THÈSE

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Marielle Simon

Problèmes de diffusion pour des chaînes d'oscillateurs harmoniques perturbées

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Directeurs de thèse :

Cédric BERNARDIN
Stefano OLLA

Après avis de :

Tadahisa FUNAKI
Claudio LANDIM

Devant la commission d'examen formée de :

Christophe BAHADORAN	*membre*
Vincent BEFFARA	*membre*
Cédric BERNARDIN	*membre*
Thierry BODINEAU	*membre*
Claudio LANDIM	*rapporteur*

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[1] J'ai peur que la liste ne soit pas exhaustive... tout oubli devra être signalé et sera compensé sans délai !

[2] Pour plus de détails sur la vie du bureau S429, on pourra consulter [58].

Introduction (FR)

The qualitative laws of natural phenomena and their quantitative relations under very simple circumstances, for example the conditions of equilibrium of a heavy parallelepiped of edges in the ratio 1 : 2 : 3*, can of course be pictured in the mind without starting from a very large finite number of elements. However, as soon as one wants to specify the quantitative laws for complicated conditions one always must start from differential equations, that is first imagine a large finite number of points in the manifold, in short one must think atomistically, and this is not altered by the fact that afterwards we can increase the number of imagined points and so come arbitrarily close to the continuum without ever reaching it.*

BOLTZMANN, 1897[3]

Prouver mathématiquement la loi de Fourier pour la conduction de la chaleur reste un problème totalement inachevé. Pour le résoudre, il est nécessaire de comprendre les phénomènes de transport sous-jacents qui impliqués au niveau microscopique. L'équation de la chaleur est connue pour être un phénomène macroscopique, émergeant après une remise à l'échelle diffusive, en espace et en temps. Il existe des modèles microscopiques pour lesquels l'énergie se comporte de manière balistique : par exemple, il est bien connu que la conductivité thermique est infinie pour des systèmes linéaires d'oscillateurs de dimension 1. Puisque la loi de Fourier n'est pas vérifiée lorsque les interactions sont linéaires, la dynamique microscopique doit prendre en compte certaines *non-linéarités*. Plus précisément, ces dernières doivent apporter suffisamment de " chaoticité " pour que le système (à l'échelle macroscopique) soit dans un état d'*équilibre local*. Cette notion est sous-entendue avec une remise à l'échelle : dans une région de dimension N^{-1}, à une échelle de temps tN^{a}, le système devrait être proche d'un équilibre, paramétré par une certaine température – cette dernière s'exprimant comme moyenne locale de l'énergie cinétique. Autrement dit, la validité des *équations hydrodynamiques* (telles que l'équation de la chaleur) découlerait des propriétés suffisamment "mélangeantes" de la dynamique microscopique.

[3]*Lectures on the Principles of Mechanics*, as translated in *Theoretical Physics and Philosophical Problems*, D. Reidel Publishing Company, Dordrecht, Holland (1974), p. 227-8.

Du monde microscopique au monde macroscopique

⊡ Équation de la Chaleur pour un Système Isolé

On considère un système macroscopique isolé, muni d'une température initiale non uniforme $T_0(x)$: par exemple, un fluide ou un solide entouré de parois adiabatiques. À l'instant $t > 0$, la température évolue à cause de flux thermiques, et la température interne satisfait l'équation de conservation :

$$\frac{\partial T(x,t)}{\partial t} = \nabla \cdot [D(T)\nabla T]$$

où $D(T)$ est le *coefficient de diffusion*. La condition initiale s'écrit : $T(x,0) = T_0(x)$, et les conditions au bord doivent être choisies convenablement. L'état stationnaire, atteint au bout d'un temps infiniment long, est donné par une température uniforme T^*. Le flux $J(T) := -D(T)\nabla T$ est la quantité de chaleur traversant une unité de surface par unité de temps, et $T(x,t)$ est la température locale. Cette loi expérimentale a été proposée pour la première fois par Fourier dans *Théorie analytique de la chaleur* (Oeuvre de Fourier, Gauthier-Villars, Paris, 1822). Une telle équation est supposée valide proche de l'équilibre. La définition du flux d'énergie local $J(T)(x,t)$ et du champ de température $T(x,t)$ repose sur l'hypothèse d'*équilibre local*.

Plaçons-nous maintenant à l'échelle microscopique, et laissons le système de $N \geqslant 1$ particules évoluer et interagir selon les lois de Newton. L'objectif final (mais encore non atteint) consisterait à prouver que l'énergie empirique du système converge dans l'échelle diffusive lorsque N tend vers $+\infty$ vers la solution de l'équation de la chaleur précédente. Autrement dit, si le système se trouve dans un état proche de l'équilibre à l'instant initial, il devrait progressivement relaxer vers un état stationnaire complètement décrit par la loi de Fourier.

⚁ Équilibre Thermique Local

Prouver un équilibre local revient à définir une température de manière locale, pour un volume macroscopiquement petit, mais microscopiquement grand, en tout point x et à tout instant t. Plus généralement, les quantités utilisées pour décrire des systèmes à l'état d'équilibre local sont supposées être des fonctions continues du temps et de l'espace. Pour cela, on doit être capable d'extraire un "petit" volume V (d'un point de vue macroscopique) autour d'un point x, c'est-à-dire petit comparé aux échelles de longueur L pour lesquelles les quantités macroscopiques typiques changent de manière notable. On doit également être sûr qu'un nombre suffisamment "grand" de particules se trouvent dans V. Enfin, le temps nécessaire pour atteindre l'état d'équilibre local doit être petit devant les échelles de temps pour lesquelles les changements macroscopiques ont lieu. Chaque petite région macroscopique donnée atteint un équilibre, mais plusieurs régions différentes peuvent être dans plusieurs états d'équilibre différents, chacun correspondant à une valeur donnée des paramètres.

⚃ Modèle Microscopique

Au niveau microscopique, on suppose que le système physique satisfait les lois de la mécanique classique, et possède un nombre fini N de degrés de libertés. Les états possibles du système sont représentés par des points ω appartement à un espace de dimension 2N : les N premières coordonnées $\{q_x\}$ sont les positions des atomes, et les N suivantes $\{p_x\}$ sont les moments. Puisque l'on recherche des modèles qui conservent l'énergie, le point $\omega = (q_1, ..., q_N, p_1, ..., p_N)$ se situe sur la surface d'énergie constante $\mathcal{S}_E^N := \{H_N(\omega) = E\}$, où H_N est l'Hamiltonien, et $E > 0$ l'énergie initiale. Par exemple, dans le cas d'oscillateurs harmoniques, l'Hamiltonien est une forme quadratique, et les surfaces d'énergie constante sont des ellipsoïdes de dimension $2N-1$.

Plus précisément, la dynamique Hamiltonienne est donnée par les équations de mouvement suivantes :

$$\begin{cases} \dfrac{dp_x(t)}{dt} = -\dfrac{\partial H_N}{\partial q_x}\big(\omega(t)\big) \\ \dfrac{dq_x(t)}{dt} = +\dfrac{\partial H_N}{\partial p_x}\big(\omega(t)\big) \end{cases} \qquad \text{pour } t > 0 \text{ et } x \in \{1, ..., N\}.$$

Rappelons que l'énergie totale du système est égale à $H_N(\omega)$: on peut alors facilement vérifier que le point ω reste bien sur une surface $\mathcal{S}_E^N$ lorsque le temps évolue. On dit que H_N est une *quantité conservée* pour le système dynamique. La *distribution microcanonique* est la loi de probabilité naturelle pour les systèmes conservatifs. Elle est concentrée sur les points ω qui possèdent une énergie fixée E, et est égale à la mesure uniforme sur la sphère S_N^E.

Tous les modèles microscopiques que l'on étudie ici sont construits pour qu'une famille d'états de Gibbs canoniques soit associée aux lois de conservation du système. Si H_N est l'unique quantité conservée, cette famille s'écrit

$$d\mu_T^N(\omega) := \frac{1}{Z_N} \exp(-T^{-1}H_N) \prod_{i=1}^{N} dp_i dq_i,$$

où $T > 0$ et Z_N est la constante de normalisation. Si d'autres quantités sont constantes au cours de l'évolution, les états de Gibbs doivent être modifiés afin de prendre en compte ces lois de conservations additionnelles.

⚃ Ensemble Microcanonique et Ergodicité

L'existence d'un état d'équilibre local est fortement reliée à la notion d'*ergodicité* pour des systèmes de dimension infinie, même si aucune définition ne fait encore consensus (voir par exemple [79]). Dans le cas de la dimension finie, un système dynamique est ergodique si, de manière grossière, il parvient à atteindre presque tous les états possibles (parmi ceux qui conservent l'énergie) au bout d'un temps très long. Pour les systèmes finis, ceci revient à montrer que la distribution microcanonique est la seule mesure invariante (en temps) pour la dynamique [3]. Si le système est ergodique, la loi microcanonique peut alors être utilisée pour calculer des valeurs à l'équilibre : prenons f une observable macroscopique du système, et notons ω l'état initial de la dynamique, pour lequel $f(\omega)$ peut prendre une valeur loin de sa valeur moyenne à l'équilibre. Lorsque le temps évolue, on s'attend à ce que cette quantité s'approche puis reste très proche de la moyenne temporelle $f^\star$. L'ergodicité implique que cette valeur d'équilibre est presque toujours égale à $\langle f \rangle_{\mathrm{mc}}$, la moyenne de f par rapport à la loi microcanonique.

La question de l'ergodicité pour des systèmes Hamiltoniens quelconques de dimension finie est toujours sans réponse (voir par exemple [66, 82]). Depuis les travaux de Kolmogorov, Arnold et Moser dans les années 1960, on ne peut pas s'attendre à ce que des systèmes Hamiltoniens génériques suffisamment réguliers soient ergodiques. Par ailleurs, d'un point de vue mathématique, la dérivation d'équations hydrodynamiques macroscopiques est basée sur la conservation de la propriété d'équilibre local à tout instant $t > 0$. La méthode la plus aboutie pour prouver cette conservation a été développée par Varadhan et ses co-auteurs [70]. Une condition suffisante (dans certains modèles) pour appliquer leurs techniques est reliée à une certaine forme d'ergodicité, et se formule de la manière suivante :

> *Les seuls états "réguliers" infinis*[4]*, invariants en temps et en espace pour la dynamique, sont des combinaisons convexes de mesures de Gibbs canoniques (infini-dimensionnelles).*

En particulier, on n'a pas réellement besoin d'ergodicité pour le système fini-dimensionnel sous-jacent. Seulement le système infini doit être ergodique au sens ci-dessus. Par conséquent, les résultats de KAM ne vont pas à l'encontre de la dérivation des limites hydrodynamiques. Néanmoins, Fritz et al. [40] soulignent que cette condition d'ergodicité est particulièrement difficile à obtenir pour des systèmes Hamiltoniens déterministes.

⚄ Conductivité Thermique

Donnons à présent un second exemple de problèmes de diffusion : on considère un système uni-dimensionnel en contact avec des réservoirs de chaleur à ses extrémités. Les réservoirs imposent une température constante aux deux points extrémaux : T_L et T_R. Lorsque le système atteint un état stationnaire, un courant de chaleur non nul $J(T)$ apparait, donné par la loi de Fourier

$$J(T) = -\kappa(T)\nabla T,$$

où $\kappa(T)$ représente la *conductivité thermique*. Pour un système uni-dimensionnel de longueur N, la conductivité thermique peut être définie en fonction du flux moyen stationnaire de chaleur. Dans [33] il est prouvé que l'état stationnaire hors équilibre de ce système dynamique est unique, et nous le notons μ_{ss}^N. On définit d'abord $\Delta T = T_R - T_L$ la différence de température, puis la conductivité thermique $\kappa_{N,\Delta T}$ pour le système fini de la manière suivante :

$$\kappa_{N,\Delta T} := -\frac{\int J_N \, d\mu_{ss}^N}{\Delta T/N} = \frac{\text{“courant d'énergie stationnaire”}}{\text{“gradient de température moyen”}}.$$

Dans le cas où

$$\kappa(T) := \lim_{N\longrightarrow\infty} \lim_{\Delta T\longrightarrow 0} \kappa_{N,\Delta T}$$

existe et est fini, la diffusion est normale et on dit que le système vérifie la loi de Fourier [22].

[4]Un état régulier est un état qui possède une entropie relative finie (par unité de volume) par rapport aux mesures de Gibbs. En particulier, ceci implique que la mesure conditionnelle de tout volume fini Λ, étant donnée la configuration à l'extérieur de Λ, est absolument continue par rapport à la mesure de Lebesgue.

La théorie de la réponse linéaire fournit une autre définition de $\kappa(\mathrm{T})$, appelée la *formule de Green-Kubo*. Reprenons l'exemple précédent, et supposons que les deux températures aux extrémités soient égales : $\mathrm{T_L} = \mathrm{T_R} = \mathrm{T}$. Dans ce cas, l'unique mesure invariante du système est un vrai état d'équilibre, noté $\mu_{\mathrm{T}}^{\mathrm{N}}$ (il n'y a pas de courant de chaleur au travers du système). On peut alors voir l'état stationnaire hors équilibre μ_{ss}^{N} comme une perturbation de la mesure d'équilibre μ_t^{N}, lorsque la différence $\Delta\mathrm{T} = \mathrm{T_R} - \mathrm{T_L}$ est petite. On définit f_{ss} comme étant la densité de μ_{ss}^{N} par rapport à la mesure $\mu_{\mathrm{T}}^{\mathrm{N}}$ (voir [16] pour l'existence et la régularité de f_{ss}), et on écrit un développement de Taylor formel jusqu'à l'ordre 1 :

$$f_{ss} = 1 + \Delta\mathrm{T} \cdot u + o(\Delta\mathrm{T}),$$

où u est une fonction *a priori* non explicite. Formellement, en utilisant le fait que le courant d'énergie est de moyenne nulle par rapport à $\mu_{\mathrm{T}}^{\mathrm{N}}$, on obtient

$$\int \mathrm{J_N}\ \mathrm{d}\mu_{ss}^{\mathrm{N}} = \Delta\mathrm{T} \cdot \int (\mathrm{J_N} u)\ \mathrm{d}\mu_{\mathrm{T}}^{\mathrm{N}} + o(\Delta\mathrm{T}).$$

La *conductivité thermique de Green-Kubo* est alors définie comme suit

$$\kappa_{\mathrm{GK}}(\mathrm{T}) = -\lim_{\mathrm{N}\longrightarrow\infty} \mathrm{N} \cdot \int (\mathrm{J_N} u)\ \mathrm{d}\mu_{\mathrm{T}}^{\mathrm{N}}.$$

De plus longs calculs montrent que les *corrélations courant-courant* sont impliqués dans cette formule. Plus précisément, imaginons que le système microscopique est formé d'une chaîne d'atomes indexée par $\mathbb{Z}$. On note e_x l'énergie de la particule x, définie par

$$e_x := \frac{p_x^2}{2m_x} + \mathrm{V}(q_{x+1} - q_x),$$

avec m_x la masse de l'atome x, $p_x^2/(2m_x)$ l'énergie cinétique, et V le potentiel d'interaction entre les atomes. Puisque la dynamique conserve l'énergie totale, il existe des *courants microscopiques d'énergie* $j_{x,x+1}$ (qui sont des fonctions locales des coordonnées du système), tels que

$$\frac{\mathrm{d}e_x}{\mathrm{d}t} = j_{x-1,x}(t) - j_{x,x+1}(t).$$

Le courant s'écrit de manière explicite

$$j_{x,x+1} = -\frac{p_{x+1}}{m_{x+1}} \mathrm{V}'(q_{x+1} - q_x).$$

En suivant par exemple [78], on peut alors écrire

$$\kappa_{\mathrm{GK}}(\mathrm{T}) = \frac{1}{\mathrm{T}^2} \sum_{x\in\mathbb{Z}} \int_0^{+\infty} \left\{ \int j_{x,x+1}(t) j_{0,1}(0)\ \mathrm{d}\mu_{\mathrm{T}} \right\}\ \mathrm{d}t.$$

Dans la formule ci-dessus, deux limites apparaissent, en temps et en espace. Pour prouver leur existence, on a besoin d'un bon contrôle de la décroissante temporelle des corrélations courant-courant : cette question est très difficile, même pour des systèmes dynamiques de dimension finie. Nous renvoyons le lecteur aux ouvrages [16, Chapitres 5-6], [17, 55] pour des dérivations heuristiques de la formule de Green-Kubo.

Des simulations numériques ainsi que certaines considérations analytiques montrent que la conductivité thermique diverge pour des systèmes uni-dimensionnels d'oscillateurs qui conservent le moment total (en plus de l'énergie) [64]. Ces résultats confirment les mesures expérimentales effectuées sur des nanotubes de carbone [27, 80]. Dans le cas d'oscillateurs harmoniques (la plus simple, et presque unique, classe de systèmes pour lesquels des calculs explicites peuvent être effectués), le flux d'énergie stationnaire peut être exprimé, et on montre qu'il ne décroit pas lorsque la taille N du système augmente : cette particularité est due au transport ballistique de l'énergie, portée par des phonons qui n'interagissent pas [60].

Quelques questions étudiées dans cette thèse

⚀ Limites hydrodynamiques

Les limites hydrodynamiques reposent sur des changements d'échelle, à la fois en temps et en espace, et permettent d'obtenir des équations différentielles partielles non linéaires. Comme déjà évoqué, on aimerait expliquer les relations qui existent entre le monde microscopique et le monde macroscopique. Puisque ce programme se situe au-delà des techniques mathématiques actuelles, il a été proposé ces dernières années d'ajouter à la dynamique déterministe une perturbation stochastique qui conserve l'énergie. Ces forces stochastiques sont censées apporter des propriétés ergodiques au système, sans modifier le comportement macroscopique typique de l'énergie. En particulier, les systèmes harmoniques purement Hamiltoniens transportent l'énergie indépendamment de la longueur de la chaîne, car ils conservent un nombre infini de quantités. Dans cette thèse, nous nous focaliserons sur le cas harmonique, et nous étudierons l'impact de différents types de perturbation.

La dérivation des limites hydrodynamiques est basée sur des principes de moyennisation : sur une grande échelle de temps, la dynamique restreinte à chaque boîte *mesoscopique* (c'est-à-dire grande d'un point de vue microscopique, mais petite d'un point de vue macroscopique) est proche de l'équilibre, celui-ci étant paramétrisé par l'énergie propre de la boîte. Habituellement, ces énergies évoluent selon des courants qui sont de moyenne nulle par rapport à toutes les mesures d'équilibre. Par conséquent, une simple moyennisation de ces courants effectuée à une échelle de temps d'ordre N ne disperse aucune énergie. Pour cette raison, on se place à l'échelle de temps N^2, là où l'énergie évolue grâce aux fluctuations du courant par rapport à l'équilibre. On établit un théorème central limite pour les courants de l'énergie, et la conductivité thermique est donnée par une double intégrale en temps et en espace des corrélations courant-courant : c'est la *formule de Green-Kubo*. Cette conductivité devrait être bien définie lorsque le système à l'équilibre possède suffisamment de propriétés mélangeantes.

⚁ Modèles non-gradients

Lorsque les courants microscopiques de l'énergie $j_{x,x+1}$ peuvent être écrits comme des gradients discrets, le comportement diffusif de l'énergie est obtenu relativement facilement. Dans ce cas, le système est dit *gradient*. Cependant, les modèles physiques naturels, en particulier les systèmes Hamiltoniens, sont *non-gradient*. Pour ces systèmes, la modélisation mathématique est beaucoup plus ardue.

Les techniques habituelles utilisées dans les modèles gradients remplacent des quantités microscopiques par leurs moyennes temporelles, grâce à des propriétés d'ergodicité locale. Cette procédure n'est cependant pas suffisante pour traiter les modèles non-gradient. Certains d'entre eux sont plus simples à étudier : il est parfois possible de remplacer le courant de l'énergie par la somme d'un gradient et d'un terme de fluctuations. Un exemple de ce type de modèle sera étudié au chapitre II : on introduit un système Hamiltonien d'oscillateurs couplés, dont la dynamique est perturbée par un bruit stochastique dégénéré. Ce dernier transforme aléatoirement les vitesses des oscillateurs en leurs opposés, grâce à des processus Poissoniens. L'évolution de ce système est caractérisé macroscopiquement par un système parabolique non linéaire couplé pour les deux lois de conservation du modèle : l'énergie, et la longueur totale de la chaîne.

Les systèmes non-gradient généraux sont plus ardus. Sans entrer dans les détails, la loi de Fourier doit être établie à un petit terme fluctuant près. Un exemple naturel de ce type de modèle peut être obtenu en ajoutant du désordre au système Hamiltonien précédent : dans le chapitre III, on suppose que les oscillateurs évoluent dans un environnement aléatoire. Puisque la perturbation stochastique est très dégénérée, les limites hydrodynamiques demandent beaucoup plus d'effort, et ne sont encore pas bien comprises. Pour cette raison, nous prouvons uniquement que les fluctuations de l'énergie à l'équilibre évoluent selon un processus d'Ornstein-Uhlenbeck infini dimensionnel. Nous concluons le chapitre en expliquant pourquoi les limites hydrodynamiques ne peuvent pas être obtenues directement.

⚂ Diffusion anormale et fluctuations macroscopiques

Ces dernières années, des comportements anormaux ont été observés pour les systèmes unidimensionnels. On s'attend par exemple à ce que la conductivité thermique diverge pour les systèmes Hamiltoniens déterministes lorsqu'ils sont "unpinned"[5], et plus génériquement, pour les systèmes dynamiques qui conservent le moment total en plus de l'énergie (voir les articles [31, 64]). Une superdiffusion de l'énergie doit être observée, plus précisément la conductivité thermique diverge comme $\kappa_N \sim N^\alpha$, pour un certain $\alpha \in (0,1)$.

Nous nous intéressons toujours à la chaîne harmonique d'oscillateurs, sans désordre, et nous introduisons une nouvelle perturbation stochastique dégénérée. De la même façon que dans [18], nous construisons un modèle simplifié qui présente plusieurs similarités avec les chaînes standards (notamment la linéarité des interactions, ainsi que la conservation de l'énergie). Une diffusion anormale peut être observée et elle est causée par la conservation d'une quantité supplémentaire.

Donnons un peu de détails. L'état du système est noté $(\omega_1, ..., \omega_N)$. La nouvelle perturbation stochastique que nous considérons est de type *échange* : les valeurs voisines ω_x et ω_y sont échangées à des temps Poissoniens aléatoires. Cette perturbation a la particularité de conserver ce qui est appelé le *volume* de la chaîne $\sum \omega_x$, en plus de l'énergie totale $\sum \omega_x^2$. Bernardin et al. [18] prouvent que la conductivité thermique donnée par la formule de Green-Kubo est infinie.

Récemment, Bernardin et al. [12] sont allés plus loin et ont montré que le champ de fluctuation de l'énergie évolue selon un processus d'Ornstein-Uhlenbeck infini dimensionnel et 3/4–fractionnaire, en utilisant certaines idées introduites dans [46]. Avec C. Bernardin, P. Gonçalves, M. Jara et M. Sasada, nous suivons leur approche, en s'inspirant de [5, 11], et nous observons deux phénomènes

[5]Une chaîne d'oscillateurs est appelée "unpinned" lorsque le potentiel de pinning, souvent noté $W(q)$, est nul.

distincts à partir d'un seul système microscopique.

Plus précisément, nous considérons la chaîne simplifiée perturbée par le bruit "flip" d'intensité γ, et le bruit "échange" d'intensité $\lambda > 0$. Les deux bruits conservent l'énergie $\sum \omega_x^2$, mais seulement le deuxième conserve le volume total $\sum \omega_x$. Si $\gamma = 0$, le volume est conservé, le transport de l'énergie est superdiffusif et décrit par un processus de Lévy dirigé par un Laplacien fractionnaire. Si $\gamma > 0$, le volume n'est plus conservé, et on peut prouver que le transport de l'énergie devient diffusif. Notre objectif est d'étudier le cas $\gamma \longrightarrow 0$, avec λ d'ordre 1, et d'obtenir un "crossover" pour le champ de fluctuations de l'énergie, dans une échelle de temps adaptée entre ces deux différents régimes. Les résultats détaillés sont expliqués dans le Chapitre IV.

Note pour le lecteur – Les Chapitres II, III et IV peuvent être lus de manière indépendante. Les notations sont rappelées lorsque nécessaires. Le Chapitre I donne une introduction plus détaillée aux trois problèmes proposés dans cette thèse.

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Introduction (EN)

The qualitative laws of natural phenomena and their quantitative relations under very simple circumstances, for example the conditions of equilibrium of a heavy parallelepiped of edges in the ratio $1:2:3$*, can of course be pictured in the mind without starting from a very large finite number of elements. However, as soon as one wants to specify the quantitative laws for complicated conditions one always must start from differential equations, that is first imagine a large finite number of points in the manifold, in short one must think atomistically, and this is not altered by the fact that afterwards we can increase the number of imagined points and so come arbitrarily close to the continuum without ever reaching it.*

BOLTZMANN, 1897[6]

Deriving the Fourier law for heat conduction is a totally unsolved problem, which assumes a good understanding of the underlying transport phenomena that are involved at a microscopic level. The heat equation is known to be a macroscopic phenomenon, emerging after a diffusive rescaling of space and time. There exist microscopic models for which the energy ballistically disperses: for instance, it is well-known that the thermal conductivity is infinite in a linear system of interacting oscillators [60]. Since the Fourier law is not valid for linear interactions, non-linearities in the microscopic dynamics are needed. Precisely, they should give enough "chaoticity" such that locally the system (in the macroscopic time scale) is in a state of so-called *local equilibrium*. This notion involves a scale parameter N: in a region of linear size N^{-1}, at a large time scale $N^a t$ $(a > 0)$, the system is close to the equilibrium given by the temperature equal to the local average of kinetic energy. In other words, the validity of the *hydrodynamic equations* (such as the heat equation) should be due to good mixing properties of the microscopic dynamics.

From the Microscopic World to the Macroscopic World

⊡ Heat Equation for an Isolated System

Let us consider an isolated macroscopic system, with an initial non-uniform local temperature $T_0(x)$, e.g. a fluid or solid surrounded by adiabatic walls. At $t > 0$, the local temperature evolves,

[6] *Lectures on the Principles of Mechanics*, as translated in *Theoretical Physics and Philosophical Problems*, D. Reidel Publishing Company, Dordrecht, Holland (1974), p. 227-8.

due to heat current, and the bulk temperature satisfies the conservation equation:

$$\frac{\partial T(x,t)}{\partial t} = \nabla \cdot [D(T)\nabla T]$$

where D(T) is the *diffusion coefficient*. This equation is to be thought with the initial condition $T(x,0) = T_0(x)$, and suitable boundary conditions. The stationary state, achieved in the large time limit, is given by a uniform temperature T^*. The flux $J(T) := -D(T)\nabla T$ is the amount of heat transported through a unit surface per unit time and $T(x,t)$ is the local temperature. This phenomenological relation was first proposed by Fourier in *Théorie analytique de la chaleur* (Oeuvre de Fourier, Gauthier-Villars, Paris, 1822). Such an equation is expected to be valid close to equilibrium. The very definition of the local energy flux $J(T)(x,t)$ and of the temperature field $T(x,t)$ relies on the *local thermal equilibrium hypothesis*.

At the microscopic scale, let a system of $N \gg 1$ particles evolve and interact according to Newton laws. The ultimate (and still unachieved) goal would be to prove that in the large N limit, the empirical energy converges in the diffusive time scale to the solution of the heat equation above. In other words, starting with an initial state close to equilibrium, the system should relax towards a stationary state, described by the Fourier law.

⚁ Local Thermal Equilibrium (LTE)

Proving local thermal equilibrium consists in defining a local temperature, for a macroscopically small but microscopically large volume, at every point x for every time t. The quantities that are used to describe systems in thermal equilibrium are assumed to be continuous functions of space and time. One should be able to exhibit a macroscopically small volume V at a macroscopic point x, namely small compared to the length scales on which typical macroscopic quantities change noticeably, but large enough so that there are "many" particles in V. In addition, the time needed to reach LTE should be small compared to the time scales on which macroscopic changes occur. Eventually, each given small macroscopic region of the system reaches equilibrium, but different regions may be in different equilibrium states, corresponding to different values of the parameters.

⚂ Microscopic Models

At the microscopic level, we assume that the physical system obeys the classical mechanics' laws, and has a finite number N of degrees of freedom. Its possible dynamical states can be viewed as points ω in a 2N-dimensional space, with N position coordinates $\{q_x\}$ and N momentum coordinates $\{p_x\}$. Since we are looking for energy conservative systems, its dynamical state $\omega = (q_1, ..., q_N, p_1, ..., p_N)$ must lie on the energy surface $\mathcal{S}_E^N := \{H_N(\omega) = E\}$, where H_N is the Hamiltonian function and $E > 0$ is the initial energy of the system. For example, in the case of a harmonic oscillators, the Hamiltonian is a quadratic form, and the energy surfaces are $(2N-1)$ – dimensional ellipsoids.

More precisely, the Hamiltonian dynamics is given by the following equations of motions

$$\begin{cases} \dfrac{\mathrm{d}p_x(t)}{\mathrm{d}t} = -\dfrac{\partial \mathrm{H_N}}{\partial q_x}\big(\omega(t)\big) \\ \dfrac{\mathrm{d}q_x(t)}{\mathrm{d}t} = +\dfrac{\partial \mathrm{H_N}}{\partial p_x}\big(\omega(t)\big) \end{cases} \qquad \text{for } t > 0 \text{ and } x \in \{1,\dots,\mathrm{N}\}.$$

Since the total energy equals $\mathrm{H_N}(\omega)$, then one can easily check that the point ω always stays on the energy surface along the time evolution of this conservative system. We say that $\mathrm{H_N}$ is a *conserved quantity* for the dynamical system. The *microcanonical distribution* is the natural probability law for conservative systems, as it is concentrated on points ω with a definite energy E, i.e. the uniform measure on the sphere $\mathcal{S}_{\mathrm{E}}^{\mathrm{N}}$.

All microscopic models are constructed in such a way that a family of canonical (Gibbs) states is associated to the conservation laws of the underlying system. If $\mathrm{H_N}$ is the only conserved quantity, they are given by

$$\mathrm{d}\mu_{\mathrm{T}}^{\mathrm{N}}(\omega) := \frac{1}{\mathrm{Z_N}} \exp(-\mathrm{T}^{-1}\mathrm{H_N}) \prod_{i=1}^{\mathrm{N}} \mathrm{d}p_i \mathrm{d}q_i,$$

where $\mathrm{T} > 0$ and $\mathrm{Z_N}$ is the normalization constant. If there are other quantities that remain constant over the time evolution, the Gibbs states shall be modified to take into account the extra conservation laws.

Microcanonical Ensemble and Ergodicity

The existence of LTE is strongly related to the notion of *ergodicity* for infinite systems, even if a consensual definition of that notion is still missing, as explained for example in [79]. Roughly speaking, in the finite-dimensional case, one wonder whether the system, after a long time evolution, passes close to almost all the dynamical states compatible with energy conservation. For finite systems, this is equivalent to prove that the microcanonical distribution is the only time-invariant law of the dynamics [3]. If the system is ergodic, the microcanonical distribution can then be used to calculate equilibrium values: suppose that f is some macroscopic observable and that the system is started at time zero from a dynamical state ω, for which $f(\omega)$ has a value that may be very far from its equilibrium value. As time evolves, we expect the current value to approach and stay very close to an equilibrium value, which is equal to the time average $f^\star$. Ergodicity tells us that this equilibrium value is almost always equal to $\langle f \rangle_{\mathrm{mc}}$, the average of f with respect to the microcanonical law.

Proving ergodicity for generic finite dimensional Hamiltonian systems is an unsolved problem (see for instance [66,82]). More precisely, since the work of Kolmogorov, Arnold and Moser in the 60's, we cannot expect ergodicity for generic sufficiently regular (and finite dimensional) Hamiltonians. From a mathematical point of view, the derivation of macroscopic hydrodynamic equations relies on the fact that the microscopic system stays in LTE for $t > 0$. The so far strongest method worked out in the last decade was initiated by Varadhan and his coworkers [70]. A sufficient condition for their method to work (in some cases) is the following ergodicity type condition:

> *Every "regular" infinite state*[7]*, invariant with respect to both translations in the space and the dynamics, is a mixture of canonical (infinite dimensional) Gibbs measures.*

[7] Regularity means that the state has finite relative entropy (per unit volume) with respect to the Gibbs measure.

In particular, ergodicity for finite dimensional systems is not really needed, and only the infinite system has to be ergodic in the sense above. Thus, KAM results do not really impede the derivation of hydrodynamic limits. Nevertheless, Fritz et al. [40] remark that such an ergodicity condition is still very challenging for deterministic Hamiltonian systems.

⚄ Thermal Conductivity

As a second example of diffusion problems, let us consider a one-dimensional system in contact with heat reservoirs at its extremities. The reservoirs specify a time invariant temperature at the two boundary points: T_L and T_R. When the system comes to a stationary state, there is a non-zero heat current $J(T)$, given by the Fourier law:

$$J(T) = -\kappa(T)\nabla T,$$

where $\kappa(T)$ is the *thermal conductivity*. For a one-dimensional system of length N, the thermal conductivity can be defined through the stationary flux of energy. In [33] it is shown that the non-equilibrium stationary state for this dynamical system is unique, and we denote it by μ_{ss}^N. We define $\Delta T = T_R - T_L$ as the temperature difference, and the thermal conductivity of the finite system, denoted by $\kappa_{N,\Delta T}$, as the following

$$\kappa_{N,\Delta T} := -\frac{\int J_N \, d\mu_{ss}^N}{\Delta T/N} = \frac{\text{“stationary energy current”}}{\text{“mean temperature gradient”}}.$$

Whenever

$$\kappa(T) := \lim_{N\longrightarrow\infty} \lim_{\Delta T\longrightarrow 0} \kappa_{N,\Delta T}$$

exists and is finite, then the conductivity is normal and the system is said to satisfy the Fourier law [22].

The linear response theory gives another formula for $\kappa(T)$, called the *Green-Kubo formula*. In the previous example, suppose that the two boundary temperatures are equal: $T_L = T_R = T$. In this case, the unique invariant measure is a real equilibrium state, denoted by μ_T^N (there is no heat current across the system). One may consider that the non-equilibrium stationary state μ_{ss}^N is a small perturbation of the equilibrium measure μ_T^N when the difference $\Delta T = T_R - T_L$ is small. Let us define f_{ss} as the density of μ_{ss}^N with respect to the measure μ_T^N (see [16] for the existence and regularity of f_{ss}), and write a formal Taylor expansion up to order 1:

$$f_{ss} = 1 + \Delta T \cdot u + o(\Delta T),$$

where u is a formal function hardly computable. Formally, since the energy current has zero average with respect to μ_T^N, one gets

$$\int J_N \, d\mu_{ss}^N = \Delta T \cdot \int (J_N u) \, d\mu_T^N + o(\Delta T).$$

The *Green-Kubo thermal conductivity* is defined as

$$\kappa_{GK}(T) = -\lim_{N\longrightarrow\infty} N \cdot \int (J_N u) \, d\mu_T^N.$$

This assumption implies, in particular, that the conditional distribution in any finite volume Λ, given the configuration outside Λ, is absolutely continuous with respect to the Lebesgue measure.

Further computations show that this formula involves *current-current correlations*. Let us consider that the microscopic system is constituted by a chain of interacting atoms indexed by $\mathbb{Z}$. We denote by e_x the energy of atom x, which reads

$$e_x := \frac{p_x^2}{2m_x} + \mathrm{V}(q_{x+1} - q_x),$$

where m_x is the mass of the atom x, then $p_x^2/(2m_x)$ states for the kinetic energy, and V is the potential associated to the interaction between atoms. Since the dynamics conserves the total energy, there exist *energy currents* $j_{x,x+1}$ (local functions of the system coordinates) such that

$$\frac{\mathrm{d}e_x}{\mathrm{d}t} = j_{x-1,x}(t) - j_{x,x+1}(t).$$

Here, the current explicitly writes as

$$j_{x,x+1} = -\frac{p_{x+1}}{m_{x+1}} \mathrm{V}'(q_{x+1} - q_x).$$

Following for instance [78], one can rewrite

$$\kappa_{\mathrm{GK}}(\mathrm{T}) = \frac{1}{\mathrm{T}^2} \sum_{x \in \mathbb{Z}} \int_0^{+\infty} \left\{ \int j_{x,x+1}(t) j_{0,1}(0) \, \mathrm{d}\mu_{\mathrm{T}} \right\} \mathrm{d}t.$$

In the above formula, two formal limits have to be taken, in space and time. For proving its well-posedness, one needs a good control of time decay of the current-current correlations, a difficult problem even for finite dimensional dynamical systems. For heuristic derivations of the Green-Kubo formula, we refer the reader to [16, Chapters 5-6], [17, 55].

It is well known, by numerical experiments and certain analytical considerations, that the thermal conductivity diverges for one-dimensional systems of anharmonic oscillators with a momentum conserving dynamics [64]. This is also consistent with some experimental results on the length dependence of the thermal conductance of carbon nanotubes [27, 80]. For a chain of harmonic oscillators (the simplest and almost unique class of systems for which we can perform explicit calculations), the stationary energy flux can be computed explicitly and does not decrease when the size N of the system increases. This is due to the ballistic transport of energy carried by the non-interacting phonons [60].

Main Issues Addressed in this Thesis

⊡ Hydrodynamic Limits

Hydrodynamic limits hold when non-linear partial differential equations are obtained through a limiting procedure that involves scale changes, both in space and time. As already explained, the challenge is to elucidate the relation between the microscopic world and the macroscopic world. Since this program is out of the range of current mathematical techniques for purely Hamiltonian systems, it has been proposed over the past few years to superpose a stochastic energy conserving perturbation to the underlying deterministic dynamics. The purpose of these stochastic forces is to give ergodic and chaotic properties to the system, without modifying the macroscopic behavior of the energy. In particular, purely harmonic Hamiltonian systems have energy transport independent of the length of the chain, because of their infinitely many conserved quantities. In this thesis, we focus on the harmonic case, and investigate the effect of different kinds of perturbation.

The proof for hydrodynamic limits is based on averaging principles: at a large time scale the dynamics of each *mesoscopic box*, namely microscopically large, but macroscopically small, is close to the equilibrium dynamics parametrized by its own energy. Usually, these energies evolve through their currents, which have null averages with respect to all equilibrium measures. Hence, a simple averaging of these currents (which would occur in a time scale of order N) would not disperse any energy. We then look at the time scale N^2, when the energy evolves due to the fluctuations of the currents in equilibrium. We establish a central limit theorem for the energy currents, and the thermal conductivity is given by the Green-Kubo formula. This conductivity should be well-defined if the system at equilibrium has enough mixing properties.

⚂ Non-gradient Models

When the microscopic energy current $j_{x,x+1}$ can be written as a discrete gradient, the diffusive behavior of the energy is easily guessed. In this case, the system is called *gradient*. However, the models that are natural from the physical point of view, in particular the Hamiltonian systems, are *non-gradient*. For these systems, the mathematical setting is hard to be rigorously analyzed.

For gradient models, the main strategy consists in replacing microscopic quantities by their ensemble averages over a long period of time, thanks to local ergodicity. This procedure is not sufficient for non-gradient models. Some of them have helpful properties that permit to replace the energy current with the sum of a gradient plus an explicit fluctuating term. An example of such models will be investigated in Chapter II: we introduce a Hamiltonian system of coupled oscillators, whose dynamics is perturbed by a degenerate stochastic noise, which randomly flips the sign of the velocities. The evolution yields two conservation laws (the energy and the length of the chain), and the macroscopic behavior is given by a non-linear parabolic system.

General non-gradient models are even more challenging. Roughly speaking, the Fourier law is established microscopically up to a small fluctuating term. One natural example of these systems can be obtained by adding some disorder in the previous Hamiltonian model: in Chapter III, we suppose the harmonic oscillators to evolve in a random environment, in addition to be stochastically perturbed. Because of the high degeneracy of the noise, the hydrodynamic limits procedure needs much more effort. For that reason, we only prove a macroscopic behavior that holds at equilibrium: precisely, we show that energy fluctuations at equilibrium evolve according to an infinite dimensional Ornstein-Uhlenbeck process. We conclude the chapter by explaining what fails in the derivation of the hydrodynamic limits.

⚂ Anomalous Diffusion and Macroscopic Fluctuations

Over the last few years, anomalous behaviors have been observed for one-dimensional systems. The divergence of the thermal conductivity is expected to hold for a deterministic Hamiltonian system when unpinned[8], and more generically for dynamical systems which preserve momentum in addition to the energy (see the review papers [31, 64]). An energy superdiffusion is expected in these cases, namely the thermal conductivity diverges as $\kappa_N \sim N^{\alpha}$, for some $\alpha \in (0,1)$.

We still focus on the harmonic chain of oscillators (without disorder), and consider a new degenerate stochastic noise. Following [18], we construct a simplified model which presents several similarities with standard chains (e.g. the linearity of interactions, and the conservation of energy). An anomalous diffusion transport can be observed for this system, because of the conservation of an extra quantity.

Let us give a few details. The dynamical state is denoted by $(\omega_1, \dots, \omega_N)$. The new stochastic perturbation under investigation is of *exchange* type, namely nearest neighbour values ω_x and ω_y are exchanged at random Poissonian times. This perturbation conserves the so-called *total volume* of the chain $\sum \omega_x$, and the total energy $\sum \omega_x^2$. Bernardin et al. [18] then prove that the thermal conductivity defined by the Green-Kubo formula is infinite.

Recently, Bernardin et al. [12] went further and showed that the energy fluctuation field evolves according to an infinite dimensional 3/4-fractional Ornstein-Uhlenbeck process, by using some ideas introduced in [46]. With C. Bernardin, P. Gonçalves, M. Jara and M. Sasada, we follow their approach, use some additional ideas from [5, 11], and finally observe two distinct phenomena from one microscopic system.

More precisely, we consider the simplified chain perturbed by the flip noise with intensity γ and the exchange noise with intensity $\lambda > 0$. The two noises conserve the energy $\sum \omega_x^2$ but only the latter conserves the total volume $\sum \omega_x$. If $\gamma = 0$, the volume is conserved, the energy transport is superdiffusive and described by a Levy process governed by a fractional Laplacian. If $\gamma > 0$, the volume is no longer conserved and one can prove that the energy transport is diffusive. Our aim is to study the case $\gamma \longrightarrow 0$, with λ of order 1, and to obtain a crossover in a suitable time scale between these two very different regimes for the energy fluctuation field. The result is explained in more details in Chapter IV.

Note for the reader – Chapters II, III and IV can be read independently of each other. All notations are recalled when needed. The aim of Chapter I is to give a more detailed introduction to the three problems under investigation.

This thesis has been partially supported by the French grant L'Oréal–Unesco *Pour les Femmes et la Science*.

[8] A chain of oscillators is called *unpinned* when the pinning potential, sometimes denoted by $W(q)$, vanishes.

Contents

CHAPTER I

Preliminary

The intuitive idea behind the definition of global equilibrium by the Gibbs states is that inevitably there are small perturbations not taken into account explicitly, which, in course of time, lead to a maximally mixed state, the (mean) energy being the only conserved quantity [...]. These perturbations – "a grain of dust in the system" – act as thermalizing agents.

Roos [73]

1 Fourier Law for a Microscopic Model of Heat Conduction

1.1 Infinite Harmonic Hamiltonian Systems

We start with performing explicit calculations for the class of purely harmonic chains. We briefly recall how to derive the thermal conductivity for a harmonic crystal in dimension 1 in contact with two heat reservoirs at different temperatures. Even if it has been known for a long time that the conductivity of perfect harmonic crystals is infinite, the forthcoming computations provide a good way to understand the main features of transport energy accross the system: in particular, the latter is qualitatively very different than the diffusion predicted by Fourier law.

As Lebowitz and Bergmann [8], we can imagine the reservoirs made up of an infinite number of identical noninteracting components, each of which interacts with the system at most once. It is assumed that prior to the interaction the components of each reservoir are at equilibrium, with some fixed temperature. We assume that the regions of the system in direct contact with a given reservoir are essentially at the "temperature" of that reservoir. We refer the reader to [60, 64] for more details.

1.1.1 Modelisation

We consider a harmonic crystal containing N particles of unit mass, which can be represented as a chain of N oscillators. Let $\omega = (p_1, ..., p_N, q_1, ..., q_N) \in \mathbb{R}^{2N}$ be the point in the phase space of the system: p_x stands for the momentum of the oscillator at site x, and q_x denotes its position. The dynamics in the bulk of the chain is governed by the Hamiltonian $\mathcal{H}_N(\omega)$. We denote by $\{\cdot, \cdot\}$ the

Poisson bracket, namely: for A and B two observables of the system,

$$\{A, B\} := \sum_{x=1}^{N} \left\{ \frac{\partial A}{\partial q_x} \frac{\partial B}{\partial p_x} - \frac{\partial A}{\partial p_x} \frac{\partial B}{\partial q_x} \right\}.$$

We denote by $d\mu_t^N(\omega)$ the probability law on $\mathbb{R}^{2N}$ which describes the state of the system at time t. Under idealised assumptions, the collisions effect with the reservoirs may be represented by a Fokker-Planck term (see [59,61]). We assume the reservoirs to be attached to each extremity of the chain, one at temperature T_L, the other one at temperature T_R.

The density μ_t^N is assumed to satisfy the Liouville equation

$$\frac{\partial \mu_t^N}{\partial t} + \{\mu_t^N, \mathcal{H}_N\} = \kappa \frac{\partial}{\partial p_1} \left[p_1 \mu_t^N + T_L \frac{\partial \mu_t^N}{\partial p_1} \right] + \kappa \frac{\partial}{\partial p_N} \left[p_N \mu_t^N + T_R \frac{\partial \mu_t^N}{\partial p_N} \right], \tag{I.1}$$

where κ is the "friction constant". The right hand side of (I.1) represents the effects of collisions with reservoir components.

Under very general conditions, μ_t^N converges to a stationary distribution μ_{ss}^N as t goes to ∞. This distribution corresponds to an equilibrium if $T_L = T_R$. Otherwise it represents a stationary non-equilibrium state in which there are heat currents flowing through the system. The harmonic Hamiltonian (i.e. the total energy of the system) reads for instance

$$\mathcal{H}_N(\omega) := \sum_{x=1}^{N} \frac{p_x^2}{2} + \sum_{x=0}^{N} \frac{(q_x - q_{x+1})^2}{2},$$

with fixed boundaries, meaning that $q_0 = q_{N+1} = 0$. Equation (I.1) rewrites as

$$\frac{\partial \mu_t^N}{\partial t} = \sum_{i,j=1}^{2N} \left\{ A_{i,j} \frac{\partial}{\partial \omega_i} \left[\omega_j \mu_t^N \right] + \frac{1}{2} D_{i,j} \frac{\partial^2 \mu_t^N}{\partial \omega_i \partial \omega_j} \right\} \tag{I.2}$$

where $A = (A_{i,j})$ and $D = (D_{i,j})$ are two $(2N, 2N)$-matrices that we write in terms of $N \times N$ blocks:

$$A := \begin{pmatrix} 0 & -I \\ G & \kappa R \end{pmatrix} \qquad D := \begin{pmatrix} 0 & 0 \\ 0 & E \end{pmatrix}.$$

Here, the tridiagonal matrix G and the two matrices R and E are defined as

$$G_{i,j} := \begin{cases} 2\delta_{i,j} - \delta_{i+1,j} - \delta_{i,j+1}, & \text{if } j = 1, \dots, N-1, \\ 2\delta_{i,N} - \delta_{i,N-1} & \text{if } j = N, \end{cases}$$
$$R_{i,j} := \delta_{i,j}(\delta_{i,1} + \delta_{i,N}),$$
$$E_{i,j} := 2T_i R_{i,j}.$$

In other words, the equations of motion are given for $x = 1, \dots, N$ by

$$\begin{cases} \dot{q}_x = p_x \\ \dot{p}_x = (q_{x+1} - 2q_x + q_{x-1}) + \delta_{x,1}(\xi_L - \kappa \dot{q}_1) + \delta_{x,N}(\xi_R - \kappa \dot{q}_x) \end{cases}$$

where ξ_L and ξ_R are independent Wiener processes with zero mean and variance $2\kappa T_L$ and $2\kappa T_R$ respectively.

1.1.2 The Stationary State

The Gaussian stationary solution μ_{ss}^{N} of this equation (corresponding to $\partial\mu_{ss}^{N}/\partial t = 0$) appears to be of the form

$$d\mu_{ss}^{N}(\omega) := \frac{\det\left(C^{-1/2}\right)}{(2\pi)^{N}} \exp\left[-\frac{1}{2}\sum_{i,j}\frac{\omega_i\omega_j}{C_{i,j}}\right]d\omega,$$

where C is the symmetric covariance matrix defined as $C_{i,j} := \int \omega_i\omega_j d\mu_{ss}^{N}$. By replacing the definition of C into (I.2), one finds that

$$\dot{C} = D - AC - CA^{*}$$

and the asymptotic stationary solutions can be determined from the following equation:

$$D = AC + CA^{*}.$$

Once C is known, all the properties of the stationary state (heat flux, kinetic temperature) are available. The explicit computation is done in [60, 64]. When $T_L = T_R = T$, it is easy to see that $d\mu_{ss}^{N}(\omega) \propto \exp[-\beta\mathcal{H}_N(\omega)]d\omega$, with $\beta = T^{-1}$.

From calculations it follows that position-position and velocity-velocity correlations are equal for all pairs of particles (x, y) such that $x+y$ is constant. This fact can be explained qualitatively: the boundary effects exponentially decay with x and y. We recall the explicit results obtained in [60] and [64] without repeating the proof.

Kinetic temperature – The stationary kinetic temperature $T(x)$ of the atom x is defined as $T(x) := \int p_x^2\, d\mu_{ss}^{N}$ and is shown to be given by

$$T(x) = \frac{T_L + T_R}{2}\left(1 + 2\frac{|T_L - T_R|}{T_L + T_R}\Phi(x)\right)$$

where Φ is an explicit function of the form

$$\Phi(x) := \frac{\sinh[\alpha(N - x)]}{\sinh(\alpha N)}, \qquad \alpha > 0.$$

This unexpectedly implies that the temperature is higher near to the coldest reservoir. Because of the exponential decay of Φ, in the bulk the temperature profile is constant as if the system were at equilibrium at constant temperature.

Heat flux – Let us define the microscopic energy e_x of the atom x as

$$e_x := \frac{p_x^2}{2} + \frac{(q_{x+1} - q_x)^2}{4} + \frac{(q_x - q_{x-1})^2}{4}.$$

The stationary energy flux between particle $x - 1$ and x is then given for $x = 2, ..., N - 1$ by

$$j_{x-1,x} = \frac{1}{2}\int (q_{x-1} - q_x)(p_{x-1} + p_x)\, d\mu_{ss}^{N} = \frac{|T_L - T_R|}{\kappa}\Phi(1).$$

Therefore, $j_{x-1,x}$ is independent of the lattice position x in the stationary state, and coincides with the energy flux $j_1 = -j_N$ coming from the reservoir at the left and going to the reservoir at the right. If the local thermal equilibrium hypothesis would be valid, then it would imply that

$$\int p_x(q_{x+1} - q_{x-1}) \mathrm{d}\mu_{ss}^{\mathrm{N}} \xrightarrow[\mathrm{N}\longrightarrow\infty]{} 0.$$

This convergence does not hold for this model. Besides, the heat flux is proportional to the temperature difference rather than to the gradient. This proves that homogeneous harmonic chains do not exhibit normal transport properties since the bulk conductivity diverges.

1.2 General Introduction to the Results of Chapter II

Chapter II is based on the published article [76] and aims at proving the Fourier law for a Hamiltonian system of N coupled harmonic oscillators, when perturbed by an additional conservative mixing noise. This system is called the *velocity-flip model*. This procedure has been proposed to overcome the lack of ergodicity of purely harmonic chains. Olla, Varadhan and Yau [70] introduced a stochastic pertubation for the first time in the context of gas dynamics, and then [40] follows this idea in the context of Hamiltonian lattice dynamics. We refer to [4, 9, 14, 15, 17, 18, 37, 65] for more recent related works.

We study the macroscopic behavior of the velocity-flip model as N goes to infinity, after rescaling space and time with the diffusive scaling. The system is considered under periodic boundary conditions – more precisely we work on the one-dimensional discrete torus $\mathbb{T}_\mathrm{N} := \{0, ..., \mathrm{N}-1\}$. The configuration space is denoted by $\Omega_\mathrm{N} := (\mathbb{R}\times\mathbb{R})^{\mathbb{T}_\mathrm{N}}$. A typical configuration is given by $\omega = (p_x, r_x)_{x\in\mathbb{T}_\mathrm{N}}$ where p_x stands for the velocity of the oscillator at site x, and r_x represents the distance between oscillator x and oscillator $x+1$. The deterministic dynamics is described by the harmonic Hamiltonian

$$\mathcal{H}_\mathrm{N}(\omega) = \sum_{x\in\mathbb{T}_\mathrm{N}} \left\{ \frac{p_x^2}{2} + \frac{r_x^2}{2} \right\}.$$

The stochastic perturbation is added only to the velocities, in such a way that the energy of particles is still conserved. Nevertheless, the momentum conservation is no longer valid. The added noise can be easily described: each particle independently waits an exponentially distributed time interval and then flips the sign of velocity. The strength of the noise is regulated by the parameter $\gamma > 0$. The total deformation $\sum r_x$ and the total energy $\sum (p_x^2 + r_x^2)/2$ are the only two conserved quantities. Therefore, the Gibbs states are parametrized by two potentials, temperature and tension: for $\beta > 0$ and $\lambda \in \mathbb{R}$, the equilibrium Gibbs measures $\mu_{\beta,\lambda}^\mathrm{N}$ on the configuration space $\Omega^\mathrm{N} := (\mathbb{R}\times\mathbb{R})^{\mathbb{T}_\mathrm{N}}$ are given by the product measures

$$\mathrm{d}\mu_{\beta,\lambda}^\mathrm{N} = \prod_{x\in\mathbb{T}_\mathrm{N}} \frac{e^{-\beta e_x - \lambda r_x}}{\mathrm{Z}(\beta,\lambda)} \mathrm{d}r_x \mathrm{d}p_x,$$

where $e_x := (p_x^2 + r_x^2)/2$ is the energy of the particle at site x, and $\mathrm{Z}(\beta,\lambda)$ is the normalization constant. The temperature is equal to β^{-1} and the tension is given by λ/β.

1.3 Hydrodynamic Limits

The goal is to prove that the two empirical profiles associated to the conserved quantities converge in the thermodynamic limit $N \longrightarrow \infty$ to the macroscopic profiles $\mathbf{r}(t,\cdot)$ and $\mathbf{e}(t,\cdot)$ which satisfy an autonomous system of coupled parabolic equations. Let $\mathbf{r}_0 : \mathbb{T} \longrightarrow \mathbb{R}$ and $\mathbf{e}_0 : \mathbb{T} \longrightarrow \mathbb{R}$ be respectively the initial macroscopic deformation profile and the initial macroscopic energy profile defined on the one-dimensional torus $\mathbb{T} = [0,1]$. We shall show that the functions $\mathbf{r}(t,q)$ and $\mathbf{e}(t,q)$ defined on $\mathbb{R}_+ \times \mathbb{T}$ are solutions of

$$\begin{cases} \partial_t \mathbf{r} = \dfrac{1}{\gamma}\partial_q^2 \mathbf{r} \\ \partial_t \mathbf{e} = \dfrac{1}{2\gamma}\partial_q^2\left(\mathbf{e} + \dfrac{\mathbf{r}^2}{2}\right) \end{cases} \qquad q \in \mathbb{T},\ t \in \mathbb{R}_+ \tag{I.3}$$

with the initial conditions $\mathbf{r}(0,\cdot) = \mathbf{r}_0(\cdot)$ and $\mathbf{e}(0,\cdot) = \mathbf{e}_0(\cdot)$.

The initial probability measure μ_0^N on the space of configurations Ω_N is related to the two initial profiles $\mathbf{r}_0$ and $\mathbf{e}_0$ in the following way:

DEFINITION I.1. *A sequence $\{\mu^N\}_N$ of probability measures on Ω^N is a* local equilibrium *associated to a deformation profile $\mathbf{r}_0 : \mathbb{T} \longrightarrow \mathbb{R}$ and an energy profile $\mathbf{e}_0 : \mathbb{T} \longrightarrow (0,+\infty)$ if for every continuous function $G : \mathbb{T} \longrightarrow \mathbb{R}$ and for every $\delta > 0$, we have*

$$\begin{cases} \lim\limits_{N\longrightarrow\infty} \mu^N\left[\left|\dfrac{1}{N}\sum\limits_{x\in\mathbb{T}_N} G\left(\dfrac{x}{N}\right) r_x - \displaystyle\int_{\mathbb{T}} G(q)\mathbf{r}_0(q)dq\right| > \delta\right] = 0, \\ \lim\limits_{N\longrightarrow\infty} \mu^N\left[\left|\dfrac{1}{N}\sum\limits_{x\in\mathbb{T}_N} G\left(\dfrac{x}{N}\right) e_x - \displaystyle\int_{\mathbb{T}} G(q)\mathbf{e}_0(q)dq\right| > \delta\right] = 0. \end{cases}$$

EXAMPLE *1.1.* For any integer N we define the probability measures

$$\mu^N_{\mathbf{e}_0(\cdot),\mathbf{r}_0(\cdot)}(d\mathbf{r},d\mathbf{p}) = \prod_{x\in\mathbb{T}_N} \frac{\exp(-\beta_0(x/N)e_x - \lambda_0(x/N)r_x)}{Z(\beta_0(\cdot),\lambda_0(\cdot))} dr_x dp_x, \tag{I.4}$$

where $\beta_0(\cdot)$ and $\lambda_0(\cdot)$ are related to $\mathbf{e}_0(\cdot)$ and $\mathbf{r}_0(\cdot)$ through thermodynamical identities (see Equation (II.1)). The sequence $\{\mu^N_{\mathbf{e}_0(\cdot),\mathbf{r}_0(\cdot)}\}_N$ is a local equilibrium, and it is called the *Gibbs local equilibrium state* associated to the macroscopic profiles $\mathbf{e}_0$ and $\mathbf{r}_0$. Both profiles are assumed to be continuous.

The hydrodynamic limits procedure consists in proving that this property of local equilibrium remains in force for the probability measure $\mu^N_{tN^2}$ (which represents the state of the system at time tN^2), and with the two time dependent profiles $\mathbf{r}(t,\cdot)$ and $\mathbf{e}(t,\cdot)$ solutions of (I.3). We approach this problem by using the relative entropy method, introduced for the first time by H. T. Yau [83] for a gradient diffusive Ginzburg-Landau dynamics. Let us recall that a conservative system is called gradient if the currents corresponding to the conserved quantities are gradients. For non-gradient models, Varadhan [82] has proposed an effective approach. Funaki et al. followed his ideas in [41] to extend the relative entropy method to some non-gradient processes and introduced the concept of local equilibrium state of second order approximation.

1.4 The Relative Entropy Method

The usual relative entropy method works with two time-dependent probability measures. Let us denote by μ_0^{N} the Gibbs local equilibrium associated to a deformation profile $\mathbf{r}_0$ and an energy profile $\mathbf{e}_0$ (Definition I.1 above). As we work in the diffusive scaling, we look at the state of the process at time $t\mathrm{N}^2$. For the sake of simplicity, we now denote it by μ_t^{N}. Let $\mu_{\mathbf{e}(t,\cdot),\mathbf{r}(t,\cdot)}^{\mathrm{N}}$ be the Gibbs local equilibrium associated to the profiles $\mathbf{r}(t,\cdot)$ and $\mathbf{e}(t,\cdot)$ that are solutions of the system (I.3).

If we denote by f_t^{N} and ϕ_t^{N}, respectively, the densities of μ_t^{N} and $\mu_{\mathbf{e}(t,\cdot),\mathbf{r}(t,\cdot)}^{\mathrm{N}}$ with respect to a reference equilibrium measure $\mu_*^{\mathrm{N}} := \mu_{1,0}^{\mathrm{N}}$, we guess that ϕ_t^{N} is a good approximation of the unknown density f_t^{N}. The existence of these two densities is justified in Section 2.1, Chapter II. We measure the distance between these two densities by their relative entropy

$$\mathrm{H}_{\mathrm{N}}(t) := \int_{\Omega^{\mathrm{N}}} f_t^{\mathrm{N}}(\omega) \log \frac{f_t^{\mathrm{N}}(\omega)}{\phi_t^{\mathrm{N}}(\omega)}\, \mathrm{d}\mu_*^{\mathrm{N}}(\omega).$$

Then, the strategy is to prove that

$$\lim_{\mathrm{N}\longrightarrow\infty} \frac{\mathrm{H}_{\mathrm{N}}(t)}{\mathrm{N}} = 0, \tag{I.5}$$

and deducing that the hydrodynamic limit holds (for this last step, see [16,49,70]). In the context of diffusive systems, the relative entropy method can be used if the following conditions are satisfied.

- First, the dynamics has to be *ergodic*: the only time and space invariant measures for the infinite system, with finite local entropy, are given by mixtures of the Gibbs measures in infinite volume $\mu_{\beta,\lambda}$ (defined in (II.4)). From [40], we know that the velocity-flip model is ergodic in the sense above (see Theorem II.4, Chapter II, for a precise statement).

- Next, we need to establish the so-called *fluctuation-dissipation equations* in the mathematics literature. Such equations express the microscopic current of energy (which here is not a discrete gradient) as the sum of a discrete gradient and a fluctuating term. More precisely, the microscopic current of energy, denoted by $j_{x,x+1}$, is defined by the local energy conservation law

  $$\mathcal{L}e_x = \nabla j_{x-1,x}$$

  where $\mathcal{L}$ is the generator of the infinite dynamics. The standard approach consists in proving that there exist local functions f_x and h_x such that the following decomposition holds

  $$j_{x,x+1} = \nabla f_x + \mathcal{L}h_x. \tag{I.6}$$

  Equation (I.6) is called a microscopic fluctuation-dissipation equation. The term $\mathcal{L}h_x$, when integrated in time, is a martingale. Roughly speaking, $\mathcal{L}h_x$ represents rapid fluctuation, whereas ∇f_x represents dissipation. Gradient models are systems for which $h_x = 0$ with the previous notations. In general, these equations are not explicit but we are able to compute them in our model (see (V.9) and (V.10)).

- Finally, since we observe the system on a diffusive scale and the system is non-gradient, we need second order approximations. If we want to obtain the entropy estimate (I.5) of order $o(\mathrm{N})$, we can not work with the measure $\mu_{\mathbf{e}(t,\cdot),\mathbf{r}(t,\cdot)}^{\mathrm{N}}$, but we have to correct the Gibbs local equilibrium state with a small term. This idea was first introduced in [41] and then used in [81] for interacting Ornstein-Uhlenbeck processes, and in [56] for the asymmetric exclusion process in the diffusive scaling. However, as far as we know, it is the first time that this is applied for a system with several conservation laws.

Recently, Even et al. [37] used the relative entropy method for a stochastically perturbed Hamiltonian dynamics which is quite close to the dynamics of this work: the time evolution is governed by the same Hamiltonian of anharmonic oscillators but the process is perturbed by a different noise: velocities are exchanged and not flipped. Besides, the boundary conditions are mechanical instead of periodic. Contrary to this work, the model is studied in the hyperbolic scale, so that the authors do not need to modify the local equilibrium state.

1.5 Technical Novelties

Up to present, the derivation of hydrodynamic equations for the harmonic oscillators perturbed by the velocity-flip noise was not rigorously achieved [14], mainly because the control of large energies has not been considered so far. Indeed, to perform the relative entropy method, we need to control the moments

$$\int \left[\frac{1}{N} \sum_{x \in \mathbb{T}_N} |p_x|^k \right] d\mu_t^N, \tag{I.7}$$

for all $k \geqslant 1$, uniformly in time and with respect to N. In fact, the only first several moments are necessary to cut-off large energies (as it is explained in Section 2.2, Chapter II) and we need all the others to obtain the Taylor expansion which appears in the relative entropy method (see Proposition II.7 and Lemma V.4). Usually, the entropy inequality (II.17) reduces the control of (I.7) to the estimate of the following equilibrium exponential moments

$$\int \exp(\delta |p_x|^k)\ d\mu_{1,0}^N$$

with $\delta > 0$ small. Unfortunately, in our case these integrals are infinite for any $k \geqslant 3$ and any $\delta > 0$.

To avoid this problem, we could cut-off large velocities by taking a relativistic kinetic energy (as done in [70]). Nevertheless, we should change the physics of the problem by modifying the Liouville operator, and consequently the fluctuation-dissipation equations would not be available any more. Similar difficulties have already appeared in other models: in [19], Bertini et al. do not have these precious exponential moments to derive rigorously their results. In another context, Bonetto et al. [21] study the heat conduction in anharmonic crystals with self-consistent reservoirs, and need energy bounds to complete their results. Bernardin [9] deals with a harmonic chain perturbed by a stochastic noise which is different from ours but has the same motivation: energy is conserved, momentum is not. He derives the hydrodynamic limit for a particular value of the intensity of the noise. In this case the hydrodynamic equations are simply given by two decoupled heat equations. The author highlights that good energy bounds are necessary to extend his work to other values of the noise intensity. In fact, only the following weak form is proved in his paper:

$$\lim_{N \longrightarrow +\infty} \int \left[\frac{1}{N^2} \sum_{x \in \mathbb{T}_N} p_x^4 \right] d\mu_t^N = 0.$$

We get uniform control of (I.7) (see Theorem II.3, Chapter II), thanks to a remarkable property of our model: the set of convex combinations of Gaussian measures is preserved by the dynamics. This is one of the main technical novelties in our work.

2 Thermal Conductivity in Disordered Chains of Oscillators

2.1 Effect of Disorder for the Purely Harmonic Chain

Chapter III is based on the submitted paper [77], and addresses diffusion problems for chains of oscillators with random defects. The presence of impurities may strongly affect the thermal conductivity. Thus, without introducing anharmonic potentials (and then non-linearities), we attempt a further comprehension of the disorder impact on heat conduction.

The disordered (and purely deterministic) harmonic chain of N oscillators was introduced in [26] and since then has attracted a lot of interest. After the first analyses of [26, 30], Ajanki and Huveneers [1] study this disordered chain when coupled at the boundaries to Langevin heat baths, with respective temperatures T_R and T_L. They prove that

$$\mathbb{E}\left[\int J_N \, d\mu_{ss}^N\right] \sim (T_R - T_L) N^{-3/2}$$

in the limit $N \longrightarrow \infty$, where $\mathbb{E}$ states for the expectation with respect to the random environment. As for the ordered case, the proof relies on an explicit representation of the current in terms of matrix elements.

The aim of Chapter III is to study the diffusive behavior for the disordered harmonic chain, but still perturbed by an energy conserving noise. Thanks to the stochastic perturbation, the conductivity of the one-dimensional chain should become finite and positive. We also expect that some homogenization effect occurs and that the conductivity does not depend on the statistics of the disorder in the thermodynamic limit.

2.2 When the Disorder Chain is Perturbed by a Stochastic Noise

The disorder effect has already been investigated for lattice gas dynamics, for example in [38, 47, 68, 71]. These papers share one main feature: the models are non-gradient due to the presence of the environment. Non-gradient systems are usually solved by establishing a microscopic Fourier law up to a small fluctuating term, following the sophisticated method initially developed by Varadhan in [82], and generalized to non-reversible dynamics [51]. The previous works mainly deal with symmetric systems of particles that evolve according to an exclusion process in random environment: the particles are attempting jumps to nearest neighbor sites at rates which depend on both their position and the objective site, and the rates themselves come from a quenched random field. Different approaches are adopted to tackle this non-gradient system: whereas the standard Varadhan's method is helpful only in dimension $d \geqslant 3$ [38], the "long jump" variation developed by Quastel in [71] is valid in all dimensions.

The study of disordered chains of oscillators perturbed by a conservative noise has appeared more recently, see by instance [10, 13, 32]. In these papers, only the behavior of the thermal conductivity defined by the Green-Kubo formula is investigated. Here, the diffusion coefficient is defined through fluctuating hydrodynamics.

Our first motivation was to investigate the same chain of harmonic oscillators as in Chapter II, still perturbed by the velocity-flip noise, but now provided with i.i.d. random masses. This makes all previous computations pointless: if the system evolves in a random medium, the fluctuation-dissipation decomposition does not hold microscopically, because the fluctuations induced by the random environment are too large. As a consequence, such a decomposition can only be approximated by a sequence of local functions, in the sense that the difference has a small space-time variance with respect to the dynamics in equilibrium. The main ingredients of the usual non-gradient method are: first, a *spectral gap* for the symmetric part of the dynamics, and second, a *sector condition* for the total generator.

Our model has special features that enforce the Varadhan's method to be considered with new perspectives. In particular, the symmetric part of the generator is poorly ergodic, and does not have a spectral gap when restricted to microcanonical manifolds. Moreover, due to the degeneracy of the noise, the asymmetric part of the generator is difficult to control by its symmetric part (in technical terms, the sector condition does not hold), with the only velocity-flip noise. Besides, let us remark that the energy current depends on the disorder, and has to be approximated by a fluctuation-dissipation equation which takes into account the fluctuations of the disorder itself.

2.3 Non-Gradient Approach with Degenerate Perturbations

Because of the high degeneracy of the velocity-flip noise, we add a second stochastic perturbation, that exchanges velocities (divided by the square root of mass) and positions at random independent Poissonian times, so that a *weak sector condition* can be proved (see Proposition III.15, Chapter III). However, the spectral gap estimate and the usual sector condition still do not hold when adding the exchange noise, meaning that the stochastic is still very degenerate. The harmonic chain has helpful properties, in particular the generator of the dynamics preserves the degree of polynomials, and even a degenerate noise is sufficient to follow Varadhan's approach. The sector condition and the non-gradient decomposition are only needed for a specific class of functions. The stochastic noise still does not have a spectral gap, but it does make no harm. Contrary to the standard Varadhan's approach, we do not need to prove any general result concerning the so-called *closed forms* (we refer to [49, 75] for the general theory). As far as we know, this is the first time that the non-gradient method is used successfully without the spectral gap estimate nor the usual sector condition.

2.4 Macroscopic Energy Fluctuations and Thermal Conductivity

For the non-linear ordered chain investigated in [69], one need a less degenerate noise than ours, in particular both the spectral gap and the sector condition hold. The authors show that ideas from Varadhan's method can be used to prove a diffusive behavior of the energy: its fluctuations in equilibrium evolve following an infinite Ornstein-Uhlenbeck process. The covariances characterizing this linearised heat equation are given in terms of the diffusion coefficient, which is defined through a variational formula.

We show that the diffusion coefficient can be equivalently defined by the Green-Kubo formula. More precisely, the latter is the space-time variance of the current at equilibrium, which is only formal in the sense that a double limit (in space and time) has to be taken. As in [10], we prove here that the limit is well-defined, and that the homogenization effect occurs for the Green-Kubo formula: for almost every realization of the disorder, the thermal conductivity exists, is independent of the disorder, is positive and finite.

Finally, let us introduce $\gamma > 0$ the intensity of the flip noise, and $\lambda > 0$ the intensity of the exchange noise. We denote the diffusion coefficient by $\mathrm{D}(\lambda,\gamma)$ when obtained through the variational formula in the Varadhan's method, and by $\bar{\mathrm{D}}(\lambda,\gamma)$ when defined through the Green-Kubo formula. We prove that the two conductivities are equal: $\mathrm{D}(\lambda,\gamma) = \bar{\mathrm{D}}(\lambda,\gamma)$, when the two intensities λ,γ are positive. In addition, in Chapter III we show (Theorem III.23) that the Green-Kubo formula remains well-defined when $\lambda = 0$, namely: $\bar{\mathrm{D}}(0,\gamma)$ exists, is finite and positive. Finally, Theorem III.26 states that $\mathrm{D}(\lambda,\gamma)$ tends to $\bar{\mathrm{D}}(0,\gamma)$ as λ goes to 0. The existence question for $\mathrm{D}(0,\gamma)$, when defining through hydrodynamics (or even fluctuating hydrodynamics) remains open.

2.5 Description of the Results in Chapter III

Let us now be more precise on the model and the convergence result of Chapter III. As before, we investigate the harmonic Hamiltonian system described by the sequence $\{p_x, r_x\}_{x\in\mathbb{T}_\mathrm{N}}$. The only difference is that each atom $x \in \mathbb{Z}$ has a mass $\mathrm{M}_x > 0$, and then the velocity of atom x is given by p_x/M_x. We assume the disorder $\mathbf{M} := \{\mathrm{M}_x\}_{x\in\mathbb{Z}}$ to be a collection of real i.i.d. positive random variables such that

$$\forall\, x \in \mathbb{Z}, \quad \frac{1}{\mathrm{C}} \leqslant \mathrm{M}_x \leqslant \mathrm{C},$$

for some finite constant $\mathrm{C} > 0$. The equations of motions are given for $x \in \mathbb{T}_\mathrm{N}$ by

$$\begin{cases} \dfrac{\mathrm{d}p_x}{\mathrm{d}t} = r_x - r_{x-1}, \\ \dfrac{\mathrm{d}r_x}{\mathrm{d}t} = \dfrac{p_{x+1}}{\mathrm{M}_{x+1}} - \dfrac{p_x}{\mathrm{M}_x}. \end{cases}$$

The dynamics conserves the total energy

$$\mathcal{E} := \sum_{x\in\mathbb{T}_\mathrm{N}} \left\{ \frac{p_x^2}{2\mathrm{M}_x} + \frac{r_x^2}{2} \right\}.$$

To overcome the lack of ergodicity of deterministic chains, we add a stochastic perturbation to this new dynamics, so that the convergence of the energy fluctuations distribution holds (Theorem III.29). The noise can be easily described: at independently distributed random Poissonian times, the quantity $p_x/\sqrt{\mathrm{M}_x}$ and the interdistance r_x are exchanged with intensity λ, or the momentum p_x is flipped into $-p_x$ with intensity γ. This noise still conserves the total energy $\mathcal{E}$, and is very degenerate.

Even if Theorem III.29 could be proved *mutatis mutandis* for this stochastically perturbed disordered harmonic chain, for pedagogical reasons we now focus on a simplified model (as in [18]), which has exactly the same features and involves less painful computations. From now on, we study the dynamics on the new configurations $\{\eta_x\}_{x\in\mathbb{T}_N}$ written as

$$m_x \mathrm{d}\eta_x = (\eta_{x+1} - \eta_{x-1})\mathrm{d}t, \tag{I.8}$$

where $\mathbf{m} := \{m_x\}_{x\in\mathbb{T}_N}$ is the new disorder with the same characteristics as before. It is notationally convenient to change the variable η_x into $\omega_x := \sqrt{m_x}\eta_x$, and the total energy reads

$$\mathcal{E} = \sum_{x\in\mathbb{T}_N} \omega_x^2.$$

Let us now introduce the corresponding stochastic energy conserving dynamics: the evolution is described by (I.8) between random exponential times, and at each ring one of the following interactions can happen:
a. Exchange noise – two nearest neighbour variables ω_x and ω_{x+1} are exchanged;
b. Flip noise – the variable ω_x at site x is flipped into $-\omega_x$.

With these two perturbations, the dynamics conserves the total energy only, the other important conservation laws of the Hamiltonian part being destroyed by the stochastic noises. As a result, the following family $\{\mu_\beta^N\}_{\beta>0}$ of grand-canonical Gibbs measures is invariant for the process:

$$\mu_\beta^N(\mathrm{d}\omega) := \prod_{x\in\mathbb{T}_N} \sqrt{\frac{2\pi}{\beta}} \exp\left(-\frac{\beta}{2}\omega_x^2\right) \mathrm{d}\omega_x. \tag{I.9}$$

The index β stands for the inverse of the temperature. Notice that μ_β does not depend on the disorder, and that the dynamics is not reversible with respect to the measure μ_β. We define $\mathbf{e}_\beta$ as the thermodynamical energy associated to β, namely the expectaction of ω_0^2 with respect to μ_β, and $\chi(\beta) = 2\beta^{-2}$ as the variance of ω_0^2 with respect to μ_β.

Energy fluctuations at equilibrium – We consider the system starting with μ_β and we denote by $\mathbb{E}_\beta$ the expectation for the stochastic dynamics starting with this invariant distribution. We prove a diffusive behavior for the energy: first, define the distributions-valued energy fluctuation field

$$\mathcal{Y}^N := \frac{1}{\sqrt{N}} \sum_{x\in\mathbb{T}_N} \delta_{x/N}\big\{\omega_x^2(0) - \mathbf{e}_\beta\big\}.$$

It is well-known that $\mathcal{Y}^N$ converges in distribution as $N \longrightarrow \infty$ towards a centered Gaussian field $\mathcal{Y}$, which satisfies

$$\mathbb{E}_\beta\big[\mathcal{Y}(F)\mathcal{Y}(G)\big] = \chi(\beta)\int_0^1 F(y)G(y)\mathrm{d}y,$$

for good test functions F, G. In Chapter III we prove that these energy fluctuations evolve diffusively in time (Theorem III.29). More precisely, the following distribution-valued process

$$\mathcal{Y}_t^N = \frac{1}{\sqrt{N}} \sum_{x\in\mathbb{T}_N} \delta_{x/N}\big\{\omega_x^2(tN^2) - \mathbf{e}_\beta\big\}$$

converges in law as $N \longrightarrow \infty$ to the solution of the linear Stochastic Partial Differential Equation (SPDE)

$$\partial_t\mathcal{Y} = D\partial_y^2\mathcal{Y}\mathrm{d}t + \sqrt{2D\chi(\beta)}\partial_y B(y,t),$$

where $D := D(\lambda,\gamma)$ is the diffusion coefficient which has various expressions, and B is the standard normalized space-time white noise.

Hydrodynamic limits – Finally, we could think of using the entropy method to derive the hydrodynamic equation. For that purpose, the initial law is not the equilibrium measure μ_β^N, but a *local equilibrium measure* (Definition I.1 above). We conjecture that this property of local equilibrium propagates in time. In other words, let $\mathbf{e}_0 : \mathbb{T} \longrightarrow \mathbb{R}$ be a bounded function. The goal would be to show that the empirical energy profile converges in the thermodynamic limit to the macroscopic profile $\mathbf{e}(t,\cdot) : \mathbb{T} \longrightarrow \mathbb{R}$ solution of

$$\begin{cases} \dfrac{\partial \mathbf{e}}{\partial t}(t,u) = \mathrm{D}\dfrac{\partial^2 \mathbf{e}}{\partial u^2}(t,u), & t > 0,\ u \in \mathbb{T}, \\ \mathbf{e}(0,u) = \mathbf{e}_0(u). \end{cases}$$

Unfortunately, even if the diffusion coefficient is well-defined through the non-gradient approach, this does not straightforwardly provide a method to derive the hydrodynamic limits. We conclude Chapter III by highlighting the step where the usual techniques fail.

3 From Normal to Super Energy Diffusion in the Evanescent Flip Noise Limit

3.1 Energy Superdiffusion for One-Dimensional Chains of Oscillators

In Chapter IV, we present the results of a joint work with Cédric Bernardin (Université de Nice), Patrícia Gonçalves (PUC, Rio de Janeiro), Milton Jara (IMPA, Rio de Janeiro) and Makiko Sasada (Keio University, Tokyo).

Anomalous diffusion for one-dimensional systems has attracted a lot of interest over the last few years. Several features of these models have been investigated. In [4] the thermal conductivity is proved to be infinite for an unpinned harmonic chain of oscillators perturbed by an energy-momentum conserving noise. Let us notice that when the stochastic perturbations of harmonic systems do not conserve momentum, the thermal conductivity is always finite [15, 20]. The Green-Kubo formalism is convenient to derive transport properties from the knowledge of the equilibrium state, without any reference to heat baths. In this context the analytic results for heat conduction always involve a calculation of the current-current correlation function.

Recently, in [12] Bernardin et al. study the infinite dynamical system $\{\omega_x\}_{x\in\mathbb{Z}}$ on $\mathbb{R}^{\mathbb{Z}}$ which can be described as the following: the equations of motion are given by

$$\mathrm{d}\omega_x = (\omega_{x+1} - \omega_{x-1})\mathrm{d}t, \tag{I.10}$$

and, in addition, the nearest neighbours quantities ω_x and ω_{x+1} are exchanged at random Poissonian times. The authors present a general method to prove that under the subdiffusive scale $t\mathrm{N}^{3/2}$, the energy-energy correlation function is given at the large N limit by the solution of the fractional heat equation with exponent $3/4$. This system is very close to the one introduced in Chapter III, except that masses equal 1 and the flip noise vanishes.

3.2 Energy Fluctuation Field and Fluctuation-Dissipation Equation

Let us define the distribution-valued energy fluctuation field $\mathcal{E}_{t\mathrm{N}^a}$ in the time scale $t\mathrm{N}^a$ $(a > 0)$ as

$$\mathcal{E}_{t\mathrm{N}^a}(f) := \frac{1}{\sqrt{\mathrm{N}}} \sum_{x\in\mathbb{Z}} f\left(\frac{x}{\mathrm{N}}\right) \left\{\omega_x^2(t\mathrm{N}^a) - \beta^{-1}\right\},$$

where f is a smooth function defined on $\mathbb{R}$. If we add the flip noise of intensity $\gamma > 0$ to the previous dynamics, the results of Chapter III show that $\mathcal{E}_{t\mathrm{N}^2}$ converges as $\mathrm{N} \longrightarrow \infty$ towards an infinite dimensional Ornstein-Uhlenbeck process solution of a linear SPDE. Actually, we could prove this convergence without using the non-gradient Varadhan's approach (that we absolutely need if random masses are added).

Let us give a rough explanation. Without any disorder, the deterministic dynamics defined by (I.10) has the same features as the harmonic chain of oscillators investigated in Chapter II. With the only flip noise, the diffusive behavior of the energy can be entirely solved thanks to an explicit fluctuation-dissipation equation of the form (I.6). Since the computation is within easy reach, hereafter we go into more details.

Deterministic system (I.10) **perturbed by the only flip noise –** Let us denote by $\mathcal{L}$ the total generator of the infinite[1] dynamics $\{\omega_x(t)\,;\, t \geqslant 0\}_{x\in\mathbb{Z}}$. The generator $\mathcal{L}$ is decomposed as the sum $\mathcal{L} = \mathcal{A} + \mathcal{S}$, where $\mathcal{A}$ corresponds to the deterministic evolution (I.10) and $\mathcal{S}^{\mathrm{flip}}$ represents the stochastic perturbation. More precisely, $\mathcal{S}^{\mathrm{flip}}$ and $\mathcal{A}$ act on local, smooth and bounded functions $f : \mathbb{R}^{\mathbb{Z}} \longrightarrow \mathbb{R}$ as follows

$$\mathcal{A}f(\omega) := \sum_{x\in\mathbb{Z}} (\omega_{x+1} - \omega_{x-1}) \frac{\partial f}{\partial \omega_x}(\omega),$$
$$\mathcal{S}^{\mathrm{flip}} f(\omega) := \frac{1}{2} \sum_{x\in\mathbb{Z}} \left\{ f(\omega^x) - f(\omega) \right\},$$

where ω^x is the configuration obtained from ω by changing ω_x into $-\omega_x$. The total energy $\sum \omega_x^2$ is preserved by the evolution, and therefore there exist energy currents $j_{x,x+1}$ satisfying $\mathcal{L}(\omega_x^2) = j_{x,x+1} - j_{x-1,x}$. Here, the energy currents read

$$j_{x,x+1} = 2\omega_x\omega_{x+1}.$$

A straightforward computation show that

$$j_{x,x+1} = \nabla(\omega_x^2 + \omega_{x-1}\omega_{x+1}) - \mathcal{L}(\omega_x\omega_{x+1}),$$

where ∇ is the discrete gradient. In other words, an exact fluctuation-dissipation relation holds, and only involves local functions: the situation is exactly similar to the velocity-flip model investigated in Chapter II.

The additional exchange noise – Following [12, 18] we now add to the dynamics the exchange noise, described by the generator

$$\mathcal{S}^{\mathrm{exch}} f(\omega) = \frac{1}{2} \sum_{x\in\mathbb{Z}} \left\{ f(\omega^{x,x+1}) - f(\omega) \right\},$$

[1] We report to Chapter IV more details on the existence of the infinite system.

where $\omega^{x,x+1}$ is obtained from ω by exchanging ω_x and ω_{x+1}. The first consequence of this additional perturbation is the apparition of an extra gradient term in the current, which has no impact on the existence of the fluctuation-dissipation equation. The second consequence has a stronger effect: in fact, there is no real hope any more to write such a decomposition with *local* functions. However, we are able to obtain non-local explicit functions f and g such that $j_{0,1} = \nabla(f) + \mathcal{L}(g)$.

Recently, Basile et al. [5] show that a good control of these functions (w.r.t. suitable norms) is sufficient to prove the diffusive behavior of the energy fluctuation field. The key point of the argument is the so-called *Boltzmann-Gibbs principle*, which was first introduced by Brox and Rost [24]. Roughly speaking, this principle states that the space-time fluctuations of any field associated to an energy conservative model can be written as a linear functional of the energy field. In our case, the same ideas from [5] can be adapted to prove the convergence of $\mathcal{E}_{t\mathrm{N}^a}$. This is explained in more details in Chapter IV.

3.3 Two Regimes in the Evanescent Flip noise

Let us consider that the flip noise (resp. the exchange noise) is given with an intensity $\gamma > 0$ (resp. an intensity $\lambda > 0$). In other words, the total generator writes $\mathcal{L} = \mathcal{A} + \gamma\mathcal{S}^{\text{flip}} + \lambda\mathcal{S}^{\text{exch}}$. We are interested in the energy transport in the limit $\gamma \longrightarrow 0$. For that purpose, we assume that there exist two parameters $c, b \geqslant 0$ such that

$$\gamma = \frac{c}{\mathrm{N}^b}.$$

If $c = 0$ (or equivalently $b = +\infty$), we recover the model of [12], and the energy transport is superdiffusive. If $b = 0$, we are in the case described above, and a non-local fluctuation-dissipation equation permits to prove a diffusive behavior.

In Chapter IV we describe with more details the regimes where these two distinct phenomena hold. If $b < 2/3$, the space-time rescaling $t\mathrm{N}^{2-b/2}$ gives rise to the heat equation. If $b > 1$, in the space-time rescaling $t\mathrm{N}^{3/2}$ the energy fluctuation field is governed by the $3/4$-fractional Laplacian.

CHAPTER II

Hydrodynamic Limits for the Velocity-Flip Model

Contents

We study the diffusive scaling limit for a chain of N *coupled oscillators. In order to provide the system with good ergodic properties, we perturb the Hamiltonian dynamics with random flips of velocities, so that the energy is locally conserved. We derive the hydrodynamic equations by estimating the relative entropy with respect to the local equilibrium state, modified by a correction term* (EXTRACTS FROM [76]).

1 Introduction to the Model and Main Results

1.1 Harmonic Chain and Velocity-Flip Noise

We consider the unpinned harmonic chain perturbed by the momentum-flip noise. Each particle has the same mass that we set equal to 1. The configuration space is denoted by $\Omega^{\mathrm{N}} := (\mathbb{R}\times\mathbb{R})^{\mathbb{T}_{\mathrm{N}}}$. A typical configuration is $\omega = (\mathbf{r},\mathbf{p}) \in \Omega^{\mathrm{N}}$, where $\mathbf{r} = (r_x)_{x\in\mathbb{T}_{\mathrm{N}}}$ and $\mathbf{p} = (p_x)_{x\in\mathbb{T}_{\mathrm{N}}}$. The generator of the dynamics is given by $\mathcal{L}_{\mathrm{N}} := \mathcal{A}_{\mathrm{N}} + \gamma\mathcal{S}_{\mathrm{N}}$, where, for any continuously differentiable function $f : \Omega^{\mathrm{N}} \longrightarrow \mathbb{R}$,

$$\mathcal{A}_{\mathrm{N}}(f) := \sum_{x\in\mathbb{T}_{\mathrm{N}}} \left[(p_{x+1}-p_x)\,\partial_{r_x} f + (r_x - r_{x-1})\,\partial_{p_x} f\right]$$

and

$$\mathcal{S}_{\mathrm{N}}(f)(\mathbf{r},\mathbf{p}) := \frac{1}{2}\sum_{x\in\mathbb{T}_{\mathrm{N}}} \left[f(\mathbf{r},\mathbf{p}^x) - f(\mathbf{r},\mathbf{p})\right].$$

Here $\mathbf{p}^x$ is the configuration obtained from $\mathbf{p}$ by the flip of p_x into $-p_x$. The parameter $\gamma > 0$ regulates the strength of the random flip of momenta.

The operator $\mathcal{A}_{\mathrm{N}}$ is the Liouville operator of a chain of interacting harmonic oscillators, and $\mathcal{S}_{\mathrm{N}}$ is the generator of the stochastic part of the dynamics that flips at random time the velocity of one particle. The dynamics conserves two quantities: the total deformation of the lattice $\mathcal{R} = \sum_{x\in\mathbb{T}_{\mathrm{N}}} r_x$

and the total energy $\mathcal{E} = \sum_{x\in\mathbb{T}_N} e_x$, where $e_x = (p_x^2 + r_x^2)/2$. Observe that the total momentum is no longer conserved.

The deformation and the energy define a family of invariant measures depending on two parameters. For $\beta > 0$ and $\lambda \in \mathbb{R}$, we denote by $\mu^N_{\beta,\lambda}$ the Gaussian product measure on Ω^N given by

$$\mu^N_{\beta,\lambda}(\mathrm{d}\mathbf{r},\mathrm{d}\mathbf{p}) = \prod_{x\in\mathbb{T}_N} \frac{e^{-\beta e_x - \lambda r_x}}{Z(\beta,\lambda)} \mathrm{d}r_x \mathrm{d}p_x \; .$$

An easy computation gives that the partition function satisfies

$$Z(\beta,\lambda) = \frac{2\pi}{\beta} \exp\left(\frac{\lambda^2}{2\beta}\right) \; .$$

In the following, we shall denote by $\mu[\cdot]$ the expectation with respect to the measure μ. We introduce $\mathbf{L}^2(\mu^N_{\beta,\lambda})$, the space of functions f defined on Ω^N such that $\mu^N_{\beta,\lambda}[f^2] < +\infty$. This is a Hilbert space, on which $\mathcal{A}_N$ is antisymmetric and $\mathcal{S}_N$ is symmetric.

The thermodynamic relations between the averages of the conserved quantities $\bar{\mathbf{r}} \in \mathbb{R}$ and $\bar{\mathbf{e}} \in (0,+\infty)$, and the potentials $\beta \in (0,+\infty)$ and $\lambda \in \mathbb{R}$ are given by

$$\begin{cases} \bar{\mathbf{e}}(\beta,\lambda) := \mu^N_{\beta,\lambda}[e_x] = \dfrac{1}{\beta} + \dfrac{\lambda^2}{2\beta^2} \; , \\ \bar{\mathbf{r}}(\beta,\lambda) := \mu^N_{\beta,\lambda}[r_x] = -\dfrac{\lambda}{\beta} \; . \end{cases} \tag{II.1}$$

Let us notice that

$$\forall\, \beta \in (0,+\infty), \forall\, \lambda \in \mathbb{R},\; \bar{\mathbf{e}}(\beta,\lambda) > \frac{\bar{\mathbf{r}}^2(\beta,\lambda)}{2} \; .$$

We assume that the initial probability law μ_0^N is close to a local equilibrium (see Definition I.1, Chapter I), recalling that a local equilibrium is a sequence μ_N of probability measures that satisfies

$$\begin{cases} \lim\limits_{N\longrightarrow\infty} \mu^N\left[\left|\dfrac{1}{N}\sum\limits_{x\in\mathbb{T}_N} G\left(\dfrac{x}{N}\right) r_x - \displaystyle\int_{\mathbb{T}} G(q)\mathbf{r}_0(q)\mathrm{d}q\right| > \delta\right] = 0 \; , \\ \lim\limits_{N\longrightarrow\infty} \mu^N\left[\left|\dfrac{1}{N}\sum\limits_{x\in\mathbb{T}_N} G\left(\dfrac{x}{N}\right) e_x - \displaystyle\int_{\mathbb{T}} G(q)\mathbf{e}_0(q)\mathrm{d}q\right| > \delta\right] = 0 \; , \end{cases}$$

for two given profiles $\mathbf{e}_0 : \mathbb{T} \longrightarrow (0,+\infty)$ and $\mathbf{r}_0 : \mathbb{T} \longrightarrow \mathbb{R}$, for every continuous function $G : \mathbb{T} \longrightarrow \mathbb{R}$ and for every $\delta > 0$. We recall that the *Gibbs local equilibrium state* associated to the macroscopic profiles $\mathbf{e}_0$ and $\mathbf{r}_0$ is defined as the following:

Definition II.1. *For any integer* N *we define the Gibbs local equilibrium states as*

$$\mu^N_{\beta_0(\cdot),\lambda_0(\cdot)}(\mathrm{d}\mathbf{r},\mathrm{d}\mathbf{p}) = \prod_{x\in\mathbb{T}_N} \frac{\exp(-\beta_0(x/N)e_x - \lambda_0(x/N)r_x)}{Z(\beta_0(\cdot),\lambda_0(\cdot))} \mathrm{d}r_x \mathrm{d}p_x \; , \tag{II.2}$$

where $\beta_0(\cdot)$ and $\lambda_0(\cdot)$ are related to $\mathbf{e}_0(\cdot)$ and $\mathbf{r}_0(\cdot)$ by (II.1)

$$\begin{cases} \mathbf{e}_0(\cdot) = \bar{\mathbf{e}}(\beta_0(\cdot),\lambda_0(\cdot)) \; , \\ \mathbf{r}_0(\cdot) = \bar{\mathbf{r}}(\beta_0(\cdot),\lambda_0(\cdot)) \; . \end{cases}$$

Both profiles are assumed to be continuous.

To establish the hydrodynamic limit corresponding to the two conservation laws, we look at the process with generator $N^2\mathcal{L}_N$, namely in the diffusive scale. The configuration at time tN^2 is denoted by ω_t^N, and the law of the process $(\omega_t^N)_{t\geqslant 0}$ is denoted by μ_t^N.

1.2 The Thermodynamic Entropy

The function

$$S(\mathbf{e},\mathbf{r}) = \inf_{\beta>0,\lambda\in\mathbb{R}} \left\{\lambda\mathbf{r} + \beta\mathbf{e} + \log Z(\beta,\lambda)\right\}$$

is called the *thermodynamic entropy*. An easy computation, coming from the explicit expression of the partition function, gives

$$S(\mathbf{e},\mathbf{r}) = 1 + \log(2\pi) + \log\left(\mathbf{e} - \frac{\mathbf{r}^2}{2}\right), \text{ when } \mathbf{e} - \frac{\mathbf{r}^2}{2} > 0 .$$

The relations (II.1) can be inverted according to

$$\lambda(\mathbf{e},\mathbf{r}) = \frac{\partial S(\mathbf{e},\mathbf{r})}{\partial \mathbf{r}} , \qquad \beta(\mathbf{e},\mathbf{r}) = \frac{\partial S(\mathbf{e},\mathbf{r})}{\partial \mathbf{e}} .$$

These two equalities, together with (II.1), show that there exists a bijection between the two sets $\left\{(\beta,\lambda)\in\mathbb{R}^2 \; ; \; \beta>0\right\}$ and $\left\{(\mathbf{e},\mathbf{r})\in\mathbb{R}^2 \; ; \; \mathbf{e}>\mathbf{r}^2/2\right\}$. From the equations above, the inverted relations can be written as

$$\lambda(\mathbf{e},\mathbf{r}) = -\frac{\mathbf{r}}{\mathbf{e}-\mathbf{r}^2/2} , \qquad \beta(\mathbf{e},\mathbf{r}) = \frac{1}{\mathbf{e}-\mathbf{r}^2/2} .$$

We denote by Ψ the function

$$\begin{array}{rccc} \Psi : & \left\{(\mathbf{e},\mathbf{r})\in\mathbb{R}^2 \; ; \; \mathbf{e}>\mathbf{r}^2/2\right\} & \longrightarrow & \left\{(\beta,\lambda)\in\mathbb{R}^2 \; ; \; \beta>0\right\} \\ & (\mathbf{e},\mathbf{r}) & \mapsto & \left(\dfrac{1}{\mathbf{e}-\mathbf{r}^2/2}, -\dfrac{\mathbf{r}}{\mathbf{e}-\mathbf{r}^2/2}\right) . \end{array}$$

If $\eta = (\mathbf{e},\mathbf{r})$ and $\chi = (\beta,\lambda)$ satisfy the relations (II.1), then η and χ are said *in duality* and we have

$$-S(\mathbf{e},\mathbf{r}) + \log Z(\beta,\lambda) = -\eta\cdot\chi . \tag{II.3}$$

Here, the notation $a\cdot b$ stands for the usual scalar product between a and b.

1.3 Hydrodynamic Equations

Let μ and ν be two probability measures on the same measurable space $(X,\mathcal{F})$. We define the relative entropy $H(\mu|\nu)$ of the probability measure μ with respect to the probability measure ν by

$$H(\mu|\nu) = \sup_f \left\{\int_X f \, d\mu - \log\left(\int_X e^f \, d\nu\right)\right\} ,$$

where the supremum is carried over all bounded measurable functions f on X. The Gibbs states in infinite volume are the probability measures $\mu_{\beta,\lambda}$ on $\Omega = (\mathbb{R}\times\mathbb{R})^{\mathbb{Z}}$ given by

$$\mu_{\beta,\lambda}(d\mathbf{r},d\mathbf{p}) = \prod_{x\in\mathbb{Z}} \frac{e^{-\beta e_x - \lambda r_x}}{Z(\beta,\lambda)} dr_x dp_x . \tag{II.4}$$

We denote by $\tau_x\varphi$ the shift of φ: $(\tau_x\varphi)(\omega) = \varphi(\tau_x\omega) = \varphi(\omega(x+\cdot\,))$. In this article the following theorem is proved.

Theorem II.1. *Let $\{\mu_0^N\}_N$ be a sequence of probability measures on Ω^N which is a local equilibrium associated to a deformation profile $\mathbf{r}_0$ and an energy profile $\mathbf{e}_0$ such that $\mathbf{e}_0 > \mathbf{r}_0^2/2$ (see (II.2)). We denote by β_0 and λ_0 the potential profiles associated to $\mathbf{r}_0$ and $\mathbf{e}_0$:*

$$(\beta_0, \lambda_0) := \Psi(\mathbf{e}_0, \mathbf{r}_0) .$$

We assume that

$$\mathrm{H}\left(\mu_0^N | \mu^N_{\beta_0(\cdot),\lambda_0(\cdot)}\right) = o(N)$$

and that the initial profiles are continuous. We also assume that the energy moments are bounded: let us suppose that there exists a positive constant C which does not depend on N and t, such that

$$\forall\, k \geqslant 1,\ \mu_t^N\left[\sum_{x\in\mathbb{T}_N} e_x^k\right] \leqslant (Ck)^k\, N . \tag{II.5}$$

Let G be a continuous function on the torus $\mathbb{T}$ and φ be a local function which satisfies the following property: there exists a finite subset $\Lambda \subset \mathbb{Z}$ and a constant $C > 0$ such that, for all $\omega \in \Omega^N$, $\varphi(\omega) \leqslant C\left(1+\sum_{i\in\Lambda} e_i(\omega)\right)$. Then,

$$\mu_t^N\left[\left|\frac{1}{N}\sum_x G\left(\frac{x}{N}\right)\tau_x\varphi - \int_{\mathbb{T}} G(y)\ \tilde\varphi(\mathbf{e}(t,q),\mathbf{r}(t,q))\mathrm{d}q\right|\right] \xrightarrow[N\longrightarrow\infty]{} 0$$

where $\tilde\varphi$ is the grand-canonical expectation of φ: in other words, for any $(\mathbf{e},\mathbf{r}) \in \mathbb{R}^2$ such that $\mathbf{e} > \mathbf{r}^2/2$, let $(\beta,\lambda) = \Psi(\mathbf{e},\mathbf{r})$ then

$$\tilde\varphi(\mathbf{e},\mathbf{r}) = \mu_{\beta,\lambda}[\varphi] = \int_{(\mathbb{R}\times\mathbb{R})^{\mathbb{Z}}} \varphi(\omega)\ d\mu_{\beta,\lambda}(\omega) .$$

Besides, $\mathbf{e}$ and $\mathbf{r}$ are defined on $\mathbb{R}_+ \times \mathbb{T}$ and are solutions of

$$\begin{cases} \partial_t \mathbf{r} = \dfrac{1}{\gamma}\partial_q^2 \mathbf{r}\ , \\[2ex] \partial_t \mathbf{e} = \dfrac{1}{2\gamma}\partial_q^2\left(\mathbf{e} + \dfrac{\mathbf{r}^2}{2}\right)\ , \end{cases} \qquad q \in \mathbb{T},\ t\in\mathbb{R}, \tag{II.6}$$

with the initial conditions $\mathbf{r}(\cdot,0) = \mathbf{r}_0(\cdot)$ and $\mathbf{e}(\cdot,0) = \mathbf{e}_0(\cdot)$.

Remark *1.1.* 1. In order to prove the theorem, we shall show afterwards that

$$\mathrm{H}\left(\mu_t^N | \nu^N_{\chi_t(\cdot)}\right) = o(N).$$

Here $\nu^N_{\chi_t(\cdot)}$ is a probability measure which is close to the Gibbs local equilibrium $\mu^N_{\beta(t,\cdot),\lambda(t,\cdot)}$ (II.2). The functions $(\beta(t,\cdot),\lambda(t,\cdot))$ are still related to $\mathbf{e}(t,\cdot)$ and $\mathbf{r}(t,\cdot)$ by (II.1).

This fact allows to establish the hydrodynamic limit in the sense given in the theorem. For a proof, we refer the reader to [70, Corollary 2.2], [16, 49].

2. Let us notice that the functions $\mathbf{e}, \mathbf{r}, \beta$ and λ are smooth when $t > 0$, since the system of partial differential equations is parabolic. Moreover, the function $\beta^{-1} = \mathbf{e} - \mathbf{r}^2/2$ satisfies

$$\partial_t\left(\frac{1}{\beta}\right) = \frac{1}{2\gamma}\ \partial_q^2\left(\frac{1}{\beta}\right) + \frac{1}{\gamma}\ |\partial_q r|^2 \geqslant \frac{1}{2\gamma}\partial_q^2\left(\frac{1}{\beta}\right) .$$

The supersolutions of the heat equation follow the minimum principle. Consequently, since there exists $c > 0$ such that the initial profile β_0 has the following property

$$\forall\, q \in \mathbb{T}_N,\ \beta_0(q) \geqslant c > 0\ ,$$

then we know that the function β satisfies:

$$\forall\, q \in \mathbb{T}_N,\ \forall\, t \in [0,T],\ \beta_t(q) \geqslant c > 0\ . \tag{II.7}$$

3. After some integrations by parts, a simple computation shows that

$$\partial_t \left\{ \int_{\mathbb{T}} S(\mathbf{r}(t,q),\mathbf{e}(t,q))\, dq \right\} = \frac{1}{2\gamma}\int_{\mathbb{T}} \left\{ \left[\frac{\partial_q \beta(t,q)}{\beta(t,q)} \right]^2 + 2\beta(t,q)\, [\partial_q r(t,q)]^2 \right\} dq \geqslant 0$$

when $\mathbf{r}$ and $\mathbf{e}$ are the solutions of the hydrodynamic equations (II.6). This fact is in agreement with the second thermodynamic principle.

In Section 3, we will show that the hypothesis on moments bounds (II.5) holds for a wide class of initial local equilibrium states. Before stating the theorem, let us give some definitions.

We denote by $\mathfrak{S}_N(\mathbb{R})$ the set of real symmetric matrices of size N. The correlation matrix $C \in \mathfrak{S}_{2N}(\mathbb{R})$ of a probability measure ν on Ω^N is the symmetric matrix $C = (C_{i,j})_{1\leqslant i,j \leqslant 2N}$ defined by

$$C_{i,j} := \begin{cases} \nu[r_i r_j] & i,j \in \{1,...,N\}\ , \\ \nu[r_i p_j] & i \in \{1,...,N\},\ j \in \{N+1,...,2N\}\ , \\ \nu[p_i r_j] & i \in \{N+1,...,2N\},\ j \in \{1,...,N\}\ , \\ \nu[p_i p_j] & i,j \in \{N+1,...,2N\}\ . \end{cases} \tag{II.8}$$

Let us denote by Σ_N the subset of $\mathbb{R}^{2N} \times \mathfrak{S}_{2N}(\mathbb{R})$ defined by the following condition:

$$(m,C) \in \Sigma_N \Leftrightarrow \begin{cases} m_k = 0 & \text{for all } k = N+1\dots 2N\ , \\ C_{i,j} = 0 & \text{for all } i \neq j\ , \\ C_{i,i} > 0 & \text{for all } i = 1\dots 2N\ , \\ C_{i,i} - m_i^2 = C_{i+N,i+N} & \text{for all } i = 1\dots N\ . \end{cases}$$

Precisely, it means that m is of the form $m = (m_1,\dots,m_N,0,\dots,0)$, and C is a diagonal matrix whose diagonal components can be written as $(m_1^2+\alpha_1,\dots,m_N^2+\alpha_N,\alpha_1,\dots,\alpha_N)$, where $\alpha_i > 0$ for all $i = 1\dots N$.

For $(m,C) \in \Sigma_N$, we denote by $G_{m,C}(\cdot)$ the Gaussian measure with mean m and correlations given by the matrix C. The covariance matrix of $G_{m,C}(\cdot)$ is thus $C - m^t m$.

Lemma II.2. *Let $\lambda(\cdot)$ and $\beta(\cdot)$ be two functions of class $\mathcal{C}^1$ defined on $\mathbb{T}$, and $\mu^N_{\beta(\cdot),\lambda(\cdot)}$ be the Gibbs local equilibrium defined by* (II.2). *If we denote by $m_{\beta(\cdot),\lambda(\cdot)}$ and $C_{\beta(\cdot),\lambda(\cdot)}$ respectively the mean vector and the correlation matrix of $\mu^N_{\beta(\cdot),\lambda(\cdot)}$, then we have*

$$(m_{\beta(\cdot),\lambda(\cdot)}, C_{\beta(\cdot),\lambda(\cdot)}) \in \Sigma_N \ \text{ and } \ \mu^N_{\beta(\cdot),\lambda(\cdot)} = G_{m_{\beta(\cdot),\lambda(\cdot)},C_{\beta(\cdot),\lambda(\cdot)}}.$$

Proof. This result comes from the explicit formula of $\mu^{\mathrm{N}}_{\beta(\cdot),\lambda(\cdot)}$ given in (II.2). First, notice that each momentum p_x is centered under $\mu^{\mathrm{N}}_{\beta(\cdot),\lambda(\cdot)}$ and

$$\mu^{\mathrm{N}}_{\beta(\cdot),\lambda(\cdot)}[r_x] = -\frac{\lambda}{\beta}\left(\frac{x}{\mathrm{N}}\right) .$$

Second, we easily obtain the following expressions:

$$m_{\beta(\cdot),\lambda(\cdot)} = \left(-\frac{\lambda}{\beta}\left(\frac{0}{\mathrm{N}}\right), \cdots, -\frac{\lambda}{\beta}\left(\frac{\mathrm{N}-1}{\mathrm{N}}\right), \underbrace{0,\cdots,0}_{\mathrm{N}} \right) ,$$

$$\mathrm{C}_{\beta(\cdot),\lambda(\cdot)} = \begin{pmatrix} \mathrm{D} & 0_{\mathrm{N}} \\ 0_{\mathrm{N}} & \mathrm{D}' \end{pmatrix} \qquad \text{where} \begin{cases} \mathrm{D} = \mathrm{diag}\left(\cdots, \dfrac{1}{\beta(x/\mathrm{N})} + \dfrac{\lambda^2(x/\mathrm{N})}{\beta^2(x/\mathrm{N})}, \cdots \right), \\ \mathrm{D}' = \mathrm{diag}\left(\cdots, \dfrac{1}{\beta(x/\mathrm{N})}, \cdots \right). \end{cases}$$

□

Now we state our second main theorem, which will be proved in Section 3.

Theorem II.3. *We assume that the initial probability measure μ_0^{N} is a convex combination of Gibbs local equilibrium states. More precisely, let σ be a probability measure whose support is included in Σ_{N}. We assume that σ satisfies:*

$$\textit{for all } k \geqslant 1, \int \left[\mathrm{K}(m,\mathrm{C})\right]^k \, d\sigma(m,\mathrm{C}) < \infty ,$$

where $\mathrm{K}(m,\mathrm{C}) := \sup_{i=1\ldots\mathrm{N}} \{\mathrm{C}_{i,i}\}$. *We define the initial probability measure μ_0^{N} by*

$$\mu_0^{\mathrm{N}}(\cdot) = \int \mathrm{G}_{m,\mathrm{C}}(\cdot) \, d\sigma(m,\mathrm{C}) .$$

Then, (II.5) *holds, and the conclusions of Theorem III.34 are valid.*

Remark *1.2.* As in [14], we could consider a more general model, with a pinning potential. Instead of the deformation r_x, we now introduce the position q_x of the particle x. The new pinning Hamiltonian is given by

$$\mathcal{H}^p_{\mathrm{N}} = \sum_{x\in\mathbb{T}_{\mathrm{N}}} \frac{p_x^2}{2} + \nu^2 \sum_{x\in\mathbb{T}_{\mathrm{N}}} \frac{q_x^2}{2} + \sum_{\substack{|x-y|=1,\\ x,y\in\mathbb{T}_{\mathrm{N}}}} \frac{(q_x-q_y)^2}{4} .$$

The strength of the pinning potential is regulated by the parameter $\nu > 0$. The energy of site x is now given by

$$e_x = \frac{p_x^2}{2} + \nu^2 \frac{q_x^2}{2} + \frac{1}{4} \sum_{y;|x-y|=1} (q_x - q_y)^2 .$$

The stochastic operator $\mathcal{S}^p_{\mathrm{N}}$ remains equal to $\mathcal{S}_{\mathrm{N}}$, and the Liouville operator $\mathcal{A}^p_{\mathrm{N}}$ can be written as follows:

$$\mathcal{A}^p_{\mathrm{N}} = \sum_{x\in\mathbb{T}_{\mathrm{N}}} \left\{ p_x \, \partial_{q_x} - [(\nu^2 - \Delta)q]_x \, \partial_{p_x} \right\} ,$$

where Δ is the discrete Laplacian: $(\Delta u)_x = u_{x+1} + u_{x-1} - 2u_x$.

Because of the presence of the pinning, the bulk dynamics conserves only one quantity: the total energy $\sum_x e_x$. It follows that the Gibbs equilibrium measures μ_β^N are fully characterized by the temperature β^{-1}. Under μ_β^N, the variables p_x are independent of the q_x and are independent identically Gaussian variables of variance β^{-1}. The q_x are distributed according to a centered Gaussian process with covariances given by

$$\mu_\beta^N(q_x q_y) = \Gamma(x-y), \text{ such that } \big[(\nu^2 - \Delta)\big]\Gamma(z) = \frac{1}{\beta}\mathbb{1}_{z=0} \ .$$

Observe that there exists $C := C(\nu)$ independent of N such that $\big|\mu_\beta^N(q_x q_y)\big| \leqslant C^{-1}e^{-C|x-y|}$ for any $N \geqslant 1$.

These correlations make computations more technical, but the hydrodynamic limit can be established by following the proof here (in [14, Section 3.2], a heuristic argument is given). Assume that the system is initially distributed according to a Gibbs local equilibrium associated to the energy profile $\mathbf{e}_0(\cdot)$, and define $\mathbf{e}(t,\cdot)$ as the evolved profile in the diffusive scale. Then, if the energy moments are bounded like (II.5), $\mathbf{e}$ is the solution of the following heat equation

$$\begin{cases} \partial_t \mathbf{e} = \partial_q(D(\mathbf{e})\partial_q \mathbf{e}) \ , & q \in \mathbb{T},\ t \in \mathbb{R}, \\ \mathbf{e}(0,\cdot) = \mathbf{e}_0(\cdot) \ , \end{cases}$$

where $D(\mathbf{e})$ is the *diffusivity* given by

$$D := D(\mathbf{e}) = \frac{1/\gamma}{2 + \nu^2 + \sqrt{\nu^2(\nu^2+4)}} \ .$$

In our model, where the state space is not compact, what matters is the existence of moments bounds. We will see in Section 3 that this existence can be easily justified by following the same ideas which work for the unpinned model.

For the sake of simplicity, we will denote by $\mathbf{e}_t(\cdot)$, $\mathbf{r}_t(\cdot)$, $\lambda_t(\cdot)$ and $\beta_t(\cdot)$, respectively, the functions $q \mapsto \mathbf{e}(t,q)$, $q \mapsto \mathbf{r}(t,q)$, $q \mapsto \lambda(t,q)$, and $q \mapsto \beta(t,q)$ defined on $\mathbb{T}$.

1.4 Ergodicity of the Infinite Velocity-Flip Model

We conclude this part by giving the theorem of ergodicity, which is proved in [16, Sections 2.2, 2.4.2], by following the ideas of [40]. Let us define, for all finite subsets $\Lambda \subset \mathbb{Z}$, and for two probability measures ν and μ on $\Omega := (\mathbb{R}\times\mathbb{R})^{\mathbb{Z}}$, the restricted relative entropy

$$H_\Lambda(\nu|\mu) := H(\nu_\Lambda|\mu_\Lambda)$$

where ν_Λ and μ_Λ are the marginal distributions of ν and μ on Ω. The formal generator of the infinite dynamics is denoted by $\mathcal{L}$. The Gibbs states in infinite volume are the probability measures $\mu_{\beta,\lambda}$ on Ω given by

$$d\mu_{\beta,\lambda} := \prod_{x\in\mathbb{Z}} \frac{e^{-\beta e_x - \lambda r_x}}{Z(\beta,\lambda)} dr_x dp_x \ .$$

Theorem II.4. *Let ν be a probability measure on the configuration space Ω such that*

1. *ν has finite density entropy: there exists* $C > 0$, *such that for all finite subsets* $\Lambda \subset \mathbb{Z}$,

$$\mathrm{H}_\Lambda(\nu|\mu_*) \leqslant C|\Lambda| ,$$

with $\mu_* := \mu_{1,0}$ *a reference Gibbs measure on* $(\mathbb{R} \times \mathbb{R})^{\mathbb{Z}}$,

2. *ν is translation invariant, and stationary, i.e. for any compactly supported and differentiable function* $F(\mathbf{r}, \mathbf{p})$,

$$\int \mathcal{A}(F)\, d\nu = 0 .$$

3. *the conditional probability distribution of* $\mathbf{p}$ *given the probability distribution of* $\mathbf{r}$, *denoted by* $\nu(\mathbf{p}|\mathbf{r})$, *is invariant by any flip* $\mathbf{p} \longrightarrow \mathbf{p}^x$, *with* $x \in \mathbb{Z}$.

Then, ν is a mixture of infinite Gibbs states.

Corollary II.5. *If ν is a probability measure on Ω satisfying 1, 2 and if ν is stationary in the sense that: for any compactly supported and differentiable function* $F(\mathbf{r}, \mathbf{p})$,

$$\int \mathcal{L}(F)\, d\nu = 0 ,$$

then ν is a mixture of infinite Gibbs states.

The outline of the rest of the section is as follows. In the next section we expose the strategy of the proof. We introduce the relative entropy $H_N(t)$ of μ_t^N with respect to a corrected local equilibrium, and we prove a Gronwall estimate of the entropy production of the form

$$\partial_t H_N(t) \leqslant C\, H_N(t) + o(N) , \tag{II.9}$$

where $C > 0$ does not depend on N. In Section 3 we prove Theorem II.3. We suppose that t belongs to a compact set $[0, T]$, T fixed. All estimates are uniform in $t \in [0, T]$.

2 Entropy Production

2.1 Introduction to the Method

For the sake of simplificity, we denote all couples of the form $(\beta(\cdot), \lambda(\cdot))$ by $\chi(\cdot)$. The corrected Gibbs local equilibrium state $\nu^N_{\chi_t(\cdot)}$ is defined by

$$\nu^N_{\chi_t(\cdot)} := \frac{1}{Z(\chi_t(\cdot))} \prod_{x \in \mathbb{T}_N} \exp\left(-\beta_t\left(\frac{x}{N}\right) e_x - \lambda_t\left(\frac{x}{N}\right) r_x + \frac{1}{N} F\left(t, \frac{x}{N}\right) \cdot \tau_x h(\mathbf{r}, \mathbf{p}) \right) dr_x dp_x$$

where $Z(\chi_t(\cdot))$ is the partition function and F, h are functions which will be precised later on. The notation $a \cdot b$ still stands for the usual scalar product between a and b. An estimate of the partition function $Z(\chi_t(\cdot))$ is performed in Appendix 2.1.1.

We are going to use the relative entropy method, with the corrected local Gibbs state $\nu^N_{\chi_t(\cdot)}$ instead of the usual one $\mu^N_{\chi_t(\cdot)}$. We define

$$H_N(t) := H\left(\mu_t^N | \nu^N_{\chi_t(\cdot)}\right) = \int_{\Omega^N} f_t^N(\omega) \log \frac{f_t^N(\omega)}{\phi_t^N(\omega)} d\mu^N_{1,0}(\omega) ,$$

where f_t^{N} is the density of μ_t^{N} with respect to the reference measure $\mu_{1,0}^{\mathrm{N}}$. This is a solution, in the sense of the distributions, of the Fokker-Planck equation

$$\partial_t f_t = \mathrm{N}^2\, \mathcal{L}_{\mathrm{N}}^* f_t$$

where $\mathcal{L}_{\mathrm{N}}^* = -\mathcal{A}_{\mathrm{N}} + \gamma \mathrm{S}_{\mathrm{N}}$ is the adjoint of $\mathcal{L}_{\mathrm{N}}$ in $\mathbf{L}^2(\mu_{1,0}^{\mathrm{N}})$. In the same way, ϕ_t^{N} is the density of $\nu_{\chi_t(\cdot)}^{\mathrm{N}}$ with respect to $\mu_{1,0}^{\mathrm{N}}$ (which here is easily computable).

Thus, our purpose is now to prove (II.9). We begin with the following lemma.

Lemma II.6.

$$\partial_t \mathrm{H}_{\mathrm{N}}(t) \leqslant \int \frac{1}{\phi_t^{\mathrm{N}}} \left(\mathrm{N}^2 \mathcal{L}_{\mathrm{N}}^* \phi_t^{\mathrm{N}} - \partial_t \phi_t^{\mathrm{N}}\right) f_t^{\mathrm{N}} d\mu_{1,0} = \mu_t^{\mathrm{N}} \left[\frac{1}{\phi_t^{\mathrm{N}}} \left(\mathrm{N}^2 \mathcal{L}_{\mathrm{N}}^* \phi_t^{\mathrm{N}} - \partial_t \phi_t^{\mathrm{N}}\right)\right].$$

Proof. The case where f_t^{N} is smooth is proved in [49, Chapter 6, Lemma 1.4]. Here, we do not know that f_t^{N} is smooth, so that we refer the reader to the proof in [17, Section 3.2], which can be easily followed. □

Now, we choose the correction term. We consider

$$\begin{cases} \mathrm{F}\left(t, \dfrac{x}{\mathrm{N}}\right) := \left(-\beta_t'\left(\dfrac{x}{\mathrm{N}}\right), -\lambda_t'\left(\dfrac{x}{\mathrm{N}}\right)\right), \\ \tau_x h(\mathbf{r}, \mathbf{p}) := \left(\dfrac{r_x}{2\gamma}\left(p_{x+1} + p_x + \dfrac{\gamma}{2} r_x\right), \dfrac{p_{x+1}}{\gamma}\right). \end{cases} \tag{II.10}$$

Thus,

$$\phi_t^{\mathrm{N}}(\mathbf{r}, \mathbf{p}) = \frac{(\mathrm{Z}(1,0))^n}{\mathrm{Z}(\chi_t(\cdot))} \prod_{x \in \mathbb{T}_{\mathrm{N}}} \exp\left(e_x\left(-\beta_t\left(\frac{x}{\mathrm{N}}\right) + 1\right) - \lambda_t\left(\frac{x}{\mathrm{N}}\right) r_x + \frac{1}{\mathrm{N}} \mathrm{F}\left(t, \frac{x}{\mathrm{N}}\right) \cdot \tau_x h(\mathbf{r}, \mathbf{p})\right).$$

We define $\xi_x := (e_x, r_x)$ and $\eta(t,q) := (\mathbf{e}(t,q), \mathbf{r}(t,q))$. If f is a vectorial function, we denote its differential by $\mathrm{D}f$.

In Appendix 2.1.1, the following technical result is proved.

Proposition II.7. *The term $(\phi_t^{\mathrm{N}})^{-1}\left(\mathrm{N}^2 \mathcal{L}_{\mathrm{N}}^* \phi_t^{\mathrm{N}} - \partial_t \phi_t^{\mathrm{N}}\right)$ is given by the sum of five terms in which a microscopic expansion up to the first order appears. In other words,*

$$\begin{aligned} &\frac{1}{\phi_t^{\mathrm{N}}} \left(\mathrm{N}^2 \mathcal{L}_{\mathrm{N}}^* \phi_t^{\mathrm{N}} - \partial_t \phi_t^{\mathrm{N}}\right) = \\ &= \sum_{k=1}^{5} \sum_{x \in \mathbb{T}_{\mathrm{N}}} v_k\left(t, \frac{x}{\mathrm{N}}\right) \left[\mathrm{J}_x^k - \mathrm{H}_k\left(\eta\left(t, \frac{x}{\mathrm{N}}\right)\right) - (\mathrm{DH}_k)\left(\eta\left(t, \frac{x}{\mathrm{N}}\right)\right) \cdot \left(\xi_x - \eta\left(t, \frac{x}{\mathrm{N}}\right)\right)\right] + o(\mathrm{N}) \end{aligned} \tag{II.11}$$

where

k	J_x^k	$H_k(\mathbf{e},\mathbf{r})$	$v_k(t,q)$
1	$p_x^2 + r_x r_{x-1} + 2\gamma p_x r_{x-1}$	$\mathbf{e} + \dfrac{\mathbf{r}^2}{2}$	$\dfrac{-1}{2\gamma}\partial_q^2\beta(t,q)$
2	$r_x + \gamma p_x$	$\mathbf{r}$	$-\dfrac{1}{\gamma}\partial_q^2\lambda(t,q)$
3	$p_x^2\,(r_x + r_{x-1})^2$	$(2\mathbf{e} - \mathbf{r}^2)\left(\mathbf{e} + \dfrac{3}{2}\mathbf{r}^2\right)$	$\dfrac{1}{4\gamma}[\partial_q\beta(t,q)]^2$
4	$p_x^2\,(r_x + r_{x-1})$	$\mathbf{r}\,(2\mathbf{e} - \mathbf{r}^2)$	$\dfrac{1}{\gamma}\partial_q\beta(t,q)\;\partial_q\lambda(t,q)$
5	p_x^2	$\mathbf{e} - \dfrac{\mathbf{r}^2}{2}$	$\dfrac{1}{\gamma}[\partial_q\lambda(t,q)]^2$

A priori the first term on the right-hand side of (II.11) is of order N, but we want to take advantage of these microscopic Taylor expansions. First, we need to cut-off large energies in order to work with bounded variables only. Second, the strategy consists in performing a one-block estimate: we replace the empirical truncated current, which is averaged over a microscopic box centered at x, by its mean with respect to a Gibbs measure with the parameters corresponding to the microscopic averaged profiles.

A one-block estimate will be performed for each term of the form

$$\sum_{x\in\mathbb{T}_N} v_k\left(t,\frac{x}{N}\right)\left[J_x^k - H_k\left(\eta\left(t,\frac{x}{N}\right)\right) - (DH_k)\left(\eta\left(t,\frac{x}{N}\right)\right)\cdot\left(\xi_x - \eta\left(t,\frac{x}{N}\right)\right)\right]. \qquad \text{(II.12)}$$

In the following the index k is omitted, whenever this does not cause confusion. We follow the lines of the proof given in [16, Section 3.3], and inspired from [70]. A sketch of the proof for the one-block estimate is given in Appendix 2.1.2.

2.2 Cut-off of Large Energies

For $x \in \mathbb{T}_N$, we define $A_{x,M} := \{e_x + e_{x-1} \leqslant M\}$, $J_{x,M} := J_x\ \mathbb{1}_{A_{x,M}}$, and $\xi_{x,M} := \xi_x\ \mathbb{1}_{e_x\leqslant M}$. Then, $J_{x,M}$ and $\xi_{x,M}$ are bounded by $C(M) > 0$. We use twice the Cauchy-Schwartz inequality to write

$$\mu_t^N\left[\sum_{x\in\mathbb{T}_N} v\left(t,\frac{x}{N}\right)\ J_x\ \mathbb{1}_{A^c_{x,M}}\right] \leqslant \mu_t^N\left[\left(\sum_{x\in\mathbb{T}_N} v^2\left(t,\frac{x}{N}\right)J_x^2\right)^{1/2}\left(\sum_{x\in\mathbb{T}_N}\mathbb{1}_{A^c_{x,M}}\right)^{1/2}\right]$$
$$\leqslant \left(\mu_t^N\left[\sum_{x\in\mathbb{T}_N} v^2\left(t,\frac{x}{N}\right)J_x^2\right]\right)^{1/2}\left(\mu_t^N\left[\sum_{x\in\mathbb{T}_N}\mathbb{1}_{A^c_{x,M}}\right]\right)^{1/2}.$$

First, $v^2\left(t,x/N\right)$ is bounded by a constant which does not depend on N. Second, the term J_x^2 can be bounded above by the squared energy e_x^2. The hypothesis (II.5) shows that there exists C_0 which does not depend on N such that

$$\left(\mu_t^N\left[\sum_{x\in\mathbb{T}_N} v^2\left(t,\frac{x}{N}\right)J_x^2\right]\right)^{1/2} \leqslant C_0\ N^{1/2}.$$

Moreover, Markov inequality proves that

$$\mu_t^N \Big[\sum_{x \in \mathbb{T}_N} \mathbb{1}_{A^c_{x,M}} \Big] \leqslant \sum_{x \in \mathbb{T}_N} \mu_t^N \left[\mathbb{1}_{e_x > M/2} \right] + \mu_t^N \left[\mathbb{1}_{e_{x-1} > M/2} \right] \leqslant \frac{4}{M} \sum_{x \in \mathbb{T}_N} \mu_t^N [e_x] \leqslant \frac{C_1}{M} N \, .$$

Finally, we obtain a constant C independent of N such that

$$\mu_t^N \Big[\sum_{x \in \mathbb{T}_N} \nu \left(t, \frac{x}{N} \right) \, J_x \, \mathbb{1}_{A^c_{x,M}} \Big] \leqslant CN \, \varepsilon(M) \, .$$

Observe that this estimate is in agreement with the Gronwall inequality we want to prove, since we are going to divide by N. Thus, the error term is of order $1/M$ that goes to 0 as $M \longrightarrow \infty$. Consequently, J_x can be replaced by $J_{x,M}$ in (II.12), and similarly, ξ_x can be replaced by $\xi_{x,M}$.

2.3 One-block Estimate

Now we prove that

$$\frac{1}{N} \mu_t^N \left[\sum_{x \in \mathbb{T}_N} \nu \left(t, \frac{x}{N} \right) \left[J_{x,M} - H \left(\eta \left(t, \frac{x}{N} \right) \right) - (DH) \left(\eta \left(t, \frac{x}{N} \right) \right) \cdot \left(\xi_{x,M} - \eta \left(t, \frac{x}{N} \right) \right) \right] \right] \leqslant$$
$$\leqslant C \, \frac{H_N(t)}{N} + \varepsilon(N, M) \quad \text{(II.13)}$$

with $\varepsilon(N, M) \xrightarrow[M \longrightarrow \infty, N \longrightarrow \infty]{} 0$. We denote by $\Lambda_\ell(y)$ the box of length ℓ centered around y. We introduce the microscopic average profiles

$$\eta_{\ell,M}(y) := \frac{1}{\ell} \sum_{j \in \Lambda_\ell(y)} \xi_{j,M} \, .$$

We split $\mathbb{T}_N$ into $p = N/\ell$ boxes $\Lambda_\ell(x_j)$ centered at x_j. Here ℓ is assumed to divide N for simplicity. We will first let $N \longrightarrow \infty$, then $\ell \longrightarrow \infty$ and then $M \longrightarrow \infty$. First of all, we want to replace

$$\frac{1}{N} \sum_{x \in \mathbb{T}_N} \nu \left(t, \frac{x}{N} \right) J_{x,M}$$

by

$$\frac{1}{p} \sum_{j=1}^{p} \nu \left(t, \frac{x_k}{N} \right) \left[\frac{1}{\ell} \sum_{i \in \Lambda_\ell(x_j)} J_{i,M} \right] .$$

The error term produced during this step can be written as

$$|R_N| = \frac{1}{N} \left| \sum_{j=1}^{p} \sum_{i \in \Lambda_\ell(x_j)} \left[\nu \left(t, \frac{i}{N} \right) - \nu \left(t, \frac{x_j}{N} \right) \right] J_{i,M} \right| \leqslant C_1(M) \frac{\ell}{N} \, .$$

The last inequality comes from the smoothness of ν, more precisely

$$\left| \nu \left(t, \frac{i}{N} \right) - \nu \left(t, \frac{x_j}{N} \right) \right| \leqslant C_0 \frac{\ell}{N} \, .$$

Similarly, we perform the same estimates for the other terms and it remains to prove that

$$\mu_t^N \left[\frac{1}{p} \sum_{j=1}^{p} v\left(t, \frac{x_j}{N}\right) \left\{ \frac{1}{\ell} \sum_{i \in \Lambda_\ell(x_j)} J_{i,M} - H\left(\eta\left(t, \frac{x_j}{N}\right)\right) \right.\right.$$
$$\left.\left. -(DH)\left(\eta\left(t, \frac{x_j}{N}\right)\right) \cdot \left(\eta_{\ell,M}(x_j) - \eta\left(t, \frac{x_j}{N}\right)\right) \right\} \right] \qquad (II.14)$$

vanishes as $M, N, \ell \longrightarrow \infty$, the limit in N taken first, then the limit in ℓ and finally the limit in M. The additive term which appears after performing this replacement can be bounded above by a term $\varepsilon_{N,M,\ell}$ which depends on N, M and ℓ, but which is independent of the particular splitting of $\mathbb{T}_N$ into p boxes. This term is of order $o(N)$ in the Gronwall inequality we want to prove, in the sense that

$$\lim_{M \longrightarrow \infty} \lim_{\ell \longrightarrow \infty} \lim_{N \longrightarrow \infty} N^{-1} \mu_t^N[\varepsilon_{N,M,\ell}] = 0 .$$

Now we want to perform a one-block estimate. The main idea consists in replacing $\ell^{-1} \sum_{i \in \Lambda_\ell(x_j)} J_{i,M}$ by $H(\eta_{\ell,M}(x_j))$. This is achieved thanks to the ergodicity of the dynamics (see Theorem II.4). In order to use this ergodicity property, we have to work with a space translation invariant measure. To obtain such a probability measure, we introduce a second average over the x_j, $1 \leqslant j \leqslant p$. For each $k \in \{0, ..., \ell - 1\}$, we can split $\mathbb{T}_N$ into p disjoint boxes of length ℓ by writing

$$\forall\, k \in \{0, ..., \ell - 1\},\ \mathbb{T}_N = \bigcup_{j=1}^{p} \Lambda_\ell(x_j + k) .$$

Then, we average the different splittings mentioned above. More precisely, in Appendix 2.1.2 we recall how to prove

$$\limsup_{M \longrightarrow \infty} \limsup_{\ell \longrightarrow \infty} \limsup_{N \longrightarrow \infty} \frac{1}{\ell} \sum_{k=0}^{\ell-1} \mu_t^N \left[\frac{1}{p\ell} \sum_{j=1}^{p} \left| v\left(t, \frac{[x_j + k]}{N}\right) \sum_{i \in \Lambda_\ell(x_j+k)} J_{i,M} - H(\eta_{\ell,M}(x_j + k)) \right| \right] = 0. \qquad (II.15)$$

2.4 Large Deviations

The previous estimates are valid for any splitting of $\mathbb{T}_N$ into p boxes of length ℓ. Thus, it would be sufficient to prove (II.14) with every x_i replaced by $x_i + k$ for arbitrary $k \in \{1, ..., \ell - 1\}$. Consequently, it is sufficient to prove (II.14) in an averaged form. Then, from the one-block estimate, we have to deal with

$$\frac{1}{\ell} \sum_{k=0}^{\ell-1} \mu_t^N \left[\frac{1}{N} \sum_{j=1}^{p} v\left(t, \frac{[x_j + k]}{N}\right) \Omega\left(\eta_{\ell,M}(x_j + k), \eta\left(t, \frac{[x_j + k]}{N}\right)\right) \right], \qquad (II.16)$$

where $\Omega(\mathbf{w}, \mathbf{u}) := H(\mathbf{w}) - H(\mathbf{u}) - DH(\mathbf{u}) \cdot (\mathbf{w} - \mathbf{u})$. By definition of the entropy, for any $\alpha > 0$ and any positive measurable function f we have

$$\int f \, d\mu \leqslant \frac{1}{\alpha} \left\{ \log\left(\int e^{\alpha f} \, d\nu \right) + H(\mu|\nu) \right\} . \qquad (II.17)$$

This inequality, known as the *entropy inequality*, shows that: for any $\alpha > 0$, (II.16) is less than or equal to

$$\frac{H_N(t)}{\alpha\, N} + \frac{1}{\ell}\sum_{k=0}^{\ell-1}\frac{1}{\alpha N}\log \nu^N_{\chi_t(\cdot)}\left[e^{\alpha\ell\sum_{j=1}^{p}\nu\left(t,\frac{[x_j+k]}{N}\right)\Omega\left(\eta_{\ell,M}(x_j+k),\eta\left(t,\frac{[x_j+k]}{N}\right)\right)}\right].$$

Notice that the last integral converges because all quantities are bounded.

The first term is in agreement with the Gronwall inequality we want to obtain. We look at the second term. Since we have arranged the sum over p disjoint blocks which are independently distributed by $\nu^N_{\chi_t(\cdot)}$, the second term is equal to

$$\frac{1}{\ell}\sum_{k=0}^{\ell-1}\frac{1}{\alpha N}\sum_{j=1}^{p}\log \nu^N_{\chi_t(\cdot)}\left[e^{\alpha\ell\nu\left(t,\frac{[x_j+k]}{N}\right)\Omega\left(\eta_{\ell,M}(x_j+k),\eta\left(t,\frac{[x_j+k]}{N}\right)\right)}\right].$$

We are going to show that this expression vanishes as $M, N, \ell \longrightarrow \infty$ by using the large deviation properties of the measure $\nu^N_{\chi_t(\cdot)}$, that locally is almost homogeneous. In fact, by using the smoothness for the various involved functions, we can substitute the inhomogeneous product measure $\nu^N_{\chi_t(\cdot)}$ restricted to $\Lambda_\ell(x_j + k)$ with the homogeneous product measure $\mu^N_{\chi_t([x_j+k]/N)}$, in each expectation of the previous expression. More precisely, we prove the following lemma in Appendix 2.1.2:

Lemma II.8.

$$M_1(N,\ell,k,M) := \frac{1}{\alpha N}\sum_{j=1}^{p}\log \nu^N_{\chi_t(\cdot)}\left[e^{\alpha\ell\left|\nu\left(t,\frac{[x_j+k]}{N}\right)\Omega\left(\eta_{\ell,M}(x_j+k),\eta\left(t,\frac{[x_j+k]}{N}\right)\right)\right|}\right]$$

can be replaced by

$$M_2(N,\ell,k,M) := \frac{1}{\alpha N}\sum_{j=1}^{p}\log \mu^N_{\chi_t([x_j+k]/N)}\left[e^{\alpha\ell\left|\nu\left(t,\frac{[x_j+k]}{N}\right)\Omega\left(\eta_{\ell,M}(x_j+k),\eta\left(t,\frac{[x_j+k]}{N}\right)\right)\right|}\right].$$

The difference between these two terms is less than or equal to a small term which depends on ℓ (but not on k) and vanishes in the N *limit: there exists a constant* $C(\ell, M, N)$ *which does not depend on k such that*

$$M_1(N,\ell,k,M) - M_2(N,\ell,k,M) \leqslant C(\ell,M,N) \;\; \textit{and} \;\; C(\ell,M,N) \xrightarrow[N\longrightarrow\infty]{} 0\,.$$

Remark *2.1.* In the following, we will prove that

$$\limsup_{M\longrightarrow\infty}\limsup_{\ell\longrightarrow\infty}\limsup_{N\longrightarrow\infty} M_2(N,\ell,k,M) = 0\,.$$

In addition to this lemma, this implies that

$$\limsup_{M\longrightarrow\infty}\limsup_{\ell\longrightarrow\infty}\limsup_{N\longrightarrow\infty} M_1(N,\ell,k,M) = 0\,,$$

since $M_1(N,\ell,k,M)$ is always nonnegative, and we know that, for all sequences $\{a_n\}$ and $\{b_n\}$,

$$\limsup a_n \leqslant \limsup(a_n - b_n) + \limsup b_n\,.$$

Lastly, we have to show that the limit

$$\limsup_{M\longrightarrow\infty}\limsup_{\ell\longrightarrow\infty}\limsup_{N\longrightarrow\infty}\frac{1}{\ell}\sum_{k=0}^{\ell-1}\frac{1}{\alpha N}\sum_{j=1}^{p}\log\mu^{N}_{\chi_t([x_j+k]/N)}\left[e^{\alpha\ell v\left(t,\frac{[x_j+k]}{N}\right)\,\Omega\left(\eta_{\ell,M},\eta\left(t,\frac{[x_j+k]}{N}\right)\right)}\right]$$

vanishes. Here, $\eta_{\ell,M}:=\eta_{\ell,M}(0)=\ell^{-1}\sum_{i\in\Lambda_\ell(0)}\xi_{i,M}$.

The limit in p results in an integral over $\mathbb{T}$ because we have a Riemann sum. Moreover, the integral does not depend on k so that the averaging over k disappears in the p limit. Hence, the point is to estimate

$$\limsup_{M\longrightarrow\infty}\limsup_{\ell\longrightarrow\infty}\frac{1}{\alpha\ell}\int_{\mathbb{T}}\log\mu^{N}_{\chi_t(q)}\left[e^{\alpha\ell v(t,q)\,\Omega\left(\eta_{\ell,M},\eta(t,q)\right)}\right]\,dq\ .$$

According to Laplace-Varadhan theorem applied to these product measures $\mu^N_{\chi_t(q)}$, and according to the dominated convergence theorem, the previous limit is equal to

$$\limsup_{M\longrightarrow\infty}\frac{1}{\alpha}\int_{\mathbb{T}}\sup_{\mathbf{z}\in\mathbb{R}^2}\left\{\alpha v(t,q)\,\Omega(\mathbf{z},\eta(t,q))-I_M(\mathbf{z},\eta(t,q))\right\}dq\ , \tag{II.18}$$

where $I_M(\mathbf{z},\eta(t,q))$ is the rate function of the sequence $\left\{k^{-1}\sum_{i=1}^{k}\xi_{i,M}\right\}_k$ as $(r_x,p_x)_{x\in\mathbb{T}_N}$ are distributed according to the homogeneous product measure $\mu^N_{\chi_t(q)}$.

The function I_M is the Legendre transform of the cumulant-generating function of $\xi_{0,M}$:

$$I_M(\mathbf{z},\eta(t,q))=\sup_{\mathbf{y}\in\mathbb{R}^2}\left\{\mathbf{y}\cdot\mathbf{z}-\log\mu^N_{\chi_t(q)}[e^{\mathbf{y}\cdot\xi_{0,M}}]\right\}\ .$$

Hence

$$\liminf_{M\longrightarrow\infty}I_M(\mathbf{z},\eta(t,q))\geqslant\sup_{\mathbf{y}\in\mathbb{R}^2}\left\{\mathbf{y}\cdot\mathbf{z}-\log\mu^N_{\chi_t(q)}[e^{\mathbf{y}\cdot\xi_0}]\right\}=I(\mathbf{z},\eta(t,q))\ ,$$

where $I(\mathbf{z},\eta(t,q))$ is the rate function of $\left\{k^{-1}\sum_{i=1}^{k}\xi_i\right\}_k$ as $(r_y,p_y)_y$ are distributed according to the homogeneous product measure $\mu^N_{\chi_t(q)}$.

It follows, by Fatou's lemma, that (II.18) is smaller than or equal to

$$\frac{1}{\alpha}\int_{\mathbb{T}}\sup_{\mathbf{z}}\left\{\alpha v(t,q)\,\Omega(\mathbf{z},\eta(t,q))-I(\mathbf{z},\eta(t,q))\right\}dq\ .$$

From now on we omit the dependance in (t,q) of the involved functions v and η. Recall that χ and η are in duality (see (II.3)). An easy computation gives that

$$\begin{aligned}I(\mathbf{z},\eta)&=\sup_{\mathbf{y}}\left\{\mathbf{y}\cdot\mathbf{z}-\log\left(\int_{\mathbb{R}^2}e^{\mathbf{y}\cdot\xi}e^{\chi\cdot\xi-\log Z(\chi)}d\mathbf{r}d\mathbf{p}\right)\right\}\\&=\sup_{\mathbf{y}}\{\mathbf{y}\cdot\mathbf{z}-\log Z(\chi+\mathbf{y})+\log Z(\chi)\}\\&=\log Z(\chi)+\mathbf{z}\cdot\chi-S(\mathbf{z})\ ,\end{aligned}$$

where the last equality follows from the equality between the Fenchel-Legendre transform of $\log Z$ and the function $-S$. We observe that $I(\eta,\eta)=0$ and $D_{\mathbf{z}}I(\mathbf{z},\eta)=0$. Furthermore, I is strictly convex in $\mathbf{z}$:

$$(D^2_{\mathbf{z}}I)(\mathbf{z},\eta)=(D^2_{\mathbf{z}}\{-S\})(\mathbf{z})>0\ .$$

Since $\Omega(\eta,\eta)=0$ and $(D_{\mathbf{z}}\Omega)(\mathbf{z},\eta)=(DH)(\mathbf{z})-DH(\eta)$, we also get: $(D_{\mathbf{z}}\Omega)(\eta,\eta)=0$.

Lemma II.9. *For $\alpha > 0$ sufficiently small,*

$$\forall\, \mathbf{z} \in \mathbb{R}^2,\ \forall\, q \in \mathbb{T},\ \alpha v(t,q)\Omega(\mathbf{z},\eta(t,q)) \leqslant \mathrm{I}(\mathbf{z},\eta(t,q))\ .$$

Proof. An easy computation provides an explicit expression for the rate function: if $\mathbf{z} = (z_1, z_2)$ and $\eta = (e,r)$ with $e - r^2/2 > 0$ then

$$\mathrm{I}(\mathbf{z},\eta) = \frac{1}{e - r^2/2}\left(\frac{r^2}{2} - z_2 r + z_1\right) - \log\left(\frac{z_1 - z_2^2/2}{e - r^2/2}\right) - 1\ .$$

From the inequality $-\log x \geqslant -x + 1$ (satisfied for any $x > 0$), we get

$$\mathrm{I}(\mathbf{z},\eta) \geqslant \frac{1}{2(e - r^2/2)}(r - z_2)^2\ .$$

Thus, for a given η, the rate function $\mathbf{z} \longrightarrow \mathrm{I}(\mathbf{z},\eta)$ is such that $\mathrm{I}(\mathbf{z},\eta) \geqslant c_\eta |\mathbf{z} - \eta|^2$, where c_η is a positive constant. Moreover, according to (II.7),

$$\forall\, t \in [0,\mathrm{T}],\ \forall\, q \in \mathbb{T},\ c_{\eta(t,q)} \geqslant c > 0$$

Let us fix $\mathbf{z} \in \mathbb{R}^2$. From the Taylor-Lagrange theorem, there exists a positive constant C such that

$$\Omega(\mathbf{z},\eta(t,q)) \leqslant \mathrm{C}|\mathbf{z} - \eta(t,q)|^2 \leqslant \mathrm{I}(\mathbf{z},\eta(t,q))\ .$$

More precisely, C is equal to

$$\sup_{(t,q)\in[0,\mathrm{T}]\times\mathbb{T}} \|\mathrm{D}^2\mathrm{H}(\eta(t,q))\|^2\ .$$

Since v is uniformly bounded, the result is proved. □

Consequently, for α small enough,

$$\sup_{\mathbf{z}} \left\{\alpha v(t,q)\ \Omega(\mathbf{z},\eta(t,q)) - \mathrm{I}(\mathbf{z},\eta(t,q))\right\} = 0\ ,$$

and we have finally proved that

$$\partial_t \mathrm{H}_\mathrm{N}(t) \leqslant \mathrm{C}\ \mathrm{H}_\mathrm{N}(t) + \mathrm{R}_{\mathrm{N},\ell,\mathrm{M}}(t)$$

with

$$\lim_{\mathrm{M}\longrightarrow\infty} \lim_{\ell\longrightarrow\infty} \lim_{\mathrm{N}\longrightarrow\infty} \frac{1}{\mathrm{N}} \int_0^t \mathrm{R}_{\mathrm{N},\ell,\mathrm{M}}(s)\ \mathrm{d}s = 0\ .$$

By Gronwall's inequality we obtain: $\mathrm{H}_\mathrm{N}(t)/\mathrm{N} \xrightarrow[\mathrm{N}\longrightarrow\infty]{} 0$ and Theorem III.34 is proved.

3 Proof of Moments Bounds

In the following, we prove the two conditions on the moments bounds for a class of local equilibrium states. First, we assume that the initial law μ_0^N is exactly the Gibbs local equilibrium measure $\mu^\mathrm{N}_{\beta_0(\cdot),\lambda_0(\cdot)}$. Second, we extend the proof to the case where μ_0^N is a convex combination of Gibbs local equilibrium measures.

We need to control the moments $\mu_t^{\mathrm{N}}\left[\sum_x e_x^k\right]$ for all $k \geqslant 1$. The first two bounds ($k = 1, 2$) would be sufficient to justify the cut-off of the currents, but here we need more because of Lemma V.4 (which is necessary to prove Proposition II.7). Since the chain is harmonic, Gibbs states are Gaussian. We recall that all Gaussian moments can be expressed in terms of variances and covariances. In the following, we first give an other representation of the dynamics of the process, and then we prove the bounds and precise their dependence on k.

From now on, we consider the process generated $\mathcal{L}_{\mathrm{N}}$ (i.e. the process is not accelerated any more). The law of this new process $(\tilde{\omega}_t)_{t\geqslant 0}$ is denoted by $\tilde{\mu}_t^{\mathrm{N}}$. At the end of this part, Theorem II.3 will be easily deduced since all estimates will not depend on t, and the following equality still holds:

$$\mu_t^{\mathrm{N}} = \tilde{\mu}_{t\mathrm{N}^2}^{\mathrm{N}} \ .$$

REMARK *3.1.*

1. In the following, we always respect the decomposition of the space $\Omega^{\mathrm{N}} = \mathbb{R}^{\mathrm{N}} \times \mathbb{R}^{\mathrm{N}}$. Let us recall that the first N components stand for $\mathbf{r}$ and the last N components stand for $\mathbf{p}$. All vectors and matrices are written according to this decomposition. Let ν be a measure on Ω^{N}. We denote by $m \in \mathbb{R}^{2\mathrm{N}}$ its mean vector and by $\mathrm{C} \in \mathfrak{M}_{2\mathrm{N}}(\mathbb{R})$ its correlation matrix (see (II.8)). We can write m and C as

$$m = (\rho, \pi) \in \mathbb{R}^{2\mathrm{N}} \ \text{ and } \ \mathrm{C} = \begin{pmatrix} \mathrm{U} & \mathrm{Z}^* \\ \mathrm{Z} & \mathrm{V} \end{pmatrix} \in \mathfrak{S}_{2\mathrm{N}}(\mathbb{R}) \ ,$$

where $\rho := \nu[\mathbf{r}] \in \mathbb{R}^{\mathrm{N}}$, $\pi := \nu[\mathbf{p}] \in \mathbb{R}^{\mathrm{N}}$ and $\mathrm{U}, \mathrm{V}, \mathrm{Z} \in \mathfrak{M}_{\mathrm{N}}(\mathbb{R})$.

2. Thanks to the convexity inequality $(a+b)^k \leqslant 2^{k-1}\,(a^k + b^k)$, for $a, b > 0$, we can write

$$e_x^k \leqslant \frac{1}{2}\,\left(p_x^{2k} + r_x^{2k}\right) \ .$$

Thus, instead of proving (II.5) we will show

$$\mu_t^{\mathrm{N}}\left[\sum_{x\in\mathbb{T}_{\mathrm{N}}} p_x^{2k}\right] \leqslant (\mathrm{C}k)^k\,\mathrm{N} \quad \text{and} \quad \mu_t^{\mathrm{N}}\left[\sum_{x\in\mathbb{T}_{\mathrm{N}}} r_x^{2k}\right] \leqslant (\mathrm{C}k)^k\,\mathrm{N} \ .$$

3.1 Poisson Process and Gaussian Measures

We are going to use a graphical representation of the process $(\tilde{\omega}_t)_{t\geqslant 0}$. Let us define

$$\mathrm{A} := \begin{pmatrix} 0 & \cdots & \cdots & 0 & -1 & 1 & & (0) \\ \vdots & & & \vdots & 0 & \ddots & \ddots & \\ \vdots & & & \vdots & 0 & & \ddots & 1 \\ 0 & \cdots & \cdots & 0 & 1 & 0 & 0 & -1 \\ 1 & 0 & 0 & -1 & 0 & \cdots & \cdots & 0 \\ -1 & \ddots & & 0 & \vdots & & & \vdots \\ & \ddots & \ddots & 0 & \vdots & & & \vdots \\ (0) & & -1 & 1 & 0 & \cdots & \cdots & 0 \end{pmatrix} \in \mathfrak{M}_{2\mathrm{N}}(\mathbb{R}) \ . \tag{II.19}$$

We now consider $(m_t, \mathrm{C}_t)_{t\geqslant 0}$, a Markov process on $\mathbb{R}^{2\mathrm{N}} \times \mathfrak{S}_{2\mathrm{N}}(\mathbb{R})$ whose generator is denoted by $\mathcal{G}$ and defined as follows.

Take $m := (\rho, \pi) \in \mathbb{R}^{2N}$ and $C := \begin{pmatrix} U & Z^* \\ Z & V \end{pmatrix} \in \mathfrak{S}_{2N}(\mathbb{R})$, where ρ, π are two vectors in $\mathbb{R}^N$, U, V are two symmetric matrices in $\mathfrak{S}_N(\mathbb{R})$ and Z is a matrix in $\mathfrak{M}_N(\mathbb{R})$. Hereafter, we denote by Z^* the transpose of the matrix Z.

The generator $\mathcal{G}_N$ is given by

$$(\mathcal{G}_N v)(m, C) := (\mathcal{K}_N v)(m, C) + \gamma\ (\mathcal{H}_N v)(m, C)\ , \tag{II.20}$$

where

$$\mathcal{K}_N := \sum_{i,j \in \mathbb{T}_N} (-AC + CA)_{i,j}\ \partial_{C_{i,j}} + \sum_{i \in \mathbb{T}_N} \left\{ (\pi_{i+1} - \pi_i)\partial_{\rho_i} + (\rho_i - \rho_{i-1})\partial_{\pi_i} \right\} ,$$

and

$$(\mathcal{H}_N v)(m, C) := \frac{1}{2} \sum_{k \in \mathbb{T}_N} [v(m^k, C^k) - v(m, C)]\ .$$

Here,

$$m^k = (\rho, \pi^k) \ \text{ and } \ C^k = \Sigma_k^* \cdot C \cdot \Sigma_k = \begin{pmatrix} U & Z^{k*} \\ Z^k & V^k \end{pmatrix} .$$

In these last two formulas, π^k is the vector obtained from π by the flip of π_k into $-\pi_k$, and Σ_k is defined as

$$\Sigma_k = \begin{pmatrix} I_n & 0_n \\ 0_n & I_n - 2E_{k,k} \end{pmatrix} .$$

More precisely,

$$Z^k_{i,j} = (-1)^{\delta_{k,i}} Z_{i,j} \ \text{ and } \ V^k_{i,j} = (-1)^{(\delta_{k,i} + \delta_{k,j})} V_{i,j}\ .$$

We denote by $\mathbb{P}_{m_0, C_0}$ the law of the process $(m_t, C_t)_{t \geqslant 0}$ starting from (m_0, C_0), and by $\mathbb{E}_{m_0, C_0}[\cdot]$ the expectation with respect to $\mathbb{P}_{m_0, C_0}$. For $t \geqslant 0$ fixed, let $\theta^t_{m_0, C_0}(\cdot, \cdot)$ be the law of the random variable $(m_t, C_t) \in \mathbb{R}^{2N} \times \mathfrak{S}_{2N}(\mathbb{R})$, knowing that the process starts from (m_0, C_0).

Recall that we denote by $G_{m,C}(\cdot)$ the Gaussian measure on Ω^N with mean $m \in \mathbb{R}^{2N}$ and correlation matrix $C \in \mathfrak{S}_{2N}(\mathbb{R})$.

Lemma II.10. *Let $\mu_0^N := \mu^N_{\beta_0(\cdot), \lambda_0(\cdot)}$ be the Gibbs equilibrium state defined by* (II.2)*, where $\lambda_0(\cdot)$ and $\beta_0(\cdot)$ are the two macroscopic potential profiles.*

Then,

$$\tilde{\mu}_t^N = \int G_{m,C}(\cdot)\ d\theta^t_{m_0, C_0}(m, C) \tag{II.21}$$

where

$$m_0 := \left(-\frac{\lambda_0}{\beta_0}\left(\frac{0}{N}\right), \cdots, -\frac{\lambda_0}{\beta_0}\left(\frac{N-1}{N}\right), \underbrace{0, \cdots, 0}_{N} \right)$$

and

$$C_0 := \begin{pmatrix} D & 0_N \\ 0_N & D' \end{pmatrix} \qquad \text{with} \begin{cases} D = \mathrm{diag}\left(\cdots, \dfrac{1}{\beta_0(x/N)} + \dfrac{\lambda_0^2(x/N)}{\beta_0^2(x/N)}, \cdots \right), \\ D' = \mathrm{diag}\left(\cdots, \dfrac{1}{\beta_0(x/N)}, \cdots \right). \end{cases}$$

Proof. We begin with the graphical representation of the process $(\tilde{\omega}_t)_{t\geqslant 0}$, which is based on the Harris description. Let $\{N_i\}_{i\in\mathbb{T}_N}$ be a sequence of independent standard Poisson processes of intensity γ. In other words, we put on each site $i \in \mathbb{T}_N$ an exponential clock of mean $1/\gamma$. At time 0 the process has an initial state ω_0. Let $T_1 = \inf_{t\geqslant 0}\left\{\exists\, i \in \mathbb{T}_N,\ N_i(t) = 1\right\}$ and i_1 the site where the infimum is achieved.

During the interval $[0, T_1)$, the process follows the deterministic evolution given by the generator $\mathcal{A}_N$. More precisely, let $F : (\mathbf{r},\mathbf{p}) \in \mathbb{T}_N^2 \longrightarrow A\cdot(\mathbf{r},\mathbf{p}) \in \mathbb{T}_N^2$ where A is given by (II.19). Then, for any continuously differentiable function $f : \Omega^N \longrightarrow \mathbb{R}$,

$$\mathcal{A}_N f(\omega) = A \cdot Df(\omega)\ ,$$

and during the time interval $[0, T_1)$, $\tilde{\omega}_t$ follows the evolution given by the system: $dy/dt = F(y)$. At time T_1, the momentum p_{i_1} is flipped, and gives a new configuration. Then, the system starts again with the deterministic evolution up to the time of the next flip, and so on. Let $\xi := \left\{(i_1, T_1), \dots, (i_k, T_k), \dots\right\}$ be the sequence of sites and ordered times for which we have a flip, and let us denote its law by $\mathbb{P}$. Conditionally to ξ, the evolution is deterministic, and the state of the process $\tilde{\omega}_t^\xi$ is given by

$$\forall\ t \in [T_k, T_{k+1}),\ \tilde{\omega}_t^\xi = e^{(t-T_k)A} \circ F_{i_k} \circ e^{(T_k-T_{k-1})A} \circ F_{i_{k-1}} \circ \dots \circ e^{T_1 A}\omega_0\ , \tag{II.22}$$

where F_i is the map $\omega = (\mathbf{r},\mathbf{p}) \longrightarrow (\mathbf{r},\mathbf{p}^i)$.

If initially the process starts from ω_0 which is distributed according to a Gaussian measure μ_0^N, then $\tilde{\omega}_t^\xi$ is distributed according to a Gaussian measure $\tilde{\mu}_t^\xi$. Then, the density $\tilde{\mu}_t^N$ is given by

$$\tilde{\mu}_t^N(\cdot) = \int \tilde{\mu}_t^\xi(\cdot)\ d\mathbb{P}(\xi)\ . \tag{II.23}$$

More precisely, the mean vector m_t^ξ and the correlation matrix C_t^ξ of $\tilde{\mu}_t^\xi$ can be related to the mean vector m_0 and the correlation matrix C_0 of μ_0^N:

$$m_t^\xi = e^{(t-T_k)A}\cdot\Sigma_{i_k}\cdot e^{(T_k-T_{k-1})A}\cdot\Sigma_{i_{k-1}}\cdots e^{T_1A}\cdot m_0\ , \tag{II.24}$$

and

$$C_t^\xi = e^{(t-T_k)A}\cdot\Sigma_{i_k}\cdot e^{(T_k-T_{k-1})A}\dots\Sigma_{i_1}\cdot e^{T_1A}\cdot C_0\cdot e^{-T_1A}\cdot\Sigma_{i_1}^*\cdots e^{-(T_k-T_{k-1})A}\cdot\Sigma_{i_k}^* e^{-(t-T_k)A}\ . \tag{II.25}$$

Equations (II.24) and (II.25) also give a graphical representation of the process $(m_t, C_t)_{t\geqslant 0}$: during the interval $[0, T_1)$, m_t follows the evolution given by the (vectorial) system

$$\frac{dy}{dt} = F(y)$$

(where F has been previously introduced for the process $\tilde{\omega}_t$). At time T_1, the component m_{i_1+N} (which corresponds to the mean of p_{i_1}) is flipped, and gives a new mean vector. Then, the deterministic evolution goes on up to the time of the next flip, and so on.

In the same way, during the interval $[0, T_1)$, C_t follows the evolution given by the (matrix) system:

$$\frac{dM}{dt} = -AM + MA$$

(where A has been previously defined). At time T_1, all the components $C_{i_1,j}$ and C_{i,i_1} when $j \neq i_1$ and $i \neq i_1$ are flipped and the matrix C_{T_1} becomes $\Sigma_{i_1} \cdot C_{T_1} \cdot \Sigma^*_{i_1}$. The generator of this Markov process $(m_t, C_t)_{t\geqslant 0}$ is exactly the one defined by (II.20). Consequently, for $t \geqslant 0$, the law of the random variable (m_t, C_t) is $\theta^t_{m_0,C_0}$, where

$$m_0 = \left(-\frac{\lambda_0}{\beta_0}\left(\frac{0}{N}\right), \dots, -\frac{\lambda_0}{\beta_0}\left(\frac{N-1}{N}\right), \underbrace{0, \dots, 0}_{N} \right)$$

and

$$C_0 = \begin{pmatrix} D & 0_N \\ 0_N & D' \end{pmatrix} \text{ where } \begin{cases} D = \operatorname{diag}\left(\cdots, \dfrac{1}{\beta_0(x/N)} + \dfrac{\lambda_0^2(x/N)}{\beta_0^2(x/N)}, \cdots \right) , \\ D' = \operatorname{diag}\left(\cdots, \dfrac{1}{\beta_0(x/N)}, \cdots \right) , \end{cases}$$

as it can be deduced from Lemma II.2. Recall that in this section, μ_0^N is given by

$$\mu_0^N(d\mathbf{r}, d\mathbf{p}) = \prod_{x\in\mathbb{T}_N} \frac{\exp\left(-\beta_0\left(x/N\right) e_x - \lambda_0(x/N) r_x\right)}{Z(\beta_0(\cdot), \lambda_0(\cdot))} dr_x dp_x .$$

It follows that the density $\tilde{\mu}_t^N$ is equal to

$$\tilde{\mu}_t^N(\cdot) = \int \tilde{\mu}_t^\xi(\cdot)\, d\mathbb{P}(\xi) = \int G_{m,C}(\cdot)\, d\theta^t_{m_0,C_0}(m, C) . \tag{II.26}$$

□

REMARK *3.2.* Observe that

$$\tilde{\mu}_t^N[p_x] = \int G_{m,C}(p_x)\, d\theta^t_{m_0,C_0}(m, C) = \int \pi_x\, d\theta^t_{m_0,C_0}(m, C) = \mathbb{E}_{m_0,C_0}[\pi_x(t)] ,$$

$$\tilde{\mu}_t^N[r_x] = \int G_{m,C}(r_x)\, d\theta^t_{m_0,C_0}(m, C) = \int \rho_x\, d\theta^t_{m_0,C_0}(m, C) = \mathbb{E}_{m_0,C_0}[\rho_x(t)] .$$

LEMMA II.11. *Let $(m_t, C_t)_{t\geqslant 0}$ be the Markov process defined above. As previously done, we introduce $\rho(t), \pi(t) \in \mathbb{R}^N$ and $U(t), V(t), Z(t) \in \mathfrak{M}_N(\mathbb{R})$ such that*

$$m_t = (\rho(t), \pi(t)) \text{ and } C_t = \begin{pmatrix} U(t) & Z^*(t) \\ Z(t) & V(t) \end{pmatrix}$$

Then,

$$\mathbb{P}_{m_0,C_0}\text{ - a. s. },\ \forall\, t \geqslant 0,\ \begin{cases} \pi_y^2(t) \leqslant V_{y,y}(t) , \\ \rho_y^2(t) \leqslant U_{y,y}(t) . \end{cases}$$

Proof. First of all, let us notice that the quantities $V_{y,y}(t) - \pi_y^2(t)$ and $U_{y,y}(t) - \rho_y^2(t)$ are the diagonal components of the symmetric matrix $S_t := m_t \cdot {}^t m_t - C_t$. From Lemma II.10, we have

$$S_t = \int S_t^\xi\, d\mathbb{P}(\xi) .$$

For any sequence of sites and ordered times $\xi = \{(i_1, T_1), \dots, (i_k, T_k), \dots\}$, the symmetric matrix S_t^ξ is positive because this is the matrix of covariances of $\tilde{\omega}_t^\xi$. It follows that S_t is positive, and its diagonal components are all positive. □

REMARK *3.3.* In the case of the pinned chain, the matrix A is slightly different, but all the notations and conclusions are still valid. The initial correlation matrix for the pinned model is not more diagonal, but has non-trivial values on the upper and lower diagonals. The initial mean vector is equal to $0_{\mathbb{R}^{2N}}$.

3.2 Evolution of $(m_t, C_t)_{t\geqslant 0}$

Thanks to the regularity of β_0 and λ_0, we know that there exists a constant K which does not depend on N such that

$$\begin{cases} \frac{1}{N}\sum_{i,j}\Big[(U_{i,j})^2(0)+(V_{i,j})^2(0)+2(Z_{i,j})^2(0)\Big]\leqslant K\,, \\ \frac{1}{N}\sum_{i}\big[U_{i,i}(0)+V_{i,i}(0)\big]\leqslant K\,, \\ \frac{1}{N}\sum_{i}\big[(U_{i,i})^k(0)+(V_{i,i})^k(0)\big]\leqslant K^k\,,\ \text{for all } k\geqslant 1\,. \end{cases} \tag{II.27}$$

Moreover, one can easily show that

$$\mathcal{G}\bigg(\sum_{i,j}(U_{i,j})^2+(V_{i,j})^2+2(Z_{i,j})^2\bigg)=0 \quad \text{and} \quad \mathcal{G}\bigg(\sum_{i}U_{i,i}+V_{i,i}\bigg)=0\,.$$

It results that the two first inequalities of (II.27) are actually uniform in t, in the sense that

$$\begin{cases} \frac{1}{N}\mathbb{E}_{m_0,C_0}\bigg[\sum_{i,j}(U_{i,j}(t))^2+(V_{i,j}(t))^2+2(Z_{i,j}(t))^2\bigg]\leqslant K\,, \\ \frac{1}{N}\mathbb{E}_{m_0,C_0}\bigg[\sum_{i}U_{i,i}(t)+V_{i,i}(t)\bigg]\leqslant K\,. \end{cases} \tag{II.28}$$

We are going to see how this last inequality can be used in order to show (II.5). We denote by $u_k(t)$ and $v_k(t)$ the two quantities

$$\begin{cases} u_k(t)=\mathbb{E}_{m_0,C_0}\bigg[\sum_{i\in\mathbb{T}_N}U_{i,i}^k(t)\bigg]\,, \\ v_k(t)=\mathbb{E}_{m_0,C_0}\bigg[\sum_{i\in\mathbb{T}_N}V_{i,i}^k(t)\bigg]\,. \end{cases}$$

Let us make the link with (II.5). In view of (II.26), we can write

$$\tilde{\mu}_t^N\left[p_y^{2k}\right]=\int G_{m,C}\left[p_y^{2k}\right]\ d\theta_{m_0,C_0}^t(m,C)\,,$$

$$\tilde{\mu}_t^N\left[r_y^{2k}\right]=\int G_{m,C}\left[r_y^{2k}\right]\ d\theta_{m_0,C_0}^t(m,C)\,.$$

We use the convexity inequality $(a+b)^{2k}\leqslant 2^{2k-1}\,(a^{2k}+b^{2k})$ - which is true for all $a,b\in\mathbb{R}$ - to get

$$\begin{aligned}\tilde{\mu}_t^N\left[p_y^{2k}\right]&=\int G_{m,C}\left[(p_y-\pi_y+\pi_y)^{2k}\right]\ d\theta_{m_0,C_0}^t(m,C)\\ &\leqslant 2^{2k-1}\int G_{m,C}\left[(p_y-\pi_y)^{2k}\right]\ d\theta_{m_0,C_0}^t(m,C)+2^{2k-1}\int \pi_y^{2k}\ d\theta_{m_0,C_0}^t(m,C)\,.\end{aligned}$$

We deal with the two terms of the sum, separately. First, observe that Gaussian centered moments are easily computable:

$$\mathrm{G}_{m,\mathrm{C}}\left[(p_y-\pi_y)^{2k}\right]=\left(\mathrm{V}_{y,y}-\pi_y^2\right)^k\frac{(2k)!}{k!\,2^k}\,.$$

Then,

$$\sum_{y\in\mathbb{T}_\mathrm{N}}\int\left(\mathrm{V}_{y,y}-\pi_y^2\right)^k\frac{(2k)!}{k!\,2^k}\,\mathrm{d}\theta^t_{m_0,\mathrm{C}_0}(m,\mathrm{C})\leqslant\frac{(2k)!}{k!\,2^k}\left(v_k(t)+\mathbb{E}_{m_0,\mathrm{C}_0}\left[\sum_{y\in\mathbb{T}_\mathrm{N}}\pi_y^{2k}(t)\right]\right)\,.$$

In the same way,

$$\sum_{y\in\mathbb{T}_\mathrm{N}}\int\left(\mathrm{U}_{y,y}-\rho_y^2\right)^k\frac{(2k)!}{k!\,2^k}\,\mathrm{d}\theta^t_{m_0,\mathrm{C}_0}(m,\mathrm{C})\leqslant\frac{(2k)!}{k!\,2^k}\left(u_k(t)+\mathbb{E}_{m_0,\mathrm{C}_0}\left[\sum_{y\in\mathbb{T}_\mathrm{N}}\rho_y^{2k}(t)\right]\right)\,.$$

Lemma II.11 shows that

$$\mathbb{E}_{m_0,\mathrm{C}_0}\left[\sum_{y\in\mathbb{T}_\mathrm{N}}\pi_y^{2k}(t)\right]\leqslant\mathbb{E}_{m_0,\mathrm{C}_0}\left[\sum_{y\in\mathbb{T}_\mathrm{N}}\mathrm{V}^k_{y,y}(t)\right]=v_k(t)\,,$$

$$\mathbb{E}_{m_0,\mathrm{C}_0}\left[\sum_{y\in\mathbb{T}_\mathrm{N}}\rho_y^{2k}(t)\right]\leqslant\mathbb{E}_{m_0,\mathrm{C}_0}\left[\sum_{y\in\mathbb{T}_\mathrm{N}}\mathrm{U}^k_{y,y}(t)\right]=u_k(t)\,.$$

As a result,

$$\sum_y\tilde{\mu}^\mathrm{N}_t\left[p_y^{2k}\right]\leqslant\frac{(2k)!}{k!}\,v_k(t)\sim2\left(\frac{4}{e}\right)^k k^k\,v_k(t)\,,$$

$$\sum_y\tilde{\mu}^\mathrm{N}_t\left[r_y^{2k}\right]\leqslant\frac{(2k)!}{k!}\,u_k(t)\sim2\left(\frac{4}{e}\right)^k k^k\,u_k(t)\,.$$

In a few words, to get (II.5), we need to estimate the two quantities $u_k(t)$ and $v_k(t)$, which are related to C_t. That is what we do in the next section.

REMARK *3.4.* In the case of the pinned model, the p_x and q_x remain centered during the evolution: for all $t>0$, $m_t=0_{\mathbb{R}^{2\mathrm{N}}}$. This simplifies the study since we do not need to center the variables. The result is the same: we need to estimate $u_k(t)$ and $v_k(t)$.

3.3 The Correlation Matrix

LEMMA II.12. *For any integer k not equal to 0, there exists a positive constant* K *which does not depend on* N *and t such that*

$$\begin{cases}v_k(t)\leqslant\mathrm{K}^k\,\mathrm{N}\,,\\u_k(t)\leqslant\mathrm{K}^k\,\mathrm{N}\,.\end{cases}$$

Proof. First of all, (II.28) shows that, uniformly in t,

$$\begin{cases}u_1(t)\leqslant\mathrm{KN}\\u_2(t)\leqslant\mathrm{KN}\end{cases}\quad\text{and}\quad\begin{cases}v_1(t)\leqslant\mathrm{KN}\\v_2(t)\leqslant\mathrm{KN}\,.\end{cases}$$

We observe that

$$u_k(t)+v_k(t)=\mathbb{E}_{m_0,\mathrm{C}_0}\left[\sum_{i\in\mathbb{T}_\mathrm{N}}\mathrm{C}^k_{i,i}(t)\right]=\int\sum_{i\in\mathbb{T}_\mathrm{N}}(\mathrm{C}^\xi_{i,i})^k(t)\,\mathrm{d}\mathbb{P}(\xi)\,.$$

Thanks to the dynamics description, we know the expression of the correlation matrix: conditionally to ξ, for all $t \in [T_k, T_{k+1})$,

$$C^{\xi}(t) = e^{(t-T_k)A} \cdot \Sigma_{i_k} \cdot e^{(T_k - T_{k-1})A} \cdots \Sigma_{i_1} \cdot e^{T_1 A} \cdot C_0 \cdot e^{-T_1 A} \cdot \Sigma_{i_1}^* \cdots e^{-(T_k - T_{k-1})A} \cdot \Sigma_{i_k}^* e^{-(t-T_k)A} ,$$

Consequently, since C_0 and $C^{\xi}(t)$ are similar, we have:

$$\forall\, k \in \mathbb{N},\ \mathrm{Tr}([C^{\xi}(t)]^k) = \mathrm{Tr}(C_0^k) = O(N) .$$

More precisely,

$$\mathrm{Tr}(C_0^k) = \sum_{i \in \mathbb{T}_N} U_{i,i}^k(0) + V_{i,i}^k(0) = \sum_{i \in \mathbb{T}_N} \frac{1}{\beta_0^k(i/N)} + \left(\frac{1}{\beta_0(i/N)} + \frac{\lambda_0^2(i/N)}{\beta_0^2(i/N)} \right)^k .$$

From (II.27) we get $\mathrm{Tr}(C_0^k) \leqslant NK^k$, where K does not depend on N, ξ and t:

$$K := \sup_{u \in [0,1]} \left\{ \frac{1}{\beta_0(u)} + \frac{\lambda_0^2(u)}{\beta_0^2(u)} \right\} .$$

Now we show that the same inequality holds for $\sum_i [C_{i,i}^{\xi}]^k(t)$. The matrix $C^{\xi}(t)$ is symmetric, hence diagonalizable, and after denoting its eigenvalues by $\lambda_1, ..., \lambda_{2N}$, we can write

$$\mathrm{Tr}([C^{\xi}(t)]^k) = \sum_{i=1}^{2N} \lambda_i^k .$$

We have now to compare $\sum_{i=1}^{2N} \lambda_i^k$ with $\sum_{i=1}^{2N} [C_{i,i}^{\xi}]^k(t)$. But, if we denote by P the orthogonal matrix of the eigenvectors of $C^{\xi}(t)$, then we get $C^{\xi}(t) = (P_t^{\xi})^* \cdot D \cdot P_t^{\xi}$, where D is the diagonal matrix with the eigenvalues $\lambda_1, ..., \lambda_{2N}$. For the sake of simplicity, we denote by $(P_{i,j})_{i,j}$ the components of P_t^{ξ}. Then,

$$[C_{i,i}^{\xi}]^k(t) = \left(\sum_{j,l} P_{i,j}^* D_{j,l} P_{l,i} \right)^k = \left(\sum_j P_{i,j}^* \lambda_j P_{j,i} \right)^k = \left(\sum_j P_{i,j}^* P_{j,i} \cdot \lambda_j \right)^k .$$

But, $\sum_j P_{i,j}^* P_{j,i} = 1$, since D is an orthogonal matrix. Consequently, we can use the convexity inequality, and we obtain

$$\sum_i [C_{i,i}^{\xi}]^k(t) \leqslant \sum_i \sum_j P_{i,j}^* P_{j,i} \lambda_j^k \leqslant \sum_j \lambda_j^k = \mathrm{Tr}([C^{\xi}(t)]^k) \leqslant NK^k .$$

Hence,

$$u_k(t) + v_k(t) \leqslant \int NK^k \, d\mathbb{P}(\xi) \leqslant NK^k .$$

□

REMARK *3.5.* We notice that the same proof works for the pinned case. The only difference is about the initial matrix C_0, but the smoothness of the profile β_0 is still true, and the estimate $\mathrm{Tr}(C_0^k) = O(N)$ is valid.

3.4 When μ_0^{N} is a Convex Combination of Gibbs Measures

As in Theorem II.3, we now suppose that the initial probability measure μ_0^{N} is a convex combination of Gibbs states defined by

$$\mu_0^{\mathrm{N}}(\cdot) = \int \mathrm{G}_{m_0,\mathrm{C}_0}(\cdot)\ \mathrm{d}\sigma(m_0,\mathrm{C}_0)\ . \tag{II.29}$$

If initially the process starts from ω_0 which is distributed according to a Gaussian measure $\mathrm{G}_{m_0,\mathrm{C}_0}$, we know from Lemma II.10 that $\tilde{\omega}_t$ is distributed according to a convex combination of Gaussian measures written as

$$\int \mathrm{G}_{m,\mathrm{C}}(\cdot)\ \mathrm{d}\theta^t_{m_0,\mathrm{C}_0}(m,\mathrm{C})\ .$$

Consequently, in the case where μ_0^{N} is given by (II.29), the law of the process $\tilde{\omega}_t$ is given by

$$\tilde{\mu}_t^{\mathrm{N}}(\cdot) = \int \left\{ \int \mathrm{G}_{m,\mathrm{C}}(\cdot)\ \mathrm{d}\theta^t_{m_0,\mathrm{C}_0}(m,\mathrm{C}) \right\}\ \mathrm{d}\sigma(m_0,\mathrm{C}_0)\ .$$

Let us recall that we want to control, for $k \geqslant 1$, $\tilde{\mu}_t^{\mathrm{N}}\left[\sum_{x\in\mathbb{T}_\mathrm{N}} p_x^{2k}\right]$ and $\tilde{\mu}_t^{\mathrm{N}}\left[\sum_{x\in\mathbb{T}_\mathrm{N}} r_x^{2k}\right]$. Following the lines of the previous section, we notice that it is sufficient to control two quantities:

$$\begin{cases} \displaystyle\int \mathbb{E}_{m_0,\mathrm{C}_0}\left[\sum_{i\in\mathbb{T}_\mathrm{N}} \mathrm{U}^k_{i,i}(t)\right]\mathrm{d}\sigma(m_0,\mathrm{C}_0)\ , \\ \displaystyle\int \mathbb{E}_{m_0,\mathrm{C}_0}\left[\sum_{i\in\mathbb{T}_\mathrm{N}} \mathrm{V}^k_{i,i}(t)\right]\mathrm{d}\sigma(m_0,\mathrm{C}_0)\ . \end{cases}$$

Lemma V.24 gives a constant $\mathrm{C}(\lambda_0,\beta_0)$ which does not depend on N and t such that

$$\begin{cases} \displaystyle\mathbb{E}_{m_0,\mathrm{C}_0}\left[\sum_{i\in\mathbb{T}_\mathrm{N}} \mathrm{U}^k_{i,i}(t)\right] \leqslant [\mathrm{C}(\lambda_0,\beta_0)]^k\ \mathrm{N}\ , \\ \displaystyle\mathbb{E}_{m_0,\mathrm{C}_0}\left[\sum_{i\in\mathbb{T}_\mathrm{N}} \mathrm{V}^k_{i,i}(t)\right] \leqslant [\mathrm{C}(\lambda_0,\beta_0)]^k\ \mathrm{N}\ . \end{cases}$$

More precisely,

$$\mathrm{C}(\lambda_0,\beta_0) = \sup_{u\in[0,1]} \left\{ \frac{1}{\beta_0(u)} + \frac{\lambda_0^2(u)}{\beta_0^2(u)} \right\}\ .$$

In order to keep the same control, we have to suppose that, for all $k \geqslant 1$,

$$\int [\mathrm{K}(m,\mathrm{C})]^k\ \mathrm{d}\sigma(m,\mathrm{C}) < \infty, \quad \text{where } \mathrm{K}(m,\mathrm{C}) := \sup_{i\in\mathbb{T}_\mathrm{N}} \mathrm{C}_{i,i}\ .$$

Finally, let us observe that all estimates are given for $\tilde{\mu}_t^{\mathrm{N}}$ but are still true for the accelerated law μ_t^{N}. Indeed, the constants that appear do not depend on N and t.

CHAPTER III

Effect of Disorder

Contents

We investigate the macroscopic behavior of the disordered harmonic chain of oscillators, through energy diffusion. The Hamiltonian dynamics of the system is perturbed by a degenerate conservative noise. After rescaling space and time diffusively, we prove that the energy fluctuations in equilibrium evolve according to a linear heat equation. The diffusion coefficient is obtained from the non-gradient Varadhan's approach, and is equivalently defined through the Green-Kubo formula. Since the perturbation is very degenerate and the symmetric part of the generator does not have a spectral gap, the standard non-gradient method is reviewed under new perspectives (EXTRACTS FROM [77], WITH SOME ADD-INS).

1 The Harmonic Case with an Energy Conserving Noise

1.1 Generator of the Markov Process

We describe the dynamics on the finite torus $\mathbb{T}_N := \{0,\dots,N\}$, meaning that boundary conditions are periodic. The configuration $\{\omega_x\}_{x\in\mathbb{T}_N}$ evolves according to a dynamics which can be divided into two parts, a deterministic one and a stochastic one. The space of configurations of our system is given by $\Omega_N = \mathbb{R}^N$. We recall that the disorder is an i.i.d. sequence $\mathbf{m} = \{m_x\}_{x\in\mathbb{Z}}$ which satisfies:

$$\forall\ x \in \mathbb{Z}, \quad \frac{1}{C} \leqslant m_x \leqslant C,$$

for some finite constant $C > 0$. The corresponding product and translation invariant measure on the space $\Omega_{\mathcal{D}} = [C^{-1}, C]^{\mathbb{Z}}$ is denoted by $\mathbb{P}$ and its expectation is denoted by $\mathbb{E}$. For a fixed disorder field $\mathbf{m} = \{m_x\}_{x\in\mathbb{T}_N}$, we consider the system of ODE's

$$\sqrt{m_x}\mathrm{d}\omega_x = \left(\frac{\omega_{x+1}}{\sqrt{m_{x+1}}} - \frac{\omega_{x-1}}{\sqrt{m_{x-1}}}\right)\mathrm{d}t, \quad t \geqslant 0,\, x \in \mathbb{T}_N$$

and we superpose to this deterministic dynamics a stochastic perturbation described as follows: to each atom $x \in \mathbb{T}_N$, and each bond $\{x, x+1\}, x \in \mathbb{T}_N$ is associated an exponential clock of rate one, such that each clock is independent of each other. When the clock attached to x rings, ω_x is flipped into $-\omega_x$, and when the clock attached to the bond $\{x, x+1\}$ rings, the values ω_x and ω_{x+1} are exchanged. This dynamics can be entirely defined by the generator of the Markov process $\{\omega_x(t)\,;\, x \in \mathbb{T}_N\}_{t\geqslant 0}$, that is

$$\mathcal{L}_N^{\mathbf{m}} = \mathcal{A}_N^{\mathbf{m}} + \gamma\mathcal{S}_N^{\text{flip}} + \lambda\mathcal{S}_N^{\text{exch}}$$

where, for all functions $f : \Omega_{\mathcal{D}} \times \Omega_N \longrightarrow \mathbb{R}$,

$$\mathcal{A}_N^{\mathbf{m}} f(\mathbf{m},\omega) = \sum_{x\in\mathbb{T}_N}\left(\frac{\omega_{x+1}}{\sqrt{m_x m_{x+1}}} - \frac{\omega_{x-1}}{\sqrt{m_{x-1}m_x}}\right)\frac{\partial f}{\partial \omega_x}(\mathbf{m},\omega),$$

$$\mathcal{S}_N^{\text{flip}} f(\mathbf{m},\omega) = \sum_{x\in\mathbb{T}_N} f(\mathbf{m},\omega^x) - f(\mathbf{m},\omega),$$
$$\mathcal{S}_N^{\text{exch}} f(\mathbf{m},\omega) = \sum_{x\in\mathbb{T}_N} f(\mathbf{m},\omega^{x,x+1}) - f(\mathbf{m},\omega).$$

Here, the configuration ω^x is the configuration obtained from ω by flipping the momentum of particle x:

$$(\omega^x)_z = \begin{cases} \omega_z & \text{if } z \neq x, \\ -\omega_x & \text{if } z = x. \end{cases}$$

The configuration $\omega^{x,x+1}$ is obtained from ω by exchanging the momenta of particles x and $x+1$:

$$(\omega^{x,x+1})_z = \begin{cases} \omega_z & \text{if } z \neq x, x+1, \\ \omega_{x+1} & \text{if } z = x, \\ \omega_x & \text{if } z = x+1. \end{cases}$$

We denote the total generator of the noise by $\mathcal{S}_N := \gamma\mathcal{S}_N^{\text{flip}} + \lambda\mathcal{S}_N^{\text{exch}}$, where $\gamma, \lambda > 0$ are two positive parameters which regulate the respective strengths of noises.

One quantity is conserved: the total energy $\sum \omega_x^2$. The following translation invariant product Gibbs measures μ_β^N on Ω_N are invariant for the process:

$$\mathrm{d}\mu_\beta^N(\omega) := \prod_{x\in\mathbb{T}_N}\sqrt{\frac{2\pi}{\beta}}\exp\left(-\frac{\beta}{2}\omega_x^2\right)\mathrm{d}\omega_x.$$

In the following, the expectation of f with respect to μ_β^N is denoted by $\langle f\rangle_\beta$. The index β stands for the inverse temperature, namely $\langle\omega_0^2\rangle_\beta = 1/\beta$. Let us highlight the fact that the Gibbs measures do not depend on the disorder $\mathbf{m}$. From the definition, our model is not reversible with respect to the measure μ_β^N. Precisely, $\mathcal{A}_N^{\mathbf{m}}$ is an antisymmetric operator in $\mathbf{L}^2(\mu_\beta^N)$, whereas $\mathcal{S}_N$ is symmetric.

We denote by Ω the space of configurations in the infinite line, that is $\Omega := \mathbb{R}^{\mathbb{Z}}$, and by μ_β the product Gibbs measure on $\mathbb{R}^{\mathbb{Z}}$. Hereafter, for every $\beta > 0$, we denote by $\mathbb{P}^\star_\beta$ the probability measure on $\Omega_{\mathcal{D}} \times \Omega$ defined by

$$\mathbb{P}^\star_\beta := \mathbb{P} \otimes \mu_\beta.$$

We notice that $\mathbb{P}^\star_\beta$ is translation invariant and we write $\mathbb{E}^\star_\beta$ for the corresponding expectation.

1.2 Energy Current

Since the dynamics conserves the total energy, there exist instantaneous currents of energy $j_{x,x+1}$ such that $\mathcal{L}^{\mathbf{m}}_{\mathrm{N}}(\omega_x^2) = j_{x,x+1}(\mathbf{m},\omega) - j_{x-1,x}(\mathbf{m},\omega)$. The quantity $j_{x,x+1}$ is the amount of energy between the particles x and $x+1$, and is equal to

$$j_{x,x+1}(\mathbf{m},\omega) = \frac{2\omega_x\omega_{x+1}}{\sqrt{m_x m_{x+1}}} + \lambda(\omega_{x+1}^2 - \omega_x^2).$$

The energy conservation law can be read locally as

$$\omega_x^2(t) - \omega_x^2(0) = \mathrm{J}_{x,x+1}(t) - \mathrm{J}_{x-1,x}(t),$$

where $\mathrm{J}_{x,x+1}(t)$ is the total energy current between x and $x+1$ up to time t. This can be written as

$$\mathrm{J}_{x,x+1}(t) = \int_0^t j_{x,x+1}(s)\,\mathrm{d}s + \mathrm{M}_{x,x+1}(t),$$

where $\mathrm{M}_{x,x+1}(t)$ is a martingale which can be explicitely computed as Itô stochastic integral:

$$\mathrm{M}_{x,x+1}(t) = \int_0^t \left[\omega_{x+1}^2 - \omega_x^2\right](s^-)\mathrm{d}\left[\mathrm{N}_{x,x+1}(s) - \lambda s\right] + \int_0^t \left[\omega_{x-1}^2 - \omega_x^2\right](s^-)\mathrm{d}\left[\mathrm{N}_{x-1,x}(s) - \lambda s\right].$$

Here $(\mathrm{N}_{x,x+1})_{x\in\mathbb{Z}}$ are independent Poisson processes of intensity λ. We also write $j_{x,x+1} = j^{\mathrm{A}}_{x,x+1} + j^{\mathrm{S}}_{x,x+1}$ where $j^{\mathrm{A}}_{x,x+1}$ (resp. $j^{\mathrm{S}}_{x,x+1}$) is the current associated to the antisymmetric (resp. symmetric) part of the generator:

$$j^{\mathrm{A}}_{x,x+1}(\mathbf{m},\omega) = \frac{2\omega_x\omega_{x+1}}{\sqrt{m_x m_{x+1}}}$$
$$j^{\mathrm{S}}_{x,x+1}(\mathbf{m},\omega) = j^{\mathrm{S}}_{x,x+1}(\omega) = \lambda(\omega_{x+1}^2 - \omega_x^2).$$

One can check that the current cannot be directly written as the gradient of a local function, neither by an exact fluctuation-dissipation equation involving local functions (except if masses are equal). We also define the *static compressibility* that is equal to

$$\chi(\beta) := \langle \omega_0^4\rangle_\beta - \langle\omega_0^2\rangle_\beta^2 = \frac{2}{\beta^2}.$$

1.3 Cylinder Functions

For every $x \in \mathbb{Z}$ and f a measurable function on $\Omega_{\mathcal{D}} \times \Omega$, we consider the translated function $\tau_x f$, which is the function on $\Omega_{\mathcal{D}} \times \Omega$ defined by: $\tau_x f(\mathbf{m},\omega) := f(\tau_x\mathbf{m}, \tau_x\omega)$, where $\tau_x\mathbf{m}$ and $\tau_x\omega$ are the disorder and particle configurations translated by $x \in \mathbb{Z}$, respectively:

$$(\tau_x\mathbf{m})_z := m_{x+z}, \qquad (\tau_x\omega)_z = \omega_{x+z}.$$

If f is a measurable function on $\Omega_{\mathcal{D}} \times \Omega$, the *support* of f, denoted by Λ_f, is the smallest subset of $\mathbb{Z}$ such that $f(\mathbf{m}, \omega)$ only depends on $\{m_x, \omega_x \; ; \; x \in \Lambda_f\}$ and f is called a *cylinder function* if Λ_f is finite. For every cylinder function $f : \Omega_{\mathcal{D}} \times \Omega \longrightarrow \mathbb{R}$, consider the formal sum

$$\Gamma_f := \sum_{x \in \mathbb{Z}} \tau_x f$$

which does not make sense but for which

$$\nabla_0(\Gamma_f) := \Gamma_f(\mathbf{m}, \omega^0) - \Gamma_f(\mathbf{m}, \omega),$$
$$\nabla_{0,1}(\Gamma_f) := \Gamma_f(\mathbf{m}, \omega^{0,1}) - \Gamma_f(\mathbf{m}, \omega),$$

are well defined. Similarly, we define

$$(\nabla_x f)(\mathbf{m}, \omega) := f(\mathbf{m}, \omega^x) - f(\mathbf{m}, \omega),$$
$$(\nabla_{x,x+1} f)(\mathbf{m}, \omega) := f(\mathbf{m}, \omega^{x,x+1}) - f(\mathbf{m}, \omega).$$

Let $\Lambda \Subset \mathbb{Z}$ be a finite subset of $\mathbb{Z}$, and denote by $\mathcal{F}_\Lambda$ the σ-algebra generated by $\{m_x, \omega_x \; ; \; x \in \Lambda\}$. For a fixed positive integer ℓ, we define $\Lambda_\ell := \{-\ell, ..., \ell\}$. If the box is centered at site $x \in \mathbb{Z}$, we denote it by $\Lambda_\ell(x) := \{-\ell + x, ..., \ell + x\}$.

We denote by $\mathcal{C}$ the set of cylinder functions on $\Omega_{\mathcal{D}} \times \Omega$ with compact support and null average with respect to μ_β (for $\mathbb{P}$-almost every $m \in \Omega_{\mathcal{D}}$). We also introduce the set of *quadratic* cylinder functions on $\Omega_{\mathcal{D}} \times \Omega$, denoted by $\mathcal{Q} \subset \mathcal{C}$, and defined as follows: $f \in \mathcal{Q}$ if there exists a finite sequence $(\psi_{i,j}(\mathbf{m}))_{i,j \in \mathbb{Z}}$ of real cylinder functions on $\Omega_{\mathcal{D}}$ such that

$$f(\mathbf{m}, \omega) = \sum_{i \in \mathbb{Z}} \psi_{i,i}(\mathbf{m})(\omega_{i+1}^2 - \omega_i^2) + \sum_{\substack{i,j \in \mathbb{Z} \\ i \neq j}} \psi_{i,j}(\mathbf{m}) \omega_i \omega_j. \tag{III.1}$$

In other words, quadratic functions are homogeneous polynomials of degree two in the variable ω, that have null average with respect to μ_β for every $\mathbf{m} \in \Omega_{\mathcal{D}}$. An other definition through *Hermite polynomials* is given in Appendix 2.2.1.

For $f \in \mathcal{C}$, denote by s_f the smallest positive integer s such that Λ_s contains the support of f and then $\Lambda_f = \Lambda_{s_f}$. Hereafter, we consider operators $\mathcal{L}^{\mathbf{m}}$, $\mathcal{A}^{\mathbf{m}}$ and $\mathcal{S}$ acting on functions $f \in \mathcal{C}$ as

$$\mathcal{L}^{\mathbf{m}} f = \mathcal{A}^{\mathbf{m}} f + \mathcal{S} f, \tag{III.2}$$
$$\mathcal{A}^{\mathbf{m}} f(\mathbf{m}, \omega) = \sum_{x \in \mathbb{Z}} \left(\frac{\omega_{x+1}}{\sqrt{m_x m_{x+1}}} - \frac{\omega_{x-1}}{\sqrt{m_{x-1} m_x}} \right) \frac{\partial f}{\partial \omega_x}(\mathbf{m}, \omega),$$

$$\mathcal{S} f = \gamma \mathcal{S}^{\text{flip}} f + \lambda \mathcal{S}^{\text{exch}} f,$$
$$\mathcal{S}^{\text{flip}} f(\mathbf{m}, \omega) = \sum_{x \in \mathbb{Z}} (\nabla_x f)(\mathbf{m}, \omega) = \sum_{x \in \mathbb{Z}} f(\mathbf{m}, \omega^x) - f(\mathbf{m}, \omega),$$
$$\mathcal{S}^{\text{exch}} f(\mathbf{m}, \omega) = \sum_{x \in \mathbb{Z}} (\nabla_{x,x+1} f)(\mathbf{m}, \omega) = \sum_{x \in \mathbb{Z}} f(\mathbf{m}, \omega^{x,x+1}) - f(\mathbf{m}, \omega).$$

We also denote $\mathcal{S}_x = \gamma \nabla_x + \lambda \nabla_{x,x+1}$ for $x \in \mathbb{Z}$. For $\Lambda_\ell \Subset \mathbb{Z}$ defined as above, we denote by $\mathcal{L}^{\mathbf{m}}_{\Lambda_\ell}$, resp. $\mathcal{S}_{\Lambda_\ell}$, the restriction of the generator $\mathcal{L}^{\mathbf{m}}$, resp. $\mathcal{S}$, to the finite box Λ_ℓ, assuming periodic boundary conditions.

Now we are ready to define two sets of functions that will play further a crucial role.

Definition III.1. *Let $\mathcal{C}_0$ (respectively $\mathcal{Q}_0$) be the set of cylinder (respectively quadratic cylinder) functions φ on $\Omega_{\mathcal{D}} \times \Omega$ such that there exists a finite subset $\Lambda \Subset \mathbb{Z}$, and cylinder functions $\{\mathrm{F}_x, \mathrm{G}_x\}_{x\in\Lambda}$ satisfying*

$$\varphi = \sum_{x\in\Lambda} \nabla_x(\mathrm{F}_x) + \nabla_{x,x+1}(\mathrm{G}_x).$$

If φ belongs to $\mathcal{Q}_0$, we assume the cylinder functions F_x, G_x to be quadratic.

To conclude this section we introduce the quadratic form associated to the generator: for any $x \in \mathbb{Z}$ and cylinder functions $f, g \in \mathcal{C}$, let us define

$$\mathcal{D}_\ell(\mu_\beta; f) := \big\langle (-\mathcal{L}^{\mathbf{m}}_{\Lambda_\ell}) f, f \big\rangle_\beta = \big\langle (-\mathcal{S}_{\Lambda_\ell}) f, f \big\rangle_\beta = \sum_{x\in\Lambda_\ell} \big\langle (-\mathcal{S}_x) f, g \big\rangle_\beta,$$

and notice that

$$\begin{aligned}\big\langle (-\mathcal{S}_x) f, g \big\rangle_\beta = \frac{\gamma}{2} \Big\langle \big(f(\mathbf{m}, \omega^x) - f(\mathbf{m}, \omega)\big) \big(g(\mathbf{m}, \omega^x) - g(\mathbf{m}, \omega)\big) \Big\rangle_\beta \\ + \frac{\lambda}{2} \Big\langle \big(f(\mathbf{m}, \omega^{x,x+1}) - f(\mathbf{m}, \omega)\big) \big(g(\mathbf{m}, \omega^{x,x+1}) - g(\mathbf{m}, \omega)\big) \Big\rangle_\beta,\end{aligned}$$

The symmetric form $\mathcal{D}_\ell$ is called the *Dirichlet form*, and is well-defined on $\mathcal{C}$. This is a random variable with respect to the disorder $\mathbf{m}$.

1.4 Semi-inner Products and Diffusion Coefficient

For cylinder functions $g, h \in \mathcal{C}$, let us introduce

$$\ll g, h \gg_{\beta,\star} := \sum_{x\in\mathbb{Z}} \mathbb{E}^\star_\beta[g\, \tau_x h] \quad \text{and} \quad \ll g \gg_{\beta,\star\star} := \sum_{x\in\mathbb{Z}} x\, \mathbb{E}^\star_\beta[g\, \omega_x^2] \tag{III.3}$$

which are well-defined because g and h belong to $\mathcal{C}$ and therefore all but a finite number of terms vanish. Notice that $\ll \cdot, \cdot \gg_{\beta,\star}$ is an inner-product, since the following equality holds:

$$\ll f, g \gg_{\beta,\star} = \lim_{\Lambda\uparrow\mathbb{Z}} \frac{1}{|\Lambda|} \mathbb{E}\left[\left\langle \sum_{x\in\Lambda} \tau_x f, \sum_{x\in\Lambda} \tau_x g \right\rangle_\beta \right]$$

Since $\ll f - \tau_x f, g \gg_{\beta,\star} = 0$ for all $x \in \mathbb{Z}$, this scalar product is only semidefinite. In the next proposition we give explicit formulas for elements of $\mathcal{C}_0$.

Proposition III.1. *If $\varphi \in \mathcal{C}_0$ with*

$$\varphi = \sum_{y\in\Lambda} \nabla_y(\mathrm{F}_y) + \nabla_{y,y+1}(\mathrm{G}_y),$$

then

$$\ll \varphi \gg_{\beta,\star\star} = \mathbb{E} \left\langle (\omega_0^2 - \omega_1^2) \sum_{y\in\Lambda} \tau_{-y} \mathrm{G}_y \right\rangle_\beta$$

$$\ll \varphi, g \gg_{\beta,\star} = \mathbb{E} \left\langle \nabla_0(\Gamma_g) \sum_{y\in\Lambda} \tau_{-y} \mathrm{F}_y + \nabla_{0,1}(\Gamma_g) \sum_{y\in\Lambda} \tau_{-y} \mathrm{G}_y \right\rangle_\beta \qquad \textit{for all } g \in \mathcal{C}.$$

Proof. The proof is straightforward. □

Definition III.2. *We define the* diffusion coefficient $D(\beta)$ *for* $\beta > 0$ *as*

$$D(\beta) := \lambda + \frac{1}{\chi(\beta)} \inf_{f \in \mathcal{Q}} \sup_{g \in \mathcal{Q}} \left\{ \ll f, -\mathcal{S} f \gg_{\beta,\star} + 2 \ll j^{A}_{0,1} - \mathcal{A}^{\mathbf{m}} f, g \gg_{\beta,\star} - \ll g, -\mathcal{S} g \gg_{\beta,\star} \right\}.$$

The first term in the sum is only due to the exchange noise, whereas the second one comes from the Hamiltonian part of the dynamics. Formally, this formula could be read as

$$D(\beta) = \lambda + \frac{1}{\chi(\beta)} \ll j^{A}_{0,1}, (-\mathcal{L}^{\mathbf{m}})^{-1} j^{A}_{0,1} \gg_{\beta,\star}, \tag{III.4}$$

but the last term is ill-defined because $j^{A}_{0,1}$ is not in the range of $\mathcal{L}^{\mathbf{m}}$. More rigorously, we should define $\ll j^{A}_{0,1}, (-\mathcal{L}^{\mathbf{m}})^{-1} j^{A}_{0,1} \gg_{\beta,\star}$ as

$$\limsup_{z \longrightarrow 0} \ll j^{A}_{0,1}, (z - \mathcal{L}^{\mathbf{m}})^{-1} j^{A}_{0,1} \gg_{\beta,\star}.$$

The scalar product above is now well-defined, and the problem is reduced to prove convergence as $z \longrightarrow 0$. From Hille-Yosida Theorem (see [36, Proposition 2.1] for instance) (III.4) is equal to the infinite volume Green-Kubo formula:

$$D(\beta) = \lambda + \frac{1}{\chi(\beta)} \lim_{\substack{z \longrightarrow 0 \\ z > 0}} \mathbb{E}\left[\int_0^{+\infty} e^{-zt} \left\langle \sum_{x \in \mathbb{Z}} j^{A}_{x,x+1}(t), j^{A}_{0,1}(0) \right\rangle_{\beta} dt \right]. \tag{III.5}$$

In Section 3.1, we prove that (III.5) converges, by inspiring the argument from [10], and show that the diffusion coefficient can be equivalently defined in the two ways.

Assuming the convergence in the Green-Kubo formula, one can easily see that $D(\beta)$ does not depend on β. We denote by $L(z)$ the second term of the right-hand side of (III.5), that is

$$L(z) := \frac{1}{\chi(\beta)} \int_0^{+\infty} e^{-zt} \ll j^{A}_{0,1}(t), j^{A}_{0,1}(0) \gg_{\beta,\star} dt.$$

The function L is smooth on $(0, +\infty)$ [72]. Let $\mathbf{L}^2(\ll \cdot, \cdot \gg_{\beta,\star})$ be the Hilbert space generated by the set of bounded local functions and the inner product $\ll \cdot, \cdot \gg_{\beta,\star}$, and $h_z := h_z(\mathbf{m}, \omega; \beta)$ be the solution of the resolvent equation in $\mathbf{L}^2(\ll \cdot, \cdot \gg_{\beta,\star})$ i.e.

$$(z - \mathcal{L}^{\mathbf{m}}) h_z = j^{A}_{0,1}.$$

We have that

$$L(z) = \frac{1}{\chi(\beta)} \ll h_z, j^{A}_{0,1} \gg_{\beta,\star} = \frac{\beta^2}{2} \ll h_z, j^{A}_{0,1} \gg_{\beta,\star}.$$

Observe that if ω is distributed according to μ_β then $\beta^{1/2}\omega$ is distributed according to μ_1. Since $h_z(\mathbf{m}, \omega; 1) = h_z(\mathbf{m}, \omega; \beta)$ and $j^{A}_{x,x+1}$ is a homogeneous function of degree two in ω, it follows that the diffusion coefficient does not depend on β.

2 Non-gradient Method without Spectral Gap

From now on, we assume $\beta = 1$. This assumption is justified since we are going to deal only with quadratic functions (as defined before). For instance, when one result is stated for the scalar product $\ll \cdot \gg_{1,\star}$ (meaning $\beta = 1$), the same argument in the proof can be rewritten for any $\beta > 0$, after multiplying the process $\{\omega_x(t)\}$ by $\beta^{-1/2}$.

2.1 Central Limit Theorem Variances at Equilibrium

In this section we are going to identify the diffusion coefficient D given in Definition III.2. Roughly speaking, we are going to show that D is the asymptotic component of the energy current $j_{x,x+1}$ in the direction of the gradient $\omega_{x+1}^2 - \omega_x^2$, and makes the expression below vanish:

$$\inf_{f\in\mathcal{Q}} \limsup_{N\longrightarrow\infty} \limsup_{t\longrightarrow\infty} \frac{1}{tN}\mathbb{E}_1^\star\left[\left(\int_0^t \sum_{x\in\mathbb{T}_N} \left[j_{x,x+1} - D(\omega_{x+1}^2 - \omega_x^2) - \mathcal{L}^{m}(\tau_x f)\right]ds\right)^2\right]. \tag{III.6}$$

Let us start by giving well-known tools that will help understand the forthcoming results.

2.1.1 An Insight through Additive Functionals of Markov Processes

Consider a continuous time Markov process $\{Y_s\}_{s\geqslant 0}$ on a complete and separable metric space E, which has an invariant and ergodic measure π. We denote by $\langle\cdot\rangle_\pi$ the inner product in $\mathbf{L}^2(\pi)$ and by $\mathcal{L}$ the infinitesimal generator of the process. The adjoint of $\mathcal{L}$ in $\mathbf{L}^2(\pi)$ is denoted by $\mathcal{L}^\star$. Fix a function $V : E \longrightarrow \mathbb{R}$ in $\mathbf{L}^2(\pi)$ such that $\langle V\rangle_\pi = 0$. Theorem 2.7 in [52] gives conditions on V which guarantee a central limit theorem for

$$\frac{1}{\sqrt{t}}\int_0^t V(Y_s)ds$$

and shows that the limiting variance equals

$$\sigma^2(V,\pi) = 2\lim_{\substack{z\longrightarrow 0\\ z>0}} \big\langle V, (z-\mathcal{L})^{-1}V\big\rangle_\pi.$$

Let the generator $\mathcal{L}$ be decomposed as $\mathcal{L} = \mathcal{S} + \mathcal{A}$, where $\mathcal{S} = (\mathcal{L}+\mathcal{L}^\star)/2$ and $\mathcal{A} = (\mathcal{L}-\mathcal{L}^\star)/2$ denote, respectively, the symmetric and antisymmetric parts of $\mathcal{L}$. Let $\mathcal{H}_1$ be the completion of $\mathbf{L}^2(\pi)$ with respect to the semi-norm $\|\cdot\|_1$ defined as:

$$\|f\|_1^2 := \big\langle f, (-\mathcal{L})f\big\rangle_\pi = \big\langle f, (-\mathcal{S})f\big\rangle_\pi.$$

Let $\mathcal{H}_{-1}$ be the dual space of $\mathcal{H}_1$ with respect to $\mathbf{L}^2(\pi)$, in other words, the Hilbert space generated by local functions and the norm $\|\cdot\|_{-1}$ defined by

$$\|f\|_{-1}^2 := \sup_g \Big\{2\big\langle f, g\big\rangle_\pi - \|g\|_1^2\Big\},$$

where the supremum is carried over all local functions g. Formally, $\|f\|_{-1}$ can also be thought as $\langle f, (-\mathcal{S})^{-1} f\rangle_\pi$. Notice the difference with the variance $\sigma^2(\mathrm{V},\pi)$ which formally reads

$$2\left\langle \mathrm{V}, (-\mathcal{L})^{-1}\mathrm{V}\right\rangle_\pi = 2\left\langle \mathrm{V}, \left[(-\mathcal{L})^{-1}\right]_s \mathrm{V}\right\rangle_\pi .$$

Hereafter, B_s represents the symmetric part of the operator B. We can write, at least formally, that

$$\left\{\left[(-\mathcal{L})^{-1}\right]_s\right\}^{-1} = -\mathcal{S} + \mathcal{A}^\star(-\mathcal{S})^{-1}\mathcal{S} \geqslant -\mathcal{S},$$

where $\mathcal{A}^\star$ stands for the adjoint of $\mathcal{A}$. We have therefore that $\left[(-\mathcal{L})^{-1}\right]_s \leqslant (-\mathcal{S})^{-1}$. The following result is a rigorous estimate of the time variance in terms of the $\mathcal{H}_{-1}$ norm, which is proved in [52, Lemma 2.4] .

Lemma III.2. *Given* $\mathrm{T} > 0$ *and a mean zero function* V *in* $\mathbf{L}^2(\pi) \cap \mathcal{H}_{-1}$,

$$\mathbb{E}_\pi\left[\sup_{0\leqslant t\leqslant \mathrm{T}}\left(\int_0^t \mathrm{V}(s)\mathrm{d}s\right)^2\right] \leqslant 24\mathrm{T}\|\mathrm{V}\|_{-1}^2. \tag{III.7}$$

If we compare the previous left-hand side to (III.6), the next step should be to take V proportional to

$$\sum_{x\in\mathbb{T}_\mathrm{N}}\left[j_{x,x+1} - \mathrm{D}(\omega_{x+1}^2 - \omega_x^2) - \mathcal{L}^{\mathrm{m}}(\tau_x f)\right]$$

and then take the limit as N goes to ∞. In the right-hand side of (III.7) we will obtain a variance that depends on N, and the main task will be to show that this variance converges: this is studied in more details in what follows. Precisely, we prove that the limit of the variance results in a semi-norm, which is denoted by $|||\cdot|||_1$ and defined in (III.14). We are going to see that (III.14) involves a variational formula, which formally reads

$$|||f|||_1^2 = \ll f, (-\mathcal{S})^{-1} f \gg_{1,\star} + \frac{2}{\lambda\chi(1)} \ll f \gg_{1,\star\star}^2 .$$

The final step consists in minimizing this semi-norm on a well-chosen subspace, through orthogonal projections in Hilbert spaces. The hard point is that $|||\cdot|||_1$ only depends on the symmetric part of the generator $\mathcal{S}$, and the latter is really degenerate, since it does not have a spectral gap.

In Subsection 2.1.2, we investigate the variance $\langle f, (-\mathcal{S})^{-1} f\rangle_1$, and prove its well-posedness for every function f in $\mathcal{Q}_0$. In Subsection 2.1.3, we relate the previous limiting variance (taking the limit as N goes to infinity) to the suitable semi-norm. Then, in Section 2.2 we investigate the Hilbert space generated by the semi-norm, and prove some decompositions into direct sums. Finally, Section 2.3 focuses on the diffusion coefficient and its different expressions.

2.1.2 Microcanonical Measures and Integration by Part

In this paragraph, we recall general results on microcanonical measures, and state them for every $\beta > 0$ for the safe of clarity.

Decomposition on microcanonical measures – The thermodynamic ensemble which is naturally associated with a Hamiltonian dynamics is the *microcanonical ensemble*, which describes the system at fixed energy. It is possible to devise a probability measure on the configurations $\omega \in \Omega_{\mathrm{N}}$ with constant energy $\beta^{-1} > 0$ such that the measure is stationary with respect to the Hamiltonian flow. The corresponding probability measure denoted by $\mu^{mc}_{\mathrm{N},\beta}$ is the normalized uniform probability measure on the sphere

$$\mathfrak{S}_{\mathrm{N},\beta} := \Big\{ \omega \in \Omega_{\mathrm{N}} \; ; \; \sum_{x \in \mathbb{T}_{\mathrm{N}}} \omega_x^2 = \beta^{-1} \Big\}.$$

Now, for $\beta^{-1} > 0$ fixed, we disintegrate the microcanonical measure $\mu^{mc}_{\mathrm{N},\beta}$ on $\mathfrak{S}_{\mathrm{N},\beta}$. Let $\mathcal{G}$ be the group generated by the following matrices: the *permutation matrices* P_σ, defined for any permutation σ of $\{1, ..., \mathrm{N}\}$ by

$$(\mathrm{P}_\sigma)_{i,j} = \begin{cases} 1 & \text{if } i = \sigma(j), \\ 0 & \text{otherwise,} \end{cases}$$

and the *sign matrices* S_k, defined for $k \in \{1, ..., \mathrm{N}\}$ by

$$(\mathrm{S}_k)_{i,j} = \begin{cases} 1 & \text{if } i = j \text{ and } i \neq k, \\ -1 & \text{if } i = j = k, \\ 0 & \text{otherwise.} \end{cases}$$

The group $\mathcal{G}$ acts on $\mathfrak{S}_{\mathrm{N},\beta}$. For $\mathbf{x} \in \mathfrak{S}_{\mathrm{N},\beta}$, we denote by $\mathcal{G}^{\mathrm{N},\beta}_{\mathbf{x}}$ the orbit of $\mathbf{x} = (\mathbf{x}_1, ..., \mathbf{x}_{\mathrm{N}})$ under the action of $\mathcal{G}$. More precisely,

$$\mathcal{G}^{\mathrm{N},\beta}_{\mathbf{x}} = \Big\{ \omega \in \mathfrak{S}_{\mathrm{N},\beta} \; ; \; \forall \, i \in \{1, ..., \mathrm{N}\}, \; \omega_i \in \{\pm \mathbf{x}_1; \cdots ; \pm \mathbf{x}_{\mathrm{N}}\} \Big\},$$

and each orbit is finite, with cardinality $2^{\mathrm{N}(\mathrm{N}+1)/2}$. This group action defines a projection

$$\pi : \mathfrak{S}_{\mathrm{N},\beta} \longrightarrow \mathcal{Q}_{\mathrm{N},\beta}$$

onto the quotient space $\mathcal{Q}_{\mathrm{N},\beta} := \mathfrak{S}_{\mathrm{N},\beta}/\mathcal{G}$. We can define the pushforward measure $\nu_{\mathrm{N},\beta} := \pi \star \mu^{mc}_{\mathrm{N},\beta}$ on $\mathcal{Q}_{\mathrm{N},\beta}$. Then, the disintegration of $\mu^{mc}_{\mathrm{N},\beta}$ with respect to π writes as follows: for all test functions $f : \mathfrak{S}_{\mathrm{N},\beta} \longrightarrow \mathbb{R}$, the measure $\mu^{mc}_{\mathrm{N},\beta}(\cdot|\mathbf{x})$ with support on $\mathcal{G}^{\mathrm{N},\beta}_{\mathbf{x}}$ satisfies

$$\int_{\mathfrak{S}_{\mathrm{N},\beta}} f(\omega) \, d\mu^{mc}_{\mathrm{N},\beta}(\omega) = \int_{\mathcal{Q}_{\mathrm{N},\beta}} \int_{\mathfrak{S}_{\mathrm{N},\beta}} f(\omega) \, d\mu^{mc}_{\mathrm{N},\beta}(\omega|\mathbf{x}) \, d\nu_{\mathrm{N},\beta}(\mathbf{x}).$$

It is not difficult to see that $\mu_{\mathrm{N},\beta,\mathbf{x}}(\cdot) := \mu^{mc}_{\mathrm{N},\beta}(\cdot|\mathbf{x})$ is the uniform measure on the orbit $\mathcal{G}^{\mathrm{N},\beta}_{\mathbf{x}}$, since its support is invariant under a subgroup of rotations (of the total sphere). Let us denote by $\langle \cdot \rangle_{\mathrm{N,E},\mathbf{x}}$ the corresponding expectation. We obtain that, for all test functions $f : \mathfrak{S}_{\mathrm{N},\beta} \longrightarrow \mathbb{R}$,

$$\langle f \rangle_{\mathrm{N},\beta,\mathbf{x}} = \frac{1}{2^{\mathrm{N}(\mathrm{N}+1)/2}} \sum_{y \in \mathcal{G}^{\mathrm{N},\beta}_{\mathbf{x}}} f(y).$$

To conclude, let us fix the energy $\beta^{-1} > 0$, take $\mathbf{x}$ in the microcanonical sphere $\mathfrak{S}_{\mathrm{N},\beta}$, and look at the dynamics generated by $\mathcal{L}_{\mathrm{N}}$ restricted on the orbit $\mathcal{G}^{\mathrm{N},\beta}_{\mathbf{x}}$. Then, observe that the kernel of $\mathcal{S}_{\mathrm{N}}$ in the Hilbert space $\mathbf{L}^2(\mu_{\mathrm{N},\beta,\mathbf{x}})$ has dimension 1. As a result, the range of $\mathcal{S}_{\mathrm{N}}$ in $\mathbf{L}^2(\mu_{\mathrm{N},\beta,\mathbf{x}})$ has codimension 1, and is equal to the mean-zero functions.

Properties of $\mathcal{C}_0$ and $\mathcal{Q}_0$ – In the sequel, we give some properties of the two spaces $\mathcal{C}_0$ and $\mathcal{Q}_0$: for instance, the energy current is among the elements of $\mathcal{Q}_0$ (Proposition III.3). We also prove an *integration by parts* formula for the functions of $\mathcal{C}_0$ (Proposition III.4).

PROPOSITION III.3. *Every $\varphi \in \mathcal{C}_0$ has zero mean with respect to $\mu_{s_\varphi,\mathrm{E},\mathbf{x}}$ namely*

$$\langle \varphi \rangle_{s_\varphi,\mathrm{E},\mathbf{x}} = 0, \textit{ for } \mathbb{P} - \textit{almost all disorder } \mathbf{m}, \textit{ for all } \mathrm{E} > 0, \textit{ and } \mathbf{x} \in \mathfrak{S}_{s_\varphi,\mathrm{E}}.$$

Moreover, the following elements belong to $\mathcal{Q}_0$

(a) $j^{\mathrm{S}}_{0,1}, \quad j^{\mathrm{A}}_{0,1}$.

(b) $\mathcal{L}^{\mathbf{m}} f, \quad \mathcal{S} f$ *and* $\mathcal{A}^{\mathbf{m}} f, \quad$ *for all* $f \in \mathcal{Q}$.

Proof. The first statement is a consequence of the definition. Besides, (a) is directly obtain from the following identities: for $x \in \mathbb{Z}$, and $k \geqslant 1$,

$$\omega_{x+1}^2 - \omega_x^2 = \nabla_{x,x+1}\left(\omega_x^2\right) \tag{III.8}$$

$$\omega_x \omega_{x+k} = \mathcal{S}_x\left(\frac{-\omega_x\omega_{x+1}}{\gamma}\right) + \sum_{\ell=1}^{k-1} \mathcal{S}_{x+\ell}\left(\frac{-\omega_x\omega_{x+\ell+1}}{\lambda}\right). \tag{III.9}$$

Then, if $f \in \mathcal{Q}$, it is easy to see that (III.8) and (III.9) are sufficient to prove (b). For instance,

$$\mathcal{L}^{\mathbf{m}}(\omega_x\omega_{x+1}) = \frac{\omega_x\omega_{x+2}}{\sqrt{m_{x+1}m_{x+2}}} - \frac{\omega_{x+1}\omega_{x-1}}{\sqrt{m_x m_{x-1}}} + \frac{\omega_{x+1}^2 - \omega_x^2}{\sqrt{m_x m_{x+1}}} - 4\gamma\omega_x\omega_{x+1} + \lambda(\omega_{x+2} - \omega_{x+1})\omega_x + \lambda(\omega_{x-1} - \omega_x)\omega_{x+1}.$$

□

Conversely, let us now consider a function $\varphi \in \mathcal{C}_0$. From the previous subsection together with Proposition III.3, we can write the cylinder function φ as $\varphi = (-\mathcal{S}_{\Lambda_\varphi})(-\mathcal{S}_{\Lambda_\varphi})^{-1}\varphi$ for some mean-zero function $(-\mathcal{S}_{\Lambda_\varphi})^{-1}\varphi$, measurable with respect to the variables $\{m_x, \omega_x \; ; \; x \in \Lambda_\varphi\}$. The reversibility of the measure $\mu_{\ell,\beta,\mathbf{x}}$ implies that the following decomposition holds in $\mathbf{L}^2(\mu_{\ell,\beta,\mathbf{x}})$

$$\varphi = \sum_{x \in \Lambda_\varphi} \nabla_x(\mathrm{F}_x) + \nabla_{x,x+1}(\mathrm{G}_x),$$

with

$$\begin{cases} \mathrm{F}_x = \dfrac{\gamma}{2}\nabla_x\left[\left(-\mathcal{S}_{\Lambda_\varphi}\right)^{-1}\varphi\right] \\ \mathrm{G}_x = \dfrac{\lambda}{2}\nabla_{x,x+1}\left[\left(-\mathcal{S}_{\Lambda_\varphi}\right)^{-1}\varphi\right]. \end{cases}$$

The following proposition is a direct consequence of these comments.

PROPOSITION III.4 (Integration by parts formula). *Let φ be a cylinder function in $\mathcal{C}_0$. There exists a family of cylinder functions $\{\mathrm{F}^\varphi_x, \mathrm{G}^\varphi_x \; ; \; x \in \Lambda_\varphi\}$ measurable with respect to $\mathcal{F}_{\Lambda_\varphi}$ such that*

$$\langle \varphi, g\rangle_{\ell,\beta,\mathbf{x}} = \sum_{x \in \Lambda_\varphi} \langle \mathrm{F}^\varphi_x, \nabla_x g\rangle_{\ell,\beta,\mathbf{x}} + \langle \mathrm{G}^\varphi_x, \nabla_{x,x+1} g\rangle_{\ell,\beta,\mathbf{x}} \tag{III.10}$$

for all rectangles Λ_ℓ *that contain* Λ_φ, *for all* $\beta > 0$, *and for all functions* $g \in \mathbf{L}^2(\mu_{\ell,\beta,\mathbf{x}})$. *For all* $y \in \mathbb{Z}$,

$$\tau_y \mathrm{F}_x^\varphi = \mathrm{F}_{x+y}^{\tau_y \varphi},$$
$$\tau_y \mathrm{G}_x^\varphi = \mathrm{G}_{x+y}^{\tau_y \varphi}.$$

Moreover,

$$\big\langle \varphi, g \big\rangle_{\ell,\beta,\mathbf{x}}^2 \leqslant \mathrm{C}(\varphi,\beta,\mathbf{x}) \big\langle g, \big(-\mathcal{S}_{\Lambda_\varphi}\big) g \big\rangle_{\ell,\beta,\mathbf{x}} \tag{III.11}$$

where $\mathrm{C}(\varphi,\beta,\mathbf{x})$ *is equal to*

$$\mathrm{C}(\varphi,\beta,\mathbf{x}) := 2\big\langle \varphi, \big(-\mathcal{S}_{\Lambda_\varphi}\big)^{-1} \varphi \big\rangle_{\ell,\beta,\mathbf{x}}.$$

By reintegration of the disintegrated measure $\mu_{\ell,\beta,\mathbf{x}}$ *the same result* (III.10) *may be restated with microcanonical measures* $\mu_{\ell,\beta,\mathbf{x}}$ *replaced by* μ_β *and* $\mathbb{P}_\beta^\star$ *and* (III.11) *becomes:*

$$\big\langle \varphi, g \big\rangle_\beta^2 \leqslant \mathrm{C}_1(\varphi) \big\langle g, \big(-\mathcal{S}_{\Lambda_\varphi}\big) g \big\rangle_\beta \tag{III.12}$$
$$\mathbb{E}\big\langle \varphi, g \big\rangle_\beta^2 \leqslant \mathrm{C}_2(\varphi)\, \mathbb{E}\big\langle g, \big(-\mathcal{S}_{\Lambda_\varphi}\big) g \big\rangle_\beta \tag{III.13}$$

for some constants $\mathrm{C}_1, \mathrm{C}_2$ *which can be written in terms of variances and do not depend on* β.

Proof. Inequalities (III.11) and (III.12) follow from Cauchy-Schwarz inequality applied to (III.10). Let us notice that the last inequality (III.13) uses the translation invariance of the measure $\mathbb{P}_\beta^\star$. □

To conclude this paragraph, we give the variational formula that defines the variance in the case of quadratic functions. The remarkable fact is its restriction on quadratic functions.

Proposition III.5 (Variance of quadratic functions). *If* $\varphi \in \mathcal{Q}_0$, *then*

$$\big\langle \varphi, (-\mathcal{S}_{\Lambda_\varphi})^{-1} \varphi \big\rangle_\beta = \sup_{g \in \mathcal{Q}} \Big\{ 2 \big\langle \varphi, g \big\rangle_\beta - \mathcal{D}_{s_\varphi}(\mu_\beta; g) \Big\}.$$

This result can be restated with μ_β *replaced with* $\mathbb{P}_\beta^\star$ *as*

$$\mathbb{E}\big\langle \varphi, (-\mathcal{S}_{\Lambda_\varphi})^{-1} \varphi \big\rangle_\beta = \sup_{g \in \mathcal{Q}} \Big\{ 2\, \mathbb{E}\big\langle \varphi, g \big\rangle_\beta - \mathbb{E}\big[\mathcal{D}_{s_\varphi}(\mu_\beta; g)\big] \Big\}.$$

Proof. This follows from the decomposition of every function in $\mathbf{L}^2(\mu_\beta)$ over the Hermite polynomials basis: see Proposition V.13 (Appendix 2.2.1). □

2.1.3 Limiting Variance and Semi-norm

We return to the case $\beta = 1$. In the following, we deliberately keep the notation $\chi(1)$, even if the latter could be replaced with its exact value. We are going to obtain a variational formula for the variance

$$(2\ell)^{-1} \mathbb{E} \left\langle \Big(-\mathcal{S}_{\Lambda_\ell} \Big)^{-1} \sum_{|x| \leqslant \ell_\varphi} \tau_x \varphi, \sum_{|x| \leqslant \ell_\varphi} \tau_x \varphi \right\rangle_1$$

where $\varphi \in \mathcal{Q}_0$ and $\ell_\varphi = \ell - s_\varphi - 1$. We first introduce a semi-norm on $\mathcal{Q}_0$. For any cylinder function φ in $\mathcal{Q}_0$, let us define

$$\|\!|\varphi|\!\|_1^2 := \sup_{g\in\mathcal{Q}} \left\{ 2 \ll \varphi, g \gg_{1,\star} + \frac{2}{\lambda}\frac{\ll \varphi \gg_{1,\star\star}^2}{\chi(1)} - \frac{\lambda}{2}\mathbb{E}_1^\star\left[\left(\nabla_{0,1}\Gamma_g\right)^2\right] - \frac{\gamma}{2}\mathbb{E}_1^\star\left[\left(\nabla_0\Gamma_g\right)^2\right]\right\} \quad \text{(III.14)}$$

$$= \sup_{\substack{g\in\mathcal{Q}\\ a\in\mathbb{R}}} \left\{ 2 \ll \varphi, g \gg_{1,\star} + 2a \ll \varphi \gg_{1,\star\star} - \mathbb{E}\left[\mathcal{D}_0\left(\mu_1; a\omega_0^2 + \Gamma_g\right)\right]\right\}. \quad \text{(III.15)}$$

As we previously noticed, this formula can be restated as

$$\|\!|\varphi|\!\|_1^2 = \ll \varphi, (-\mathcal{S})^{-1}\varphi \gg_{1,\star} + \frac{2}{\lambda\,\chi(1)} \ll \varphi \gg_{1,\star\star}^2. \quad \text{(III.16)}$$

Since φ belongs to $\mathcal{Q}_0$, the results of Subsection 2.1.2 are valid, namely: the first term in the right-hand side of (III.16) is well-defined (Proposition III.4), and the supremum in the variational formula (III.14) can be restricted over functions in $\mathcal{Q}$ (Proposition III.5). We are now in position to state the main result of this subsection.

Theorem III.6. *Consider a quadratic cylinder function $\varphi \in \mathcal{Q}_0$. Then*

$$\lim_{\ell\longrightarrow\infty} (2\ell)^{-1}\mathbb{E}\left\langle \left(-\mathcal{S}_{\Lambda_\ell}\right)^{-1} \sum_{|x|\leqslant \ell_\varphi} \tau_x\varphi, \sum_{|x|\leqslant\ell_\varphi} \tau_x\varphi \right\rangle_1 = \|\!|\varphi|\!\|_1^2.$$

Here, ℓ_φ stands for $\ell - s_\varphi - 1$ so that the support of $\tau_x\varphi$ is included in Λ_ℓ for every $x \in \Lambda_{\ell_\varphi}$.

This theorem is the key of the standard non-gradient Varadhan's method. As usual, the proof is done in two steps that we separate as two different lemmas for the sake of clarity.

First, we bound the variance of a cylinder function $\varphi \in \mathcal{Q}_0$, with respect to the canonical measure μ_1, by the semi-norm $\|\!|\varphi|\!\|_1^2$. Precisely,

Lemma III.7. *Under the assumptions of Theorem III.6,*

$$\limsup_{\ell\longrightarrow\infty} (2\ell)^{-1}\mathbb{E}\left\langle \left(-\mathcal{S}_{\Lambda_\ell}\right)^{-1} \sum_{|x|\leqslant \ell_\varphi} \tau_x\varphi, \sum_{|x|\leqslant\ell_\varphi} \tau_x\varphi \right\rangle_1 \leqslant \|\!|\varphi|\!\|_1^2.$$

In this step, one need to know the weak limits of some particular sequences in $\mathcal{Q}_0$. In the typical approach, these weak limits are viewed as *germs of closed forms*, but for the harmonic chain, this way of thinking is not necessary. In Appendix 2.2.2, we describe the link between the point of view of closed forms and the theorem below.

Theorem III.8. *Let $\{f_n\}_{n\in\mathbb{N}}$ a sequence of quadratic functions in $\mathbf{L}^2(\mu_1)$. Let us define*

$$g_n := \nabla_0\left(\Gamma_{f_n}\right) \quad \text{and} \quad h_n := \nabla_{0,1}\left(\Gamma_{f_n}\right).$$

If $\{g_n\}$, respectively $\{h_n\}$, weakly converges in $\mathbf{L}^2(\mu_1)$ towards g, respectively h, then there exist $a \in \mathbb{R}$ and $f \in \mathcal{Q}$ such that

$$g(\omega) = \nabla_0(\Gamma_f)(\omega), \quad \text{(III.17)}$$

$$h(\omega) = a(\omega_0^2 - \omega_1^2) + \nabla_{0,1}(\Gamma_f)(\omega), \quad \text{(III.18)}$$

considering that the above equalities are stated in $\mathbf{L}^2(\mu_1)$ sense. This result remains in force if μ_1 is replaced with the product measure $\mathbb{P}_1^\star = \mathbb{P}\otimes\mu_1$, where $\mathbb{P}$ is the law of the disorder.

Lemma III.7 and Theorem III.8 are both proved in Appendix 2.2.2.

In the second step, a lower bound for the variance can be easily deduced from the variational formula which expresses the variance as a supremum:

Lemma III.9. *Under the assumptions of Theorem III.6,*

$$\limsup_{\ell\longrightarrow\infty}(2\ell)^{-1}\mathbb{E}\left\langle \big(-\mathcal{S}_{\Lambda_\ell}\big)^{-1}\sum_{|x|\leqslant \ell_\varphi}\tau_x\varphi,\ \sum_{|x|\leqslant \ell_\varphi}\tau_x\varphi\right\rangle_1 \geqslant |||\varphi|||_1^2.$$

This result is very close to the standard method, and we postpone its proof to Appendix 2.2.2.

2.2 Hilbert Space and Projections

We now focus on the semi-norm $|||\cdot|||_1$ that was introduced in the previous section (III.14). We can easily define from $|||\cdot|||_1$ a semi-inner product on $\mathcal{C}_0$ through polarization. Denote by $\mathcal{N}$ the kernel of the semi-norm $|||\cdot|||_1$ on $\mathcal{C}_0$. Then, the completion of $\mathcal{Q}_0|_{\mathcal{N}}$ denoted by $\mathcal{H}_1$ is a Hilbert space. Let us explain how the well-known Varadhan's approach is modified. Usually, the Hilbert space on which orthogonal projections are performed is the completion of $\mathcal{C}_0|_{\mathcal{N}}$, in other words it involves all local functions. Then, the standard procedure aims at proving that each element of that Hilbert space can be approximated by a sequence of functions in the range of the generator plus an additional term which is proportional to the current. The crucial steps for obtaining this decomposition consist in: first, controlling the antisymmetric part of the generator by the symmetric one for every cylinder function, and second, proving a strong result on germs of closed forms (see Appendix 2.2.2). These two key points are not valid in our model, but they can be adapted and then proved when restricted to quadratic functions. It turns out that these weak versions are sufficient, since we are looking for a fluctuation-dissipation approximation that involves quadratic functions only.

In Subsection 2.2.1, we show that $\mathcal{H}_1$ is the completion of $\mathcal{S}\mathcal{Q}|_{\mathcal{N}}+\{j_{0,1}^{\mathrm{S}}\}$. In other words, all elements of $\mathcal{H}_1$ can be approximated by $a j_{0,1}^{\mathrm{S}}+\mathcal{S}g$ for some $a\in\mathbb{R}$ and $g\in\mathcal{Q}$. This is not irrelevant since the symmetric part of the generator preserves the degree of polynomial functions. Moreover, the sum of the two subspaces $\{j_{0,1}^{\mathrm{S}}\}$ and $\overline{\mathcal{S}\mathcal{Q}}|_{\mathcal{N}}$ is orthogonal, and we denote it by

$$\overline{\mathcal{S}\mathcal{Q}}|_{\mathcal{N}}\oplus^{\perp}\{j_{0,1}^{\mathrm{S}}\}.$$

Nevertheless, this decomposition is not satisfactory, because we want the fluctuating term to be on the form $\mathcal{L}^{\mathbf{m}}(f)$, and not $\mathcal{S}(f)$. In order to make this replacement, we need to prove the weak sector condition, that gives a control of $|||\mathcal{A}^{\mathbf{m}}g|||_1$ by $|||\mathcal{S}g|||_1$, when g is a quadratic function. The argument is explained is Subsection 2.2.2 and 2.2.3, and the weak sector condition is proved in Appendix 2.2.3. The only trouble is that this new decomposition is not orthogonal any more, so that we can not express the diffusion coefficient as a variational formula, like (III.26). This problem is solved in Section 2.3.

2.2.1 Decomposition according to the symmetric part

We begin this subsection with a table of calculus, very useful in the sequel.

PROPOSITION III.10. *For all $g \in \mathcal{Q}_0, h \in \mathcal{Q}$,*

$$\begin{array}{rcl} \ll h, \mathcal{S}g \gg_1 & = & - \ll h, g \gg_{1,\star}, \\ \ll h, j^{\mathrm{S}}_{0,1} \gg_1 & = & - \ll h \gg_{1,\star\star}, \\ \ll j^{\mathrm{S}}_{0,1}, \mathcal{S}h \gg_1 & = & 0, \\ |||j^{\mathrm{S}}_{0,1}|||_1^2 & = & \lambda\chi(1). \end{array}$$

Proof. The first two identities are direct consequences of Theorem III.6 and of the following identity

$$\mathcal{S}\left(\sum_{x\in\Lambda} x\omega_x^2\right) = \sum_{x\in\Lambda} j_{x,x+1}.$$

The last two ones follow directly. □

COROLLARY III.11. *For all $a \in \mathbb{R}$ and $g \in \mathcal{Q}$,*

$$|||a j^{\mathrm{S}}_{0,1} + \mathcal{S}g|||_1^2 = a^2\lambda\chi(1) + \frac{\lambda}{2}\mathbb{E}_1^\star\left[(\nabla_{0,1}\Gamma_g)^2\right] + \frac{\gamma}{2}\mathbb{E}_1^\star\left[(\nabla_0\Gamma_g)^2\right].$$

In particular, the variational formula for $|||h|||_1$ when $h \in \mathcal{Q}_0$ writes

$$|||h|||_1^2 = \frac{1}{\lambda\chi(1)} \ll h, j^{\mathrm{S}}_{0,1} \gg_1 + \sup_{g\in\mathcal{Q}}\left\{-2 \ll h, \mathcal{S}g \gg_1 - |||\mathcal{S}g|||_1^2\right\}. \tag{III.19}$$

PROPOSITION III.12. *We denote by $\mathcal{SQ}$ the space $\{\mathcal{S}h \ ; \ h \in \mathcal{Q}\}$. Then,*

$$\mathcal{H}_1 = \overline{\mathcal{SQ}}|_{\mathcal{N}} \oplus^\perp \{j^{\mathrm{S}}_{0,1}\}.$$

Proof. We divide the proof into two steps.

(a) The space is well generated – The inclusion $\overline{\mathcal{SQ}}|_{\mathcal{N}} + \{j^{\mathrm{S}}_{0,1}\} \subset \mathcal{H}_1$ is obvious. Moreover, from the variational formula (III.19) we know that: if $h \in \mathcal{H}_1$ satisfies $\ll h, j^{\mathrm{S}}_{0,1} \gg_1 = 0$ and $\ll h, \mathcal{S}g \gg_1 = 0$ for all $g \in \mathcal{Q}$, then $|||h|||_1 = 0$.

(b) The sum is orthogonal – This follows from the previous proposition and from the fact that $\ll j^{\mathrm{S}}_{0,1}, \mathcal{S}h \gg_1 = 0$ for all $h \in \mathcal{Q}$.

□

2.2.2 Replacement of $\mathcal{S}$ with $\mathcal{L}$

In this subsection, we prove identities which mix the antisymmetric and the symmetric part of the generator, which will be used to get the weak sector condition (Proposition III.15). The argument is widely inspired from [69].

LEMMA III.13. *For all $g, h \in \mathcal{Q}$,*

$$\ll \mathcal{S}g, \mathcal{A}^{\mathbf{m}}h \gg_1 = - \ll \mathcal{A}^{\mathbf{m}}g, \mathcal{S}h \gg_1 . \tag{III.20}$$

$$\ll \mathcal{S}g, j^{\mathrm{A}}_{0,1} \gg_1 = - \ll \mathcal{A}^{\mathbf{m}}g, j^{\mathrm{S}}_{0,1} \gg_1 . \tag{III.21}$$

Proof. Identity (III.20) easily comes from the first identity of Proposition III.10 and from the invariance by translations of the measure $\mathbb{P}_1^\star$:

$$\begin{aligned}\ll \mathcal{S}g, \mathcal{A}^{\mathrm{m}}h \gg_1 &= - \ll g, \mathcal{A}^{\mathrm{m}}h \gg_{1,\star} = -\sum_{x\in\mathbb{Z}} \mathbb{E}_1^\star\big[\tau_x g, \mathcal{A}^{\mathrm{m}}h\big] = \sum_{x\in\mathbb{Z}} \mathbb{E}_1^\star\big[\mathcal{A}^{\mathrm{m}}(\tau_x g), h\big] \\ &= \sum_{x\in\mathbb{Z}} \mathbb{E}_1^\star\big[\tau_x(\mathcal{A}^{\mathrm{m}}g), h\big] = \sum_{x\in\mathbb{Z}} \mathbb{E}_1^\star\big[\mathcal{A}^{\mathrm{m}}g, \tau_{-x}h\big] = \sum_{x\in\mathbb{Z}} \mathbb{E}_1^\star\big[\mathcal{A}^{\mathrm{m}}g, \tau_x h\big] = - \ll \mathcal{A}^{\mathrm{m}}g, \mathcal{S}h \gg_1 .\end{aligned}$$

Then, by the first identity of Proposition III.10,

$$\begin{aligned}\ll \mathcal{S}g, j_{0,1}^{\mathrm{A}} \gg_1 &= - \ll g, j_{0,1}^{\mathrm{A}} \gg_{1,\star} = -\sum_{x\in\mathbb{Z}} \mathbb{E}_1^\star\big[\tau_x g, j_{0,1}^{\mathrm{A}}\big] = -\sum_{x\in\mathbb{Z}} \mathbb{E}_1^\star\big[g, j_{x,x+1}^{\mathrm{A}}\big] \\ &= -\sum_{x\in\mathbb{Z}} x\mathbb{E}_1^\star\big[g, j_{x-1,x}^{\mathrm{A}} - j_{x,x+1}^{\mathrm{A}}\big] = -\sum_{x\in\mathbb{Z}} x\mathbb{E}_1^\star\big[g, \mathcal{A}^{\mathrm{m}}(\omega_x^2)\big] = \sum_{x\in\mathbb{Z}} x\mathbb{E}_1^\star\big[\mathcal{A}^{\mathrm{m}}g, \omega_x^2\big] \\ &= - \ll \mathcal{A}^{\mathrm{m}}g, j_{0,1}^{\mathrm{S}} \gg_1,\end{aligned}$$

and this proves (III.21). □

This last lemma and the second identity of Proposition III.10 imply the following:

Corollary III.14. *For all $a \in \mathbb{R}$, $g \in \mathcal{Q}$,*

$$\ll a j_{0,1}^{\mathrm{S}} + \mathcal{S}g, a j_{0,1}^{\mathrm{A}} + \mathcal{A}^{\mathrm{m}}g \gg_1 = 0.$$

We are now in position to state the main result of this subsection.

Proposition III.15 (Weak sector condition). *(i) There exist two constants $\mathrm{C}_0 := \mathrm{C}(\gamma,\lambda)$ and $\mathrm{C}_1 := \mathrm{C}(\gamma,\lambda)$ such that the following inequalities hold for all $f, g \in \mathcal{Q}$:*

$$|\ll \mathcal{A}^{\mathrm{m}}g, \mathcal{S}f \gg_1| \leqslant \mathrm{C}_0 |||\mathcal{S}f|||_1\, |||\mathcal{S}g|||_1. \tag{III.22}$$

$$|\ll \mathcal{A}^{\mathrm{m}}g, \mathcal{S}f \gg_1| \leqslant \mathrm{C}_1 |||\mathcal{S}g|||_1 + \frac{1}{2} |||\mathcal{S}f|||_1. \tag{III.23}$$

(ii) There exists a positive constant C such that, for all $g \in \mathcal{Q}$,

$$|||\mathcal{A}^{\mathrm{m}}g|||_1 \leqslant \mathrm{C} |||\mathcal{S}g|||_1.$$

Proof. The proof is technical because made of explicit computations for quadratic functions. For that reason, we report it to Appendix 2.2.3. □

2.2.3 Decomposition of the Hilbert space

We now deduce from the previous two subsections the expected decomposition of $\mathcal{H}_1$.

Proposition III.16. *We denote by $\mathcal{L}^{\mathrm{m}}\mathcal{Q}$ the space $\{\mathcal{L}^{\mathrm{m}}g\ ;\ g \in \mathcal{Q}\}$. Then,*

$$\mathcal{H}_1 = \overline{\mathcal{L}^{\mathrm{m}}\mathcal{Q}}|_{\mathcal{N}} \oplus \{j_{0,1}^{\mathrm{S}}\}.$$

Proof. We first prove that $\mathcal{H}_1$ can be written as the sum of the two subspaces. Then, we show that the sum is direct.

(a) The space is well generated – The inclusion $\overline{\mathcal{L}^{\mathbf{m}}\mathcal{Q}}|_{\mathcal{N}} + \{j^{\mathrm{S}}_{0,1}\} \subset \mathcal{H}_1$ follows from Proposition III.3. To prove the converse inclusion, let $h \in \mathcal{H}_1$ so that $\ll h, j^{\mathrm{S}}_{0,1} \gg_1 = 0$ and $\ll h, \mathcal{L}^{\mathbf{m}} g \gg_1 = 0$ for all $g \in \mathcal{Q}$. From Corollary III.12, h can be written as

$$h = \lim_{k \longrightarrow \infty} \mathcal{S} g_k$$

for some sequence $\{g_k\} \in \mathcal{Q}$. More precisely, since $\ll \mathcal{S}g_k, \mathcal{A}^{\mathbf{m}} g_k \gg_1 = 0$ by Equation (III.20),

$$|||h|||_1^2 = \lim_{k \longrightarrow \infty} \ll \mathcal{S}g_k, \mathcal{S}g_k \gg_1 = \lim_{k \longrightarrow \infty} \ll \mathcal{S}g_k, \mathcal{L}^{\mathbf{m}} g_k \gg_1 .$$

Moreover, we also have by assumption that $\ll h, \mathcal{S}g_k \gg_1 = 0$ for all k, and from Proposition III.15,

$$\sup_{k \in \mathbb{N}} |||\mathcal{L}^{\mathbf{m}} g_k|||_1 \leqslant (\mathrm{C}+1) \sup_{k \in \mathbb{N}} |||\mathcal{S}g_k|||_1 =: \mathrm{C}_h$$

is finite. Therefore,

$$|||h|||_1^2 = \lim_{k \longrightarrow \infty} \ll \mathcal{S}g_k, \mathcal{L}^{\mathbf{m}} g_k \gg_1 = \lim_{k \longrightarrow \infty} \ll \mathcal{S}g_k - h, \mathcal{L}^{\mathbf{m}} g_k \gg_1 \leqslant \lim_{k \longrightarrow \infty} \mathrm{C}_h |||\mathcal{S}g_k - h|||_1 = 0.$$

(b) The sum is direct – Let $\{g_k\} \in \mathcal{Q}$ be a sequence such that, for some $a \in \mathbb{R}$,

$$\lim_{k \longrightarrow \infty} \mathcal{L}^{\mathbf{m}} g_k = a j^{\mathrm{S}}_{0,1} \quad \text{in } \mathcal{H}_1,$$

By a similar argument,

$$\limsup_{k \longrightarrow \infty} \ll \mathcal{S}g_k, \mathcal{S}g_k \gg_1 = \limsup_{k \longrightarrow \infty} \ll \mathcal{L}^{\mathbf{m}} g_k, \mathcal{S}g_k \gg_1 = \limsup_{k \longrightarrow \infty} \ll \mathcal{L}^{\mathbf{m}} g_k - a j^{\mathrm{S}}_{0,1}, \mathcal{S}g_k \gg_1 = 0,$$

where the last equality comes from the fact that $\ll j^{\mathrm{S}}_{0,1}, \mathcal{S}g_k \gg_1 = 0$ for all k. On the other hand, by Proposition III.15, $|||\mathcal{L}^{\mathbf{m}} g_k|||_1 \leqslant (\mathrm{C}+1) |||\mathcal{S}g_k|||_1^2$. Then, $a = 0$ and this concludes the proof. □

Recall that $j^{\mathrm{S}}_{0,1}(\mathbf{m}, \omega) = \lambda(\omega_1^2 - \omega_0^2)$. We have obtained the following result.

Theorem III.17. *For every $g \in \mathcal{Q}_0$, there exists a unique constant $a \in \mathbb{R}$, such that*

$$g + a(\omega_1^2 - \omega_0^2) \in \overline{\mathcal{L}^{\mathbf{m}}\mathcal{Q}} \quad \textit{in } \mathcal{H}_1. \tag{III.24}$$

In particular, this theorem states that there exists a unique number D, and a sequence of cylinder functions $\{f_k\} \in \mathcal{Q}$ such that

$$|||j_{0,1} - \mathrm{D}(\omega_1^2 - \omega_0^2) - \mathcal{L}^{\mathbf{m}} f_k|||_1 \xrightarrow[k \longrightarrow \infty]{} 0. \tag{III.25}$$

Let us notice that this convergence also holds with the same constant D and the same sequence $\{f_k\}$ if we replace the semi-norm $|||\cdot|||_1$ with $|||\cdot|||_\beta$ for all $\beta > 0$ (from the change of variables argument given at the beginning of Section 2).

2.3 On the Diffusion Coefficient

The main goal of this section is to express the diffusion coefficient in several variational formulas. First, recall Definition III.2, which can be written as

$$\mathrm{D} = \lambda + \frac{1}{\chi(1)} \inf_{f\in\mathcal{Q}} \sup_{g\in\mathcal{Q}} \mathbb{E}\Big[\mathcal{D}_0(\mu_1;\Gamma_f) + 2\big\langle j^{\mathrm{A}}_{0,1} - \mathcal{A}^{\mathbf{m}} f, \Gamma_g\big\rangle_1 - \mathcal{D}_0(\mu_1;\Gamma_g)\Big]. \tag{III.26}$$

From Theorem III.17, there exists a unique number D such that

$$j_{0,1} - \mathrm{D}(\omega_1^2 - \omega_0^2) \in \overline{\mathcal{L}^{\mathbf{m}}\mathcal{Q}} \quad \text{ in } \mathcal{H}_1.$$

We are going to obtain a more explicit formula for that D, and relate it to (III.26), by following the argument given by instance in [69]. We first rewrite the decomposition of the Hilbert space given in Proposition III.16, by replacing $j^{\mathrm{S}}_{0,1}$ with $j_{0,1}$. This new statement is based on Corollary III.14, which gives an orthogonality relation. The second step is to find an other orthogonal decomposition (see (III.27) below), which will enable us to prove the variational formula (III.26) for D.

Hereafter, we denote by $\mathcal{L}^{\mathbf{m},\star} := \mathcal{S} - \mathcal{A}^{\mathbf{m}}$ the adjoint of the generator in $\mathbf{L}^2(\mu_1)$, and

$$j^\star_{0,1} := j^{\mathrm{S}}_{0,1} - j^{\mathrm{A}}_{0,1}.$$

Lemma III.18. *The following decompositions hold*

$$\mathcal{H}_1 = \overline{\mathcal{L}^{\mathbf{m}}\mathcal{Q}}|_{\mathcal{N}} \oplus \{j_{0,1}\} = \overline{\mathcal{L}^{\mathbf{m},\star}\mathcal{Q}}|_{\mathcal{N}} \oplus \{j^\star_{0,1}\}.$$

Proof. We only sketch the proof of the first decomposition, since it is done in [69]. Let us recall from Proposition III.16 that $\overline{\mathcal{L}^{\mathbf{m}}\mathcal{Q}}$ has a complementary subspace in $\mathcal{H}_1$ which is one-dimensional. Therefore, it is sufficient to prove that $\mathcal{H}_1$ is generated by $\overline{\mathcal{L}^{\mathbf{m}}\mathcal{Q}}$ and the total current. Let $h \in \mathcal{H}_1$ such that $\ll h, j_{0,1} \gg_1 = 0$ and $\ll h, \mathcal{L}^{\mathbf{m}} g \gg_1 = 0$ for all $g \in \mathcal{Q}$. By Corollary III.12, h can be written as

$$h = \lim_{k\longrightarrow\infty} \mathcal{S} g_k + a j^{\mathrm{S}}_{0,1}$$

for some sequence $\{g_k\} \in \mathcal{Q}$, and $a \in \mathbb{R}$, and from Corollary III.14,

$$|||h|||_1^2 = \lim_{k\longrightarrow\infty} \ll a j^{\mathrm{S}}_{0,1} + \mathcal{S} g_k, a j_{0,1} + \mathcal{L}^{\mathbf{m}} g_k \gg_1 .$$

Moreover, from Proposition III.15,

$$\sup_{k\in\mathbb{N}} |||a j_{0,1} + \mathcal{L}^{\mathbf{m}} g_k|||_1^2 \leqslant 2a^2 |||j_{0,1}|||_1^2 + 2(\mathrm{C}+1) \sup_{k\in\mathbb{N}} |||\mathcal{S} g_k|||_1^2 =: \mathrm{C}_h$$

is finite. Therefore,

$$\begin{aligned} |||h|||_1^2 &= \lim_{k\longrightarrow\infty} \ll a j^{\mathrm{S}}_{0,1} + \mathcal{S} g_k - h, a j_{0,1} + \mathcal{L}^{\mathbf{m}} g_k \gg_1 \\ &\leqslant \limsup_{k\longrightarrow\infty} \mathrm{C}_h |||a j^{\mathrm{S}}_{0,1} + \mathcal{S} g_k - h|||_1^2 = 0. \end{aligned}$$

The same arguments apply to the second decomposition. □

We define bounded linear operators $\mathrm{T}, \mathrm{T}^\star : \mathcal{H}_1 \longrightarrow \mathcal{H}_1$ as

$$\mathrm{T}(a j_{0,1} + \mathcal{L}^{\mathbf{m}} f) := a j^{\mathrm{S}}_{0,1} + \mathcal{S} f,$$
$$\mathrm{T}^\star(a j^\star_{0,1} + \mathcal{L}^{\mathbf{m},\star} f) := a j^{\mathrm{S}}_{0,1} + \mathcal{S} f.$$

From the following identity

$$|||a j_{0,1} + \mathcal{L}^{\mathbf{m}} f|||_1^2 = |||a j^\star_{0,1} + \mathcal{L}^{\mathbf{m},\star} f|||_1^2 = |||a j^{\mathrm{S}}_{0,1} + \mathcal{S} f|||_1^2 + |||a j^{\mathrm{A}}_{0,1} + \mathcal{A}^{\mathbf{m}} f|||_1^2,$$

we can easily see that $\mathrm{T}^\star$ is the adjoint operator of T and we also have the relations

$$\ll \mathrm{T} j^{\mathrm{S}}_{0,1}, j^\star_{0,1} \gg_1 = \ll \mathrm{T}^\star j^{\mathrm{S}}_{0,1}, j_{0,1} \gg_1 = \lambda \chi(1)$$
$$\ll \mathrm{T} j^{\mathrm{S}}_{0,1}, \mathcal{L}^{\mathbf{m},\star} f \gg_1 = \ll \mathrm{T}^\star j^{\mathrm{S}}_{0,1}, \mathcal{L}^{\mathbf{m}} f \gg_1 = 0, \text{ for all } f \in \mathcal{Q}.$$

In particular, T maps $\{j^{\mathrm{S}}_{0,1}\}$ into a subspace orthogonal to $\overline{\mathcal{L}^{\mathbf{m},\star}\mathcal{Q}}|_{\mathcal{N}}$ i.e.

$$\mathcal{H}_1 = \overline{\mathcal{L}^{\mathbf{m},\star}\mathcal{Q}}|_{\mathcal{N}} \oplus^\perp \{\mathrm{T} j^{\mathrm{S}}_{0,1}\} \tag{III.27}$$

and there exists a unique number Q such that

$$j^\star_{0,1} - \mathrm{QT} j^{\mathrm{S}}_{0,1} \in \overline{\mathcal{L}^{\mathbf{m},\star}\mathcal{Q}} \quad \text{in } \mathcal{H}_1.$$

We are going to show that $\mathrm{D} = \lambda \mathrm{Q}$.

Lemma III.19.

$$\mathrm{Q} = \frac{\lambda\chi(1)}{|||\mathrm{T} j^{\mathrm{S}}_{0,1}|||_1^2} = \frac{1}{\lambda\chi(1)} \inf_{f \in \mathcal{Q}} |||j^\star_{0,1} - \mathcal{L}^{\mathbf{m},\star} f|||_1^2. \tag{III.28}$$

Proof. The first identity follows from the fact that

$$\ll \mathrm{T} j^{\mathrm{S}}_{0,1}, j^\star_{0,1} - \mathrm{QT} j^{\mathrm{S}}_{0,1} \gg_1 = \lambda\chi(1) - \mathrm{Q}|||\mathrm{T} j^{\mathrm{S}}_{0,1}|||_1^2 = 0.$$

The second identity is obtained from the following statement

$$\inf_{f \in \mathcal{Q}} |||j^\star_{0,1} - \mathrm{QT} j^{\mathrm{S}}_{0,1} - \mathcal{L}^{\mathbf{m},\star} f|||_1 = 0. \tag{III.29}$$

□

After an easy computation, we can also prove that $\ll \mathrm{T}g, g \gg_1 = \ll \mathrm{T}g, \mathrm{T}g \gg_1$ for all $g \in \mathcal{H}_1$. Since $j^{\mathrm{S}}_{0,1} - \mathrm{T} j^{\mathrm{S}}_{0,1}$ is orthogonal to $\mathrm{T} j^{\mathrm{S}}_{0,1}$, we have:

$$j^{\mathrm{S}}_{0,1} - \mathrm{T} j^{\mathrm{S}}_{0,1} \in \overline{\mathcal{L}^{\mathbf{m},\star}\mathcal{Q}}.$$

By the fact we obtain the variational formula for $|||\mathrm{T} j^{\mathrm{S}}_{0,1}|||_1$:

Proposition III.20.

$$|||\mathrm{T} j^{\mathrm{S}}_{0,1}|||_1^2 = \inf_{f \in \mathcal{Q}} |||j^{\mathrm{S}}_{0,1} - \mathcal{L}^{\mathbf{m},\star} f|||_1^2. \tag{III.30}$$

Proof. With a similar argument (in the proof of the previous proposition), we have

$$\inf_{f \in \mathcal{Q}} |||j^{\mathrm{S}}_{0,1} - \mathrm{T} j^{\mathrm{S}}_{0,1} - \mathcal{L}^{\mathbf{m},\star} f|||_1 = 0,$$

and

$$\inf_{f \in \mathcal{Q}} |||j^{\mathrm{S}}_{0,1} - \mathrm{T} j^{\mathrm{S}}_{0,1} - \mathcal{L}^{\mathbf{m},\star} f|||_1^2 = \inf_{f \in \mathcal{Q}} |||j^{\mathrm{S}}_{0,1} - \mathcal{L}^{\mathbf{m},\star} f|||_1^2 - \inf_{f \in \mathcal{Q}} |||\mathrm{T} j^{\mathrm{S}}_{0,1}|||_1^2,$$

which concludes the proof. □

Theorem III.21.

$$\mathrm{D} = \frac{1}{\chi(1)} \inf_{f \in \mathcal{Q}} |||j^{\star}_{0,1} - \mathcal{L}^{\mathbf{m},\star} f|||_1^2 = \frac{\chi(1)}{4 \inf_{f \in \mathcal{Q}} |||j^{\mathrm{S}}_{0,1} - \mathcal{L}^{\mathbf{m},\star} f|||_1^2}. \tag{III.31}$$

Proof. By the definition, $j_{0,1} - \mathrm{D} j^{\mathrm{S}}_{0,1}/\lambda \in \overline{\mathcal{L}^{\mathbf{m}}\mathcal{Q}}$ and therefore

$$\ll j_{0,1} - j^{\mathrm{S}}_{0,1}\frac{\mathrm{D}}{\lambda}, \mathrm{T}^{\star} j^{\mathrm{S}}_{0,1} \gg_1 = \lambda\chi(1) - \frac{\mathrm{D}}{\lambda}|||\mathrm{T} j^{\mathrm{S}}_{0,1}|||_1^2 = 0. \tag{III.32}$$

Therefore, $\mathrm{D} = \lambda \mathrm{Q}$, and the variational formula for D can be deduced from the one for Q. □

Remark *2.1.* We can rewrite the variational formula for D as:

$$\begin{aligned}
\mathrm{D} &= \frac{1}{\chi(1)} \inf_{f \in \mathcal{Q}} \left\{ |||j^{\mathrm{S}}_{0,1}|||_1^2 + |||\mathcal{S} f|||_1^2 + |||j^{\mathrm{A}}_{0,1} - \mathcal{A}^{\mathbf{m}} f|||_1^2 \right\} \\
&= \lambda + \frac{1}{\chi(1)} \inf_{f \in \mathcal{Q}} \left\{ |||\mathcal{S} f|||_1^2 + |||j^{\mathrm{A}}_{0,1} - \mathcal{A}^{\mathbf{m}} f|||_1^2 \right\} \qquad \text{(III.33)} \\
&= \lambda + \frac{1}{\chi(1)} \inf_{f \in \mathcal{Q}} \sup_{g \in \mathcal{Q}} \left\{ |||\mathcal{S} f|||_1^2 - 2 \ll j^{\mathrm{A}}_{0,1} - \mathcal{A}^{\mathbf{m}} f, \mathcal{S} g \gg_1 - |||\mathcal{S} g|||_1^2 \right\} \\
&= \lambda + \frac{1}{\chi(1)} \inf_{f \in \mathcal{Q}} \sup_{g \in \mathcal{Q}} \left\{ \ll f, -\mathcal{S} f \gg_{1,\star} + 2 \ll j^{\mathrm{A}}_{0,1} - \mathcal{A}^{\mathbf{m}} f, g \gg_{1,\star} - \ll g, -\mathcal{S} g \gg_{1,\star} \right\} \qquad \text{(III.34)} \\
&= \lambda + \frac{1}{\chi(1)} \inf_{f \in \mathcal{Q}} \sup_{g \in \mathcal{Q}} \mathbb{E}\Big[\mathcal{D}_0(\mu_1; \Gamma_f) + 2 \Big\langle j^{\mathrm{A}}_{0,1} - \mathcal{A}^{\mathbf{m}} f, \Gamma_g \Big\rangle_1 - \mathcal{D}_0(\mu_1; \Gamma_g) \Big]. \qquad \text{(III.35)}
\end{aligned}$$

We use the fact that in (III.33), we can restrict the infimum on functions f in $\mathcal{Q}$ that satisfy $\ll j^{\mathrm{A}}_{0,1} - \mathcal{A}^{\mathbf{m}} f, j^{\mathrm{S}}_{0,1} \gg_1 = 0$. Let us notice that (III.34) and (III.35) recover the variational formula (III.26).

We conclude this section with a general statement that will be used in Section 4 to prove the diffusive behavior of the macroscopic energy fluctuations.

Proposition III.22. *For any sequence* $\{f_k\} \in \mathcal{Q}$ *such that*

$$\lim_{k \longrightarrow \infty} |||j_{0,1} - \mathrm{D}(\omega_1^2 - \omega_0^2) - \mathcal{L}^{\mathbf{m}} f_k|||_1 = 0$$

we have

$$\lim_{k \longrightarrow \infty} \mathbb{E}\left\langle \lambda\Big(\nabla_{0,1}(\omega_0^2 - \Gamma_{f_k})\Big)^2 + \gamma\Big(\nabla_0(\Gamma_{f_k})\Big)^2 \right\rangle_1 = 2\mathrm{D}\chi(1).$$

Proof. By assumption,

$$\lim_{k \longrightarrow \infty} |||\mathrm{T}\big(j_{0,1} - \mathrm{D}(\omega_1^2 - \omega_0^2) - \mathcal{L}^{\mathbf{m}} f_k\big)|||_1 = 0$$

and therefore

$$\lim_{k \longrightarrow \infty} |||j^{\mathrm{S}}_{0,1} - \mathcal{S} f_k|||_1^2 = \mathrm{D}^2 |||\mathrm{T}(\omega_1^2 - \omega_0^2)|||_1^2.$$

Then, the result follows from

$$\mathrm{D} = \lambda \mathrm{Q} = \frac{\chi(1)}{|||\mathrm{T}(\omega_1^2 - \omega_0^2)|||_1^2}$$

and

$$|||j^{\mathrm{S}}_{0,1} - \mathcal{S} f_k|||_1^2 = \frac{\lambda}{2}\mathbb{E}\left\langle \Big(\omega_0^2 - \omega_1^2 - \nabla_{0,1}(\Gamma_{f_k})\Big)^2 \right\rangle_1 + \frac{\gamma}{2}\mathbb{E}\left\langle \Big(\nabla_0(\Gamma_{f_k})\Big)^2 \right\rangle_1. \tag{III.36}$$

□

3 Green-Kubo Formulas

3.1 Convergence of Green-Kubo Formula

Linear response theory predicts that the diffusion coefficient is given by the homogenized *Green-Kubo formula*. Let us define

$$\overline{\kappa}(z) = \lambda + \frac{1}{2}\int_0^{+\infty} e^{-zt} \ll j^{\mathrm{A}}_{0,1}(\mathbf{m},t), j^{\mathrm{A}}_{0,1}(\mathbf{m},0) \gg_{1,\star} \mathrm{d}t$$

where $\ll \cdot \gg_{1,\star}$ is the inner product defined by (III.3). The Laplace transform above (the second term of the right-hand side) is denoted by $\mathrm{L}(z)$, is smooth on $(0,+\infty)$, and $\overline{\kappa}(z)$ can be rewritten:

$$\overline{\kappa}(z) = \lambda + \frac{1}{2} \ll j^{\mathrm{A}}_{0,1}, (z-\mathcal{L}^{\mathbf{m}})^{-1} j^{\mathrm{A}}_{0,1} \gg_{1,\star} . \tag{III.37}$$

3.1.1 Existence of the Green-Kubo Formula

In this paragraph we prove the existence and finiteness of the Green-Kubo formula. The argument is based on the paper [10], where the author generalizes some ideas developed in [6, 50].

Theorem III.23. *The following limit* $\overline{\mathrm{D}} := \lim_{\substack{z \longrightarrow 0 \\ z>0}} \overline{\kappa}(z)$ *exists, is finite and positive.*

Proof. We investigate the existence of the limit

$$\lim_{\substack{z \longrightarrow 0 \\ z>0}} \ll j^{\mathrm{A}}_{0,1}, (z-\mathcal{L}^{\mathbf{m}})^{-1} j^{\mathrm{A}}_{0,1} \gg_{1,\star} . \tag{III.38}$$

The Hilbert space generated by the set of local functions and the inner product $\ll \cdot,\cdot \gg_{1,\star}$ is denoted by $\mathbf{L}^2_\star$. We define $h_z := h_z(\mathbf{m},\omega;1)$ as the solution of the resolvent equation in $\mathbf{L}^2_\star$

$$(z-\mathcal{L}^{\mathbf{m}})h_z = j^{\mathrm{A}}_{0,1}. \tag{III.39}$$

Then we have to prove that

$$\mathrm{L}(z) = \frac{1}{2} \ll h_z, j^{\mathrm{A}}_{0,1} \gg_{1,\star}$$

converges as z goes to 0, and that the limit is finite and non-negative. Then, from (III.37) it will follow that $\overline{\mathrm{D}} \geqslant \lambda > 0$ and $\overline{\mathrm{D}}$ is positive. We denote by $\|\cdot\|_1$ the semi-norm corresponding to the symmetric part of the generator due to the flip noise

$$\|f\|_1^2 = \ll f, (-\gamma\mathcal{S}^{\mathrm{flip}})f \gg_{1,\star}$$

and $\mathcal{H}_1$ is the Hilbert space obtained by the completion of $\mathbf{L}^2_\star$ w.r.t. that semi-norm. We multiply (III.39) by h_z and integrate with respect to $\ll \cdot \gg_{1,\star}$ and we get:

$$z \ll h_z, h_z \gg_{1,\star} + \|h_z\|_1^2 + \ll h_z, (-\lambda\mathcal{S}^{\mathrm{exch}})h_z \gg_{1,\star} = \ll h_z, j^{\mathrm{A}}_{0,1} \gg_{1,\star} .$$

Let us notice that $(-\gamma\mathcal{S}^{\mathrm{flip}})(j^{\mathrm{A}}_{0,1}) = 2\gamma j^{\mathrm{A}}_{0,1}$. As a consequence, the Cauchy-Schwarz inequality for the scalar product $\ll \cdot, (-\gamma\mathcal{S}^{\mathrm{flip}})\cdot \gg_{1,\star}$ on the right-hand side gives

$$\|h_z\|_1^2 \leqslant \mathrm{C}$$

for some positive constant C. Since $\{h_z\}_z$ is a bounded sequence in $\mathcal{H}_1$, we can extract a weakly converging subsequence in $\mathcal{H}_1$. We continue to denote this subsequence by $\{h_z\}_z$ and we denote by h_0 the limit.

Now we are going to show that the convergence is stronger (see (iv) in Lemma III.24 below) and that the limit is independent of the subsequence. Since the generator $\mathcal{L}^{\mathbf{m}}$ conserves the degree of homogeneous polynomial functions, we know that the solution of the resolvent equation is expected to be on the form

$$h_z(\omega) = \sum_{x,y\in\mathbb{Z}^2} \varphi_z(x,y)\omega_x\omega_y,$$

where $\varphi_z : \mathbb{Z}^2 \longrightarrow \mathbb{R}$ is a square-summable symmetric function. Let $h_z = h_z^= + h_z^{\neq}$ be the decomposition of h_z according to the two subspaces $\mathcal{Q}^=$ and $\mathcal{Q}^{\neq}$, where $\mathcal{Q}^=$ is generated by $\{\omega_x^2, x\in\mathbb{Z}\}$ and $\mathcal{Q}^{\neq}$ is generated by $\{\omega_x\omega_y, x\neq y\}$. The main point in the following argument is that all gradient terms vanish in $\mathbf{L}^2_\star$.

First of all, one can easily see how the spaces $\mathcal{Q}^=$ and $\mathcal{Q}^{\neq}$ are mapped by the generators:

$$\begin{array}{ll} \mathcal{A}^{\mathbf{m}} : \mathcal{Q}^= \longrightarrow \mathcal{Q}^{\neq} & \mathcal{A}^{\mathbf{m}} : \mathcal{Q}^{\neq} \longrightarrow \mathcal{Q} \\ \mathcal{S}^{\text{flip}} : \mathcal{Q}^= \longrightarrow \{0\} & \mathcal{S}^{\text{flip}} : \mathcal{Q}^{\neq} \longrightarrow \mathcal{Q}^{\neq} \\ \mathcal{S}^{\text{exch}} : \mathcal{Q}^= \longrightarrow \mathcal{Q}^= & \mathcal{S}^{\text{exch}} : \mathcal{Q}^{\neq} \longrightarrow \mathcal{Q}^{\neq} \end{array}$$

Moreover, if $f\in\mathcal{Q}^=$, then $\mathcal{A}^{\mathbf{m}}(f)$ is a gradient in $\mathcal{Q}^{\neq}$, and $\mathcal{S}^{\text{exch}}(f)$ is a gradient in $\mathcal{Q}^=$. With all these considerations, (III.39) rewrites in $\mathbf{L}^2_\star$ as

$$\begin{cases} zh_z^= - \lambda\mathcal{S}^{\text{exch}}(h_z^=) = 0 \\ zh_z^{\neq} - \lambda\mathcal{S}^{\text{exch}}(h_z^{\neq}) - \gamma\mathcal{S}^{\text{flip}}(h_z^{\neq}) - \mathcal{A}^{\mathbf{m}}(h_z^{\neq}) = j^{\mathrm{A}}_{0,1}. \end{cases}$$

The first equation means that $h_z^= = 0$ in $\mathbf{L}^2_\star$ and therefore the solution h_z of the resolvent equation is an element of $\mathcal{Q}^{\neq}$. As a consequence, we can write $(-\gamma\mathcal{S}^{\text{flip}})(h_z) = 2\gamma h_z$, and this remark is one of the key points in the following argument.

Lemma III.24. *All the properties below are satisfied:*

(i) $\lim_{z\longrightarrow 0} z \ll h_z, h_z \gg_{1,\star} = 0$

(ii) $\{h_z\}$ *weakly converges as* z *goes to 0 towards* h_0 *in* $\mathbf{L}^2_\star$

(iii) $\ll j^{\mathrm{A}}_{0,1}, h_0 \gg_{1,\star} = \ll h_0, (-\mathcal{S})h_0 \gg_{1,\star}$

(iv) $\ll (h_z - h_0), (-\mathcal{S})(h_z - h_0) \gg_{1,\star}$ *vanishes as* z *goes to 0*

(v) *the weak limit of* $\{h_z\}$ *does not depend on the subsequence.*

We briefly prove the five points: (i) and (ii) come from the fact that $\ll h_z, h_z \gg_{1,\star}$ equals $2\gamma\|h_z\|_1^2$. To get (iii), we multiply (III.39) by $h_{z'}$ and integrate:

$$z \ll h_{z'}, h_z \gg_{1,\star} + \ll h_{z'}, (-\mathcal{S})h_z \gg_{1,\star} + \ll h_{z'}, (-\mathcal{A}^{\mathbf{m}})h_z \gg_{1,\star} = \ll h_{z'}, j^{\mathrm{A}}_{0,1} \gg_{1,\star}. \qquad \text{(III.40)}$$

We first take the limit as $z' \longrightarrow 0$ and then as $z \longrightarrow 0$, and we use (i) and (ii) to obtain (iii). In the same way, multiplying (III.39) by h_z gives

$$z \ll h_z, h_z \gg_{1,\star} + \ll h_z, (-\mathcal{S})h_z \gg_{1,\star} = \ll h_z, j^{\mathrm{A}}_{0,1} \gg_{1,\star}.$$

The first term of the left-hand side vanishes as z goes to 0, and the right-hand side converges to $\ll h_0, (-\mathcal{S})h_0 \gg_{1,\star}$. This implies (iv), that is

$$\ll (h_z - h_0), (-\mathcal{S})(h_z - h_0) \gg_{1,\star} \xrightarrow[z \longrightarrow 0]{} 0.$$

The uniqueness of the limit follows by a standard argument with the same idea of (III.40). We have proved the first part: the limit (III.38) exists. To obtain its finiteness, we are going to give an upper bound, using the following variational formula:

$$\ll j^{\mathrm{A}}_{0,1}, (z - \mathcal{L}^{\mathbf{m}})^{-1} j^{\mathrm{A}}_{0,1} \gg_{1,\star} = \sup_f \left\{ 2 \ll f, j^{\mathrm{A}}_{0,1} \gg_{1,\star} - \| f \|^2_{1,z} - \| \mathcal{A}^{\mathbf{m}} f \|^2_{-1,z} \right\},$$

where the supremum is carried over local functions and the two norms $\| \cdot \|_{\pm 1,z}$ are defined by

$$\| f \|^2_{\pm 1,z} = \ll f, (z - \mathcal{S})^{\pm 1} f \gg_{1,\star}.$$

For the upper bound, we neglect the term coming from the antisymmetric part $\mathcal{A}^{\mathbf{m}} f$, that gives

$$\ll j^{\mathrm{A}}_{0,1}, (z - \mathcal{L}^{\mathbf{m}})^{-1} j^{\mathrm{A}}_{0,1} \gg_{1,\star} \leqslant \ll j^{\mathrm{A}}_{0,1}, (z - \mathcal{S})^{-1} j^{\mathrm{A}}_{0,1} \gg_{1,\star}.$$

In the right-hand side we can also neglect the part coming from the exchange symmetric part $\mathcal{S}^{\mathrm{exch}}$, and remind that $\mathcal{S}^{\mathrm{flip}}(j^{\mathrm{A}}_{0,1}) = -2 j^{\mathrm{A}}_{0,1}$. This gives an explicit finite upper bound. Then, we have from Lemma III.24, Property (iii) that the limit

$$\lim_{z \longrightarrow \infty} \ll j^{\mathrm{A}}_{0,1}, (z - \mathcal{L}^{\mathbf{m}})^{-1} j^{\mathrm{A}}_{0,1} \gg_{1,\star} = \ll j^{\mathrm{A}}_{0,1}, h_0 \gg_{1,\star} = \ll h_0, (-\mathcal{S})h_0 \gg_{1,\star} \geqslant 0,$$

and the positiveness is proved. □

3.1.2 Equivalence of the Definitions

In this subsection we rigorously prove the equality between the variational formula for the diffusion coefficient and the Green-Kubo formula (see the end of Subsection 1.4).

Theorem III.25. *For every $\lambda > 0$ and $\gamma > 0$,*

$$\overline{\mathrm{D}} := \lambda + \frac{1}{2} \lim_{\substack{z \longrightarrow 0 \\ z > 0}} \ll j^{\mathrm{A}}_{0,1}, (z - \mathcal{L}^{\mathbf{m}})^{-1} j^{\mathrm{A}}_{0,1} \gg_{1,\star},$$

coincides with the diffusion coefficient D *defined in Subsection 2.3.*

Proof. From Subsection 2.3, we know that the diffusion coefficient can be written different ways. For instance, one can easily check that

$$\mathrm{D} = \frac{2}{\| \mathrm{T}(\omega_1^2 - \omega_0^2) \|^2_1}.$$

By definition of D, there exists a sequence $\{f_\varepsilon\}_{\varepsilon > 0}$ of functions in $\mathcal{Q}$ such that

$$g_\varepsilon := j^\star_{0,1} - \mathrm{D}(\omega_1^2 - \omega_0^2) - \mathcal{L}^{\mathbf{m},\star}(f_\varepsilon)$$

satisfies $\| g_\varepsilon \|_1 \longrightarrow 0$ as ε goes to 0. By substitution in the equality above, we get

$$\mathrm{D}^{-1} = \frac{1}{2\mathrm{D}^2} \ll j^\star_{0,1} - \mathcal{L}^{\mathbf{m},\star} f_\varepsilon - g_\varepsilon, \mathrm{T}^\star (j^\star_{0,1} - \mathcal{L}^{\mathbf{m},\star} f_\varepsilon - g_\varepsilon) \gg_1$$

recalling that $\ll \mathrm{T}g, \mathrm{T}g \gg_1 = \ll g, \mathrm{T}^\star g \gg_1$ for all $g \in \mathcal{H}_1$. Therefore,

$$\begin{aligned}\mathrm{D} &= \frac{1}{2} \ll j^\star_{0,1} - \mathcal{L}^{\mathbf{m},\star} f_\varepsilon - g_\varepsilon, j^{\mathrm{S}}_{0,1} - \mathcal{S} f_\varepsilon - g_\varepsilon \gg_1 \\ &= \frac{1}{2} \ll j^\star_{0,1} - \mathcal{L}^{\mathbf{m},\star} f_\varepsilon, j^{\mathrm{S}}_{0,1} - \mathcal{S} f_\varepsilon \gg_1 + \mathrm{R}_\varepsilon\end{aligned}$$

where R_ε is bounded by $\mathrm{C}|||g_\varepsilon|||_1^2$, and then vanishes as ε goes to 0. Finally, from Proposition III.10, we can write

$$\mathrm{D} = \lambda + \frac{1}{2} \lim_{\varepsilon \longrightarrow 0} \ll f_\varepsilon, (-\mathcal{S}) f_\varepsilon \gg_{1,\star} .$$

The problem is now reduced to prove that

$$\lim_{\varepsilon \longrightarrow 0} \ll f_\varepsilon, (-\mathcal{S}) f_\varepsilon \gg_{1,\star} = \lim_{\substack{z \longrightarrow 0 \\ z>0}} \ll j^{\mathrm{A}}_{0,1}, (z - \mathcal{L}^{\mathbf{m}})^{-1} j^{\mathrm{A}}_{0,1} \gg_{1,\star} . \tag{III.41}$$

For every $z > 0$ and $\varepsilon > 0$, we have by definition above and (III.39),

$$j^{\mathrm{A}}_{0,1} = z h_z - \mathcal{L}^{\mathbf{m}} h_z \tag{III.42}$$

$$j^\star_{0,1} = \mathrm{D}(\omega_1^2 - \omega_0^2) + g_\varepsilon + \mathcal{L}^{\mathbf{m},\star} f_\varepsilon. \tag{III.43}$$

First, multiply (III.43) by f_ε and integrate with respect to $\ll \cdot \gg_{1,\star}$, keeping in mind that all gradients give no contribution. We get

$$- \ll j^{\mathrm{A}}_{0,1}, f_\varepsilon \gg_{1,\star} = \ll f_\varepsilon, g_\varepsilon \gg_{1,\star} - \ll f_\varepsilon, (-\mathcal{S}) f_\varepsilon \gg_{1,\star}$$

and using (III.42),

$$\ll \mathcal{L}^{\mathbf{m}} h_z, f_\varepsilon \gg_{1,\star} - z \ll h_z, f_\varepsilon \gg_{1,\star} = \ll f_\varepsilon, g_\varepsilon \gg_{1,\star} - \ll f_\varepsilon, (-\mathcal{S}) f_\varepsilon \gg_{1,\star} .$$

First, let z go to 0, and observe that $z \ll h_z, f_\varepsilon \gg_{1,\star}$ vanishes, from the Cauchy-Schwarz inequality together with Statement (i) of Lemma III.24. The limit of $\ll \mathcal{L}^{\mathbf{m}} h_z, f_\varepsilon \gg_{1,\star}$ exists from the weak convergence of $\{h_z\}_z$. Then, take the limit as ε goes to 0, and observe that

$$\begin{aligned}\ll f_\varepsilon, g_\varepsilon \gg_{1,\star} = \ll f_\varepsilon, (-\mathcal{S})(-\mathcal{S})^{-1} g_\varepsilon \gg_{1,\star} &\leqslant \ll f_\varepsilon, (-\mathcal{S}) f_\varepsilon \gg_{1,\star}^{1/2} \ll g_\varepsilon, (-\mathcal{S})^{-1} f_\varepsilon \gg_{1,\star}^{1/2} \\ &\leqslant \mathrm{C}|||g_\varepsilon|||_1 \xrightarrow[\varepsilon \longrightarrow 0]{} 0.\end{aligned}$$

The first equality is justified by the fact that g_ε belongs to $\mathcal{Q}_0$, and the last inequality comes from the definition of the semi-norm $|||\cdot|||_1$ given in (III.14). As a consequence, we have obtained

$$\lim_{\varepsilon \longrightarrow 0} \ll f_\varepsilon, (-\mathcal{S}) f_\varepsilon \gg_{1,\star} = \lim_{\varepsilon \longrightarrow 0} \lim_{z \longrightarrow 0} \ll -\mathcal{L}^{\mathbf{m}} h_z, f_\varepsilon \gg_{1,\star} .$$

In the same way, multiply (III.43) by h_z and integrate with respect to $\ll \cdot \gg_{\beta,\star}$ so that

$$- \ll j^{\mathrm{A}}_{0,1}, h_z \gg_{1,\star} = \ll g_\varepsilon, h_z \gg_{1,\star} + \ll \mathcal{L}^{\mathbf{m},\star} f_\varepsilon, h_z \gg_{1,\star} .$$

If we send first z to 0, then $\ll g_\varepsilon, h_z \gg_{1,\star}$ converges to $\ll g_\varepsilon, h_0 \gg_{1,\star}$ from the weak convergence of $\{h_z\}_z$. With the same argument as before, we write

$$\ll g_\varepsilon, h_0 \gg_{1,\star} \leqslant \mathrm{C}|||g_\varepsilon|||_1 \xrightarrow[\varepsilon \longrightarrow 0]{} 0.$$

Therefore,

$$\begin{aligned}\lim_{z \longrightarrow 0} \ll j^{\mathrm{A}}_{0,1}, h_z \gg_{1,\star} &= \lim_{\varepsilon \longrightarrow 0} \lim_{z \longrightarrow 0} \ll -\mathcal{L}^{\mathbf{m},\star} f_\varepsilon, h_z \gg_{1,\star} \\ &= \lim_{\varepsilon \longrightarrow 0} \ll f_\varepsilon, (-\mathcal{S}) f_\varepsilon \gg_{1,\star}\end{aligned}$$

and the claim is proved. □

3.2 Vanishing Exchange Noise

With the same ideas of the previous subsection, it can be easily shown that the homogenized Green-Kubo formula also converges if the strength λ of the exchange noise vanishes. The aim of this paragraph is to study the limit of $\overline{\mathrm{D}}(\lambda,\gamma)$ as λ goes to 0. First, we turn (III.37) into a new definition that highlights the dependence on $\lambda > 0$. For that purpose we introduce new notations: we define $\mathcal{S}_0 := \gamma\mathcal{S}^{\text{flip}}$, $\mathcal{S}_\lambda := \mathcal{S}_0 + \lambda\mathcal{S}^{\text{exch}}$, and then

$$\begin{cases} \mathcal{L}_0^{\mathbf{m}} := \mathcal{A}^{\mathbf{m}} + \mathcal{S}_0 \\ \mathcal{L}_\lambda^{\mathbf{m}} := \mathcal{A}^{\mathbf{m}} + \mathcal{S}_\lambda = \mathcal{L}_0^{\mathbf{m}} + \lambda\mathcal{S}^{\text{exch}} \end{cases} \quad \text{and} \quad \mathrm{J}_0(\mathbf{m})(\omega) := \frac{\omega_0\omega_1}{\sqrt{m_0 m_1}} = j_{0,1}^{\mathrm{A}}(\mathbf{m},\omega).$$

Let us introduce the homogenized Green-Kubo formula for both noises:

$$\overline{\kappa}(\lambda,z) := \ll \mathrm{J}_0(\mathbf{m}), (z-\mathcal{L}_\lambda^{\mathbf{m}})^{-1}\mathrm{J}_0(\mathbf{m}) \gg_{1,\star} \tag{III.44}$$

and the homogenized Green-Kubo formula for flip noise only:

$$\overline{\kappa}_0(z) := \ll \mathrm{J}_0(\mathbf{m}), (z-\mathcal{L}_0^{\mathbf{m}})^{-1}\mathrm{J}_0(\mathbf{m}) \gg_{1,\star} . \tag{III.45}$$

According to the previous paragraph, we already know that the Green-Kubo formulas (III.44) and (III.45) converge as z goes to 0. Then, the following diffusion coefficients are well defined, for all $\lambda > 0$,

$$\begin{cases} \overline{\mathrm{D}}(\lambda) := \lambda + \lim_{z\longrightarrow 0} \overline{\kappa}(\lambda,z), \\ \overline{\mathrm{D}}_0 := \lim_{z\longrightarrow 0} \overline{\kappa}_0(z). \end{cases}$$

The main result of this subsection is stated in the following theorem.

Theorem III.26. *The function $\lambda \mapsto \overline{\mathrm{D}}(\lambda)$ is continuous at 0. More precisely,*

$$\lim_{\lambda\longrightarrow 0} \overline{\mathrm{D}}(\lambda) = \overline{\mathrm{D}}_0.$$

Let us remark that the theorem above does not imply the existence of the hydrodynamics diffusion coefficient $\mathrm{D}(0,\gamma)$. This question remains open.

Proof. The proof is divided into two steps. For the sake of readability, we erase the notation $\mathbf{m}$ in $\mathrm{J}_0(\mathbf{m})$, and keep in mind its dependence on the disorder.

Step 1 - Convergence of the diffusion coefficient. Let us denote by $h_{z,0}$ and $\overline{h}_{z,\lambda}$ the two solutions of the resolvent equations in $\mathbf{L}^2_\star$:

$$(z-\mathcal{L}_0^{\mathbf{m}})h_{z,0} = \mathrm{J}_0,$$
$$(z-\mathcal{L}_\lambda^{\mathbf{m},\star})\overline{h}_{z,\lambda} = \mathrm{J}_0.$$

We look at the following difference, for $\lambda, z > 0$ fixed,

$$\begin{aligned} &\Big| \ll \mathrm{J}_0, (z-\mathcal{L}_\lambda^{\mathbf{m}})^{-1}\mathrm{J}_0 \gg_{1,\star} - \ll \mathrm{J}_0\,, (z-\mathcal{L}_0^{\mathbf{m}})^{-1}\mathrm{J}_0 \gg_{1,\star} \Big| \\ &\qquad = \Big| \ll \mathrm{J}_0\,, (z-\mathcal{L}_\lambda^{\mathbf{m}})^{-1}\mathrm{J}_0 \gg_{1,\star} - \ll \mathrm{J}_0, h_{z,0} \gg_{1,\star} \Big| \\ &\qquad = \Big| \ll \mathrm{J}_0\,, (z-\mathcal{L}_\lambda^{\mathbf{m}})^{-1}\Big[(z-\mathcal{L}_0^{\mathbf{m}})h_{z,0} - (z-\mathcal{L}_\lambda^{\mathbf{m}})h_{z,0}\Big] \gg_{1,\star} \Big| \\ &\qquad = \lambda \Big| \ll \mathrm{J}_0\,, (z-\mathcal{L}_\lambda^{\mathbf{m}})^{-1}\mathcal{S}^{\text{exch}}(h_{z,0}) \gg_{1,\star} \Big| \\ &\qquad = \lambda \Big| \ll (z-\mathcal{L}_\lambda^{\mathbf{m},\star})^{-1}\mathrm{J}_0\,, \mathcal{S}^{\text{exch}}(h_{z,0}) \gg_{1,\star} \Big| . \end{aligned}$$

To complete the proof, we are reduced to show that $\lambda\big|\ll \overline{h}_{z,\lambda}, \mathcal{S}^{\text{exch}}(h_{z,0}) \gg_{1,\star}\big|$ vanishes when we first let $z \longrightarrow 0$ and then $\lambda \longrightarrow 0$. For that purpose, we need more precise information on the two solutions $\overline{h}_{z,\lambda}$ and $h_{z,0}$. Since the generator $\mathcal{L}_\lambda^{\mathbf{m}}$ (resp. $\mathcal{L}_0^{\mathbf{m}}$) conserves the degree of homogeneous polynomial functions, we know that the solution of the resolvent equation $\overline{h}_{z,\lambda}$ (resp. $h_{z,0}$) has to be homogeneous polynomial of degree two, precisely:

$$\overline{h}_{z,\lambda}(\omega) = \sum_{x,y\in\mathbb{Z}} \varphi_{z,\lambda}(\mathbf{m},x,y)\omega_x\omega_y,$$

where $\varphi_{z,\lambda}(\mathbf{m},\cdot,\cdot) : \mathbb{Z}^2 \longrightarrow \mathbb{R}$ is a square-integrable symmetric function. As before, we decompose every degree two function h as $h = h^= + h^{\neq}$, where $h^=$ belongs to $\mathcal{Q}^=$ and $h^{\neq}$ belongs to $\mathcal{Q}^{\neq}$. We have seen in the proof of Theorem III.23 that the part belonging to $\mathcal{Q}^=$ vanishes for the two solutions, in other words, $\overline{h}_{z,\lambda}$ and $h_{z,0}$ are elements of $\mathcal{Q}^{\neq}$. As a consequence,

$$\ll \overline{h}_{z,\lambda}, \mathcal{S}^{\text{exch}}(h_{z,0}) \gg_{1,\star} =\ll \overline{h}_{z,\lambda}, \mathcal{S}^{\text{exch}}(h_{z,0}) \gg_{1,\star}$$

which is bounded by

$$\sqrt{\ll \overline{h}_{z,\lambda}, (-\mathcal{S}^{\text{exch}})(\overline{h}_{z,\lambda}) \gg_{1,\star}}\sqrt{\ll h_{z,0}, (-\mathcal{S}^{\text{exch}})(h_{z,0}) \gg_{1,\star}}$$

according to the Cauchy-Schwarz inequality for the scalar product $\ll \cdot, (-\mathcal{S}^{\text{exch}})\cdot \gg_{1,\star}$. We treat separately the two terms into the two lemmas below. We prove that the first term is bounded by $\mathrm{C}/\sqrt{\lambda}$, and the second one is uniformly bounded for $\lambda, z > 0$. Here we state the two lemmas:

Lemma III.27. *There exists a constant* $\mathrm{C} > 0$ *such that, for all* $z, \lambda > 0$,

$$\ll \overline{h}_{z,\lambda}, (-\mathcal{S}^{exch})(\overline{h}_{z,\lambda}) \gg_{1,\star} \leqslant \frac{\mathrm{C}}{\lambda}.$$

Lemma III.28. *There exists a constant* $\mathrm{C} > 0$ *such that, for all* $z > 0$,

$$\ll h_{z,0}, (-\mathcal{S}^{exch})(h_{z,0}) \gg_{1,\star} \leqslant \mathrm{C}.$$

From these statements we deduce

$$\lambda\Big|\ll \overline{h}_{z,\lambda}, \mathcal{S}^{\text{exch}}(h_{z,0}) \gg_{1,\star}\Big| \leqslant \mathrm{C}_0\sqrt{\lambda}$$

where C_0 does not depend on $\lambda, z > 0$, and Theorem III.26 follows.

Step 2 - Proofs of the two lemmas. We begin with the proof of Lemma III.27. We recall the resolvent equation in $\mathbf{L}_\star^2$:

$$z\overline{h}_{z,\lambda} - (\lambda\mathcal{S}^{\text{exch}} + \mathcal{S}_0 - \mathcal{A}^{\mathbf{m}})\overline{h}_{z,\lambda} = \mathrm{J}_0. \tag{III.46}$$

We multiply (III.46) by $h_{z,\lambda}$ and integrate with respect to $\ll \cdot \gg_{1,\star}$, in order to get

$$z \ll \overline{h}_{z,\lambda}, \overline{h}_{z,\lambda} \gg_{1,\star} + \ll \overline{h}_{z,\lambda}, (-\mathcal{S}_0)(\overline{h}_{z,\lambda}) \gg_{1,\star} +\lambda \ll \overline{h}_{z,\lambda}, (-\mathcal{S}^{\text{exch}})(\overline{h}_{z,\lambda}) \gg_{1,\star} =\ll \mathrm{J}_0, \overline{h}_{z,\lambda} \gg_{1,\star}.$$

The right-hand side rewrites as

$$(2\gamma)^{-1} \ll (-\mathcal{S}_0)(\mathrm{J}_0), h_{z,0} \gg_{1,\star}.$$

Cauchy-Schwarz inequality for the scalar product $\ll \cdot, (-\mathcal{S}_0)\cdot \gg_{1,\star}$ on the right-hand side gives

$$z \ll \overline{h}_{z,\lambda}, \overline{h}_{z,\lambda} \gg_{1,\star} \leqslant \mathrm{C}$$

with $\mathrm{C} := (2\gamma)^{-1/2} \ll \mathrm{J}_0, \mathrm{J}_0 \gg_{1,\star}^{1/2}$ and then

$$\lambda \ll \overline{h}_{z,\lambda}, (-\mathcal{S}^{\mathrm{exch}})(\overline{h}_{z,\lambda}) \gg_{1,\star} \leqslant \mathrm{C}.$$

We now turn to Lemma III.28. We prove a general result, precisely: there exists a constant $\mathrm{C} > 0$ such that, for all $g \in \mathcal{Q}^{\neq}$,

$$\ll g, (-\mathcal{S}^{\mathrm{exch}})g \gg_{1,\star} \leqslant \mathrm{C} \ll g, g \gg_{1,\star}. \tag{III.47}$$

This fact is proved through explicit computations. Let us write $g \in \mathcal{Q}^{\neq}$ in the form

$$g(\omega) = \sum_{\substack{x\in\mathbb{Z} \\ k\geqslant 1}} \phi_{x,k}(\mathbf{m})\omega_x\omega_{x+k}.$$

A straightforward computation gives that

$$\begin{aligned}\ll g, (-\mathcal{S}^{\mathrm{exch}})g \gg_{1,\star} &= \frac{1}{2}\mathbb{E}_1^{\star}\Big[\big(\nabla_{0,1}\Gamma_g\big)^2\Big] = \sum_{k\geqslant 2}\mathbb{E}\left[\left(\sum_{z\in\mathbb{Z}}\phi_{z,k}(\tau_{-z}\mathbf{m}) - \phi_{z,k}(\tau_{1-z}\mathbf{m})\right)^2\right].\\ &\leqslant 4\sum_{k\geqslant 2}\mathbb{E}\left[\left(\sum_{z\in\mathbb{Z}}\phi_{z,k}(\mathbf{m})\right)^2\right].\end{aligned}$$

In the last inequality, we use the fact that the measure $\mathbb{P}$ on the disorder is translation invariant and that $(a-b)^2 \leqslant 2(a^2+b^2)$ for all $a, b \in \mathbb{R}$. Besides, one can also check that

$$\ll g, g \gg_{1,\star} = \sum_{k\geqslant 1}\mathbb{E}\left[\sum_{x,z\in\mathbb{Z}}\phi_{z,k}(\tau_{-z}\mathbf{m})\phi_{x,k}(\tau_{-x}\mathbf{m})\right] = \sum_{k\geqslant 1}\mathbb{E}\left[\left(\sum_{z\in\mathbb{Z}}\phi_{z,k}(\mathbf{m})\right)^2\right],$$

thanks to the translation invariance of $\mathbb{P}$. The bound (III.47) follows directly, with $\mathrm{C} = 4$. To prove Lemma III.28, it remains to show that $\ll h_{z,0}, h_{z,0} \gg_{1,\star}$ is uniformly bounded in z. We recall the resolvent equation in $\mathbf{L}^2_\star$:

$$zh_{z,0} - (\mathcal{S}_0 + \mathcal{A}^{\mathbf{m}})h_{z,0} = \mathrm{J}_0. \tag{III.48}$$

Notice that we can write $\mathcal{S}_0(h_{z,0}) = -2\gamma h_{z,0}$. We multiply (III.48) by $h_{z,0}$ and integrate with respect to $\ll \cdot \gg_{1,\star}$ in order to get

$$z \ll h_{z,0}, h_{z,0} \gg_{1,\star} + 2\gamma \ll h_{z,0}, h_{z,0} \gg_{1,\star} = \ll \mathrm{J}_0, h_{z,0} \gg_{1,\star}.$$

As previously, Cauchy-Schwarz inequality for the scalar product $\ll \cdot, (-\mathcal{S}_0)\cdot \gg_{1,\star}$ on the right-hand side gives

$$\ll h_{z,0}, h_{z,0} \gg_{1,\star} \leqslant \mathrm{C},$$

with $\mathrm{C} := (2\gamma)^{-1} \ll \mathrm{J}_0, \mathrm{J}_0 \gg_{1,\star}^{1/2}$. □

4 Macroscopic Fluctuations of Energy

In this section we are interested in the fluctuations of the empirical energy, when the system is at equilibrium. We prove that the limit fluctuation process is governed by a generalized Ornstein-Uhlenbeck process, whose covariances are given in terms of the diffusion coefficient.

4.1 Energy Fluctuation Field

Recall that we denote by $\mathbf{e}_\beta$ the thermodynamical energy associated to the inverse temperature $\beta > 0$, namely $\mathbf{e}_\beta = \beta^{-1}$. We define the energy empirical distribution $\pi^N_{t,\mathbf{m}}$ on the torus $\mathbb{T} = [0,1)$ as

$$\pi^N_{t,\mathbf{m}}(du) = \frac{1}{N}\sum_{x\in\mathbb{T}_N} \omega_x^2(t)\delta_{x/N}(du), \quad t \in [0,T], \quad u \in \mathbb{T},$$

where δ_u states for the Dirac measure. We denote by $\{\omega(t)\}_{t\geqslant 0}$ the Markov process generated by $N^2\mathcal{L}_N^{\mathbf{m}}$ and by $\mathcal{M}_1$ the set of probability measures on $\mathbb{T}$, endowed with the weak topology. The space of trajectories in $\mathcal{M}_1$, which are right-continuous and left-limited (i.e. the Skorokhod space) is denoted by $\mathcal{D}\left([0,T],\mathcal{M}_1\right)$. If the initial state of the dynamics is given by the equilibrium Gibbs measure μ^N_β, then $\pi^N_{t,\mathbf{m}}$ weakly converges towards the deterministic measure on $\mathbb{T}$, equal to $\{\mathbf{e}_\beta du\}$. Our goal is to investigate the fluctuations of the empirical measure π^N with respect to this limit. Let us fix the disorder $\mathbf{m}$, and the inverse of temperature $\beta > 0$ and consider the system under the equilibrium measure μ^N_β .

Definition III.3 (Empirical energy fluctuations). *We denote by $\mathcal{Y}^N_{t,\mathbf{m}}$ the empirical energy fluctuation field defined as*

$$\mathcal{Y}^N_{t,\mathbf{m}}(H) = \frac{1}{\sqrt{N}}\sum_{x\in\mathbb{T}_N} H\left(\frac{x}{N}\right)\left\{\omega_x^2(t) - \mathbf{e}_\beta\right\},$$

where $H : \mathbb{T} \longrightarrow \mathbb{R}$ is a smooth function.

We are going to prove that the distribution $\mathcal{Y}^N_{t,\mathbf{m}}$ converges in law towards the solution of the linear SPDE:

$$\partial_t \mathcal{Y} = D\,\partial_y^2\mathcal{Y}\,dt + \sqrt{2D\chi(\beta)}\,\partial_y\mathcal{B}(y,t)$$

where $\mathcal{B}$ is a standard normalized space-time white noise, and D is the diffusion coefficient defined in Theorem III.17. Observe that there is no dependence on the statistics of the disorder $\mathbf{m}$ in the limit process. In other words, the latter is described by the stationary generalized Ornstein-Uhlenbeck process with zero mean and covariances given by

$$\left\langle \mathcal{Y}_t(H)\mathcal{Y}_0(G)\right\rangle = \frac{\chi(\beta)}{\sqrt{4\pi t D}}\int_{\mathbb{R}^2} du\,dv\,\overline{H}(u)\overline{G}(v)\exp\left(-\frac{(u-v)^2}{4tD}\right),$$

for all $t \geqslant 0$ and smooth functions $H, G : \mathbb{T} \longrightarrow \mathbb{R}$. Here, $\overline{H}$ (resp. $\overline{G}$) is the periodic extension to the real line of H (resp. G).

We denote by $\mathfrak{Y}^N_{\mathbf{m}}$ the probability measure on $\mathcal{D}([0,T],\mathcal{M}_1)$ induced by the energy fluctuation field $\mathcal{Y}^N_{t,\mathbf{m}}$ and the Markov process $\{\omega(t)\}_{t\geqslant 0}$ generated by $N^2\mathcal{L}_N^m$, starting from the equilibrium probability measure μ^N_β. Let $\mathfrak{Y}$ be the probability measure on the space $\mathcal{D}([0,T],\mathcal{M}_1)$ corresponding to the generalized Ornstein-Uhlenbeck process $\mathcal{Y}_t$. The main result of this section is the following.

Theorem III.29. *For almost all realization of the disorder $\mathbf{m} \in \Omega_{\mathcal{D}}$, the sequence $\{\mathfrak{Y}^N_{\mathbf{m}}\}_{N\geqslant 1}$ weakly converges in $\mathcal{D}([0,T],\mathcal{M}_1)$ to the probability measure $\mathfrak{Y}$.*

4.2 Strategy of the Proof

We follow the lines of [69, Section 3], and we write the proof for $\beta = 1$ (the same argument remaining in force for every $\beta > 0$). The proof of Theorem III.29 is divided into three steps. First, we need to show that the sequence $\{\mathfrak{Y}^{\mathrm{N}}_{\mathbf{m}}\}_{\mathrm{N}\geqslant 1}$ is tight. This point follows a standard argument, given for instance in [49, Section 11].

Then, we prove that the one-time marginal of any limit point $\mathfrak{Y}^\star$ of a convergent subsequence of $\{\mathfrak{Y}^{\mathrm{N}}_{\mathbf{m}}\}_{\mathrm{N}\geqslant 1}$ is the law of a centered Gaussian field $\mathcal{Y}$ with covariances given by

$$\big\langle \mathcal{Y}(\mathrm{H})\mathcal{Y}(\mathrm{G})\big\rangle = \chi(1)\int_{\mathbb{T}} \mathrm{d}u\, \mathrm{H}(u)\mathrm{G}(u),$$

where $\mathrm{H},\mathrm{G} : \mathbb{T} \longrightarrow \mathbb{R}$ are smooth functions. This statement comes from the central limit theorem for independent variables. Finally, we prove the main point in the next subsections: all limit points $\mathfrak{Y}^\star$ of convergent subsequences of $\{\mathfrak{Y}^{\mathrm{N}}_{\mathbf{m}}\}_{\mathrm{N}\geqslant 1}$ solve the martingale problems below.

Martingale problems – For each smooth function $\mathrm{H} : \mathbb{T} \longrightarrow \mathbb{R}$,

$$\mathfrak{M}_t(\mathrm{H}) := \mathcal{Y}_t(\mathrm{H}) - \mathcal{Y}_0(\mathrm{H}) - \int_0^t \mathrm{D}\mathcal{Y}_s(\mathrm{H}'')\mathrm{d}s, \tag{III.49}$$

and

$$\mathfrak{N}_t(\mathrm{H}) := \big(\mathfrak{M}_t(\mathrm{H})\big)^2 - 2t\chi(1)\mathrm{D}\int_{\mathbb{T}} \mathrm{H}'(u)^2\mathrm{d}u \tag{III.50}$$

are $\mathbb{L}^1(\mathfrak{Y})$-martingales.

4.3 Martingale Decompositions

Let us fix a smooth function $\mathrm{H} : \mathbb{T} \longrightarrow \mathbb{R}$. We rewrite $\mathcal{Y}^{\mathrm{N}}_{t,\mathbf{m}}(\mathrm{H})$ as

$$\mathcal{Y}^{\mathrm{N}}_{t,\mathbf{m}}(\mathrm{H}) = \mathcal{Y}^{\mathrm{N}}_{0,\mathbf{m}}(\mathrm{H}) + \int_0^t \sqrt{\mathrm{N}}\sum_{x\in\mathbb{T}_\mathrm{N}} \nabla_\mathrm{N}\mathrm{H}\left(\frac{x}{\mathrm{N}}\right) j_{x,x+1}(\mathbf{m},s)\,\mathrm{d}s + \mathcal{M}^{\mathrm{N}}_{t,\mathbf{m}}(\mathrm{H})$$

where $\mathcal{M}^{\mathrm{N}}_{t,\mathbf{m}}$ is the martingale defined as

$$\mathcal{M}^{\mathrm{N}}_{t,\mathbf{m}}(\mathrm{H}) = \int_0^t \frac{1}{\mathrm{N}\sqrt{\mathrm{N}}}\sum_{x\in\mathbb{T}_\mathrm{N}} \nabla_\mathrm{N}\mathrm{H}\left(\frac{x}{\mathrm{N}}\right)\left(\omega^2_{x+1}-\omega^2_x\right)(s)\,\mathrm{d}\big[\mathrm{N}_{x,x+1}(s)-\lambda s\big].$$

Hereafter, $(\mathrm{N}_{x,x+1})_{x\in\mathbb{Z}}, (\mathrm{N}_x)_{x\in\mathbb{Z}}$ are independent Poisson processes of intensity (respectively) λ and γ. The notation ∇_N states for the discrete gradient:

$$\nabla_\mathrm{N}\mathrm{H}\left(\frac{x}{\mathrm{N}}\right) = \mathrm{N}\left[\mathrm{H}\left(\frac{x+1}{\mathrm{N}}\right) - \mathrm{H}\left(\frac{x}{\mathrm{N}}\right)\right],$$

and the discrete Laplacian Δ_N is defined in a similar way:

$$\Delta_\mathrm{N}\mathrm{H}\left(\frac{x}{\mathrm{N}}\right) = \mathrm{N}^2\left[\mathrm{H}\left(\frac{x+1}{\mathrm{N}}\right) + \mathrm{H}\left(\frac{x-1}{\mathrm{N}}\right) - 2\mathrm{H}\left(\frac{x}{\mathrm{N}}\right)\right].$$

To close the equation, we are going to replace the term involving the microscopic currents with a term involving $\mathcal{Y}^{\mathrm{N}}_{t,\mathbf{m}}$. In other words, the most important part in the fluctuation field represented by

$$\int_0^t \sqrt{\mathrm{N}} \sum_{x\in\mathbb{T}_\mathrm{N}} \nabla_\mathrm{N}\mathrm{H}\left(\frac{x}{\mathrm{N}}\right) j_{x,x+1}(\mathbf{m},s)\,\mathrm{d}s$$

is its projection over the conservation field $\mathcal{Y}^{\mathrm{N}}_{t,\mathbf{m}}$ (recall that the total energy is the unique conserved quantity of the system). The non-gradient approach consists in using the fluctuation-dissipation approximation of the current $j_{x,x+1}$ given by Theorem III.17 as $\mathrm{D}\big(\omega_{x+1}^2-\omega_x^2\big)+\mathcal{L}^{\mathbf{m}}(\tau_x f)$. For that purpose, we rewrite, for any $f\in\mathcal{Q}$,

$$\mathcal{Y}^{\mathrm{N}}_{t,\mathbf{m}}(\mathrm{H})=\mathcal{Y}^{\mathrm{N}}_{0,\mathbf{m}}(\mathrm{H})+\int_0^t \mathrm{D}\mathcal{Y}^{\mathrm{N}}_{s,\mathbf{m}}(\Delta_\mathrm{N}\mathrm{H})\mathrm{d}s+\mathfrak{I}^{1,\mathrm{N}}_{t,\mathbf{m},f}(\mathrm{H})+\mathfrak{I}^{2,\mathrm{N}}_{t,\mathbf{m},f}(\mathrm{H})+\mathfrak{M}^{1,\mathrm{N}}_{t,\mathbf{m},f}(\mathrm{H})+\mathfrak{M}^{2,\mathrm{N}}_{t,\mathbf{m},f}(\mathrm{H}), \quad \text{(III.51)}$$

where

$$\mathfrak{I}^{1,\mathrm{N}}_{t,\mathbf{m},f}(\mathrm{H})=\int_0^t \sqrt{\mathrm{N}}\sum_{x\in\mathbb{T}_\mathrm{N}}\nabla_\mathrm{N}\mathrm{H}\left(\frac{x}{\mathrm{N}}\right)\Big[j_{x,x+1}(\mathbf{m},s)-\mathrm{D}\big(\omega_{x+1}^2-\omega_x^2\big)(s)-\mathcal{L}^{\mathbf{m}}(\tau_x f)(\mathbf{m},s)\Big]\,\mathrm{d}s,$$

$$\mathfrak{I}^{2,\mathrm{N}}_{t,\mathbf{m},f}(\mathrm{H})=\int_0^t \sqrt{\mathrm{N}}\sum_{x\in\mathbb{T}_\mathrm{N}}\nabla_\mathrm{N}\mathrm{H}\left(\frac{x}{\mathrm{N}}\right)\mathcal{L}^{\mathbf{m}}(\tau_x f)(\mathbf{m},s)\mathrm{d}s,$$

$$\mathfrak{M}^{1,\mathrm{N}}_{t,\mathbf{m},f}(\mathrm{H})=\int_0^t \frac{1}{\mathrm{N}\sqrt{\mathrm{N}}}\sum_{x\in\mathbb{T}_\mathrm{N}}\nabla_\mathrm{N}\mathrm{H}\left(\frac{x}{\mathrm{N}}\right)\Big\{\big[\nabla_{x,x+1}(\omega_0^2-\Gamma_f)\big](s)\,\mathrm{d}\big[\mathrm{N}_{x,x+1}(s)-\lambda s\big] - \nabla_x(\Gamma_f)(s)\,\mathrm{d}\big[\mathrm{N}_x(s)-\gamma s\big]\Big\},$$

$$\mathfrak{M}^{2,\mathrm{N}}_{t,\mathbf{m},f}(\mathrm{H})=\int_0^t \frac{1}{\mathrm{N}\sqrt{\mathrm{N}}}\sum_{x\in\mathbb{T}_\mathrm{N}}\nabla_\mathrm{N}\mathrm{H}\left(\frac{x}{\mathrm{N}}\right)\Big\{\nabla_{x,x+1}(\Gamma_f)(s)\,\mathrm{d}\big[\mathrm{N}_{x,x+1}(s)-\lambda s\big] + \nabla_x(\Gamma_f)(s)\,\mathrm{d}\big[\mathrm{N}_x(s)-\gamma s\big]\Big\}.$$

The strategy of the proof is based on the two following results.

Lemma III.30. *For every smooth function* $\mathrm{H}:\mathbb{T}\longrightarrow\mathbb{R}$, *and every function* $f\in\mathcal{Q}$,

$$\lim_{\mathrm{N}\longrightarrow\infty}\mathbb{E}\left\langle\sup_{0\leqslant t\leqslant \mathrm{T}}\left(\mathfrak{I}^{2,\mathrm{N}}_{t,\mathbf{m},f}(\mathrm{H})+\mathfrak{M}^{2,\mathrm{N}}_{t,\mathbf{m},f}(\mathrm{H})\right)^2\right\rangle_1=0.$$

Theorem III.31 (Boltzmann-Gibbs principle). *There exists a sequence of functions* $\{f_k\}_{k\in\mathbb{N}}\in\mathcal{Q}$ *such that*

(i) for every smooth function $\mathrm{H}:\mathbb{T}\longrightarrow\mathbb{R}$,

$$\lim_{k\longrightarrow\infty}\lim_{\mathrm{N}\longrightarrow\infty}\mathbb{E}\left\langle\sup_{0\leqslant t\leqslant \mathrm{T}}\left(\mathfrak{I}^{1,\mathrm{N}}_{t,\mathbf{m},f_k}(\mathrm{H})\right)^2\right\rangle_1=0, \quad \text{(III.52)}$$

(ii) and moreover

$$\lim_{k\longrightarrow\infty}\mathbb{E}\left\langle\lambda\Big(\nabla_{0,1}(\omega_0^2-\Gamma_{f_k})\Big)^2+\gamma\Big(\nabla_0(\Gamma_{f_k})\Big)^2\right\rangle_1=2\mathrm{D}\chi(1). \quad \text{(III.53)}$$

As a result, the martingale $\mathfrak{M}^{1,N}_{t,\mathbf{m},f_k}$ converges in $\mathbf{L}^2(\mathbb{P}^\star_1)$, as $N \longrightarrow \infty$ and $k \longrightarrow \infty$, to a martingale $\mathfrak{M}_t(H)$ of quadratic variation

$$2tD\chi(1)\int_{\mathbb{T}} H'(u)^2\,du,$$

and the limit $\mathcal{Y}_t(H)$ of $\mathcal{Y}^N_{t,\mathbf{m}}(H)$ satisfies the equation

$$\mathcal{Y}_t(H) = \mathcal{Y}_0(H) + \int_0^t \mathcal{Y}_s(DH'')\,ds + \mathfrak{M}_t(H).$$

We have proved that the limit solves the martingale problems (III.49) and (III.50), which uniquely characterize the generalized Ornstein-Uhlenbeck process $\mathcal{Y}_t$. The proof of Theorem III.31 is strongly related to the characterization of the diffusion coefficient given in Sections 2.1, 2.2 and 2.3.

4.4 Proof of Lemma III.30

In this paragraph we give a proof of Lemma III.30. We define

$$X^N_{\mathbf{m},f}(t) = \frac{1}{N\sqrt{N}}\sum_{x\in\mathbb{T}_N}\nabla_N H\left(\frac{x}{N}\right)\tau_x f(\mathbf{m},t)$$

As before, we can rewrite

$$\begin{aligned}\mathfrak{I}^{2,N}_{t,\mathbf{m},f}(H) + \mathfrak{M}^{2,N}_{t,\mathbf{m},f}(H) &= X^N_{\mathbf{m},f}(t) - X^N_{\mathbf{m},f}(0)\\ &+ \frac{1}{N\sqrt{N}}\int_0^t \sum_{x\in\mathbb{T}_N}\nabla_{x,x+1}\left(\left\{\sum_{z\in\mathbb{T}_N}\nabla_N H\left(\frac{z}{N}\right)\tau_z f\right\} - \nabla_N\left(\frac{x}{N}\right)\Gamma_f\right)(\mathbf{m},s)d\big[N_{x,x+1}(s)-\lambda s\big]\\ &+ \frac{1}{N\sqrt{N}}\int_0^t \sum_{x\in\mathbb{T}_N}\nabla_{x}\left(\left\{\sum_{z\in\mathbb{T}_N}\nabla_N H\left(\frac{z}{N}\right)\tau_z f\right\} - \nabla_N H\left(\frac{x}{N}\right)\Gamma_f\right)(\mathbf{m},s)d\big[N_{x}(s)-\lambda s\big].\end{aligned}$$

Therefore,

$$\begin{aligned}\left(\mathfrak{I}^{2,N}_{t,\mathbf{m},f}(H) + \mathfrak{M}^{2,N}_{t,\mathbf{m},f}(H)\right)^2 &\leqslant 3\left(X^N_{\mathbf{m},f}(t) - X^N_{\mathbf{m},f}(0)\right)^2\\ &+ 3\left(\frac{1}{N\sqrt{N}}\int_0^t \sum_{x\in\mathbb{T}_N}\nabla_{x,x+1}\left(\left\{\sum_{z\in\mathbb{T}_N}\nabla_N H\left(\frac{z}{N}\right)\tau_z f\right\} - \nabla_N H\left(\frac{x}{N}\right)\Gamma_f\right)(\mathbf{m},s)d\big[N_{x,x+1}(s)-\lambda s\big]\right)^2\\ &+ 3\left(\frac{1}{N\sqrt{N}}\int_0^t \sum_{x\in\mathbb{T}_N}\nabla_{x}\left(\left\{\sum_{z\in\mathbb{T}_N}\nabla_N H\left(\frac{z}{N}\right)\tau_z f\right\} - \nabla_N H\left(\frac{x}{N}\right)\Gamma_f\right)(\mathbf{m},s)d\big[N_{x}(s)-\lambda s\big]\right)^2\end{aligned} \tag{III.54}$$

On the one hand,

$$\mathbb{E}\left\langle\left(X^N_{\mathbf{m},f}\right)^2\right\rangle_1 = \frac{1}{N^3}\sum_{x,y\in\mathbb{T}_N}\nabla_N H\left(\frac{x}{N}\right)\nabla_N H\left(\frac{y}{N}\right)\mathbb{E}\left\langle\tau_x f,\tau_y f\right\rangle_1.$$

This last quantity is of order $1/\mathrm{N}^2$, because f is a local function of zero average, and H is smooth. On the other hand, let us define

$$\mathrm{Y}_x(\mathbf{m},\omega) := \sum_{z\in\mathbb{T}_\mathrm{N}} \nabla_\mathrm{N}\mathrm{H}\left(\frac{z}{\mathrm{N}}\right)\tau_z f - \nabla_\mathrm{N}\mathrm{H}\left(\frac{x}{\mathrm{N}}\right)\sum_{z\in\mathbb{Z}}\tau_z f.$$

Then, the expectation of the second term of (III.54) is equal to

$$\frac{3\lambda^2 t\mathrm{N}^2}{\mathrm{N}^3}\sum_{x\in\mathbb{T}_\mathrm{N}}\mathbb{E}\Big\langle\big[\nabla_{x,x+1}(\mathrm{Y}_x)\big]^2\Big\rangle_1.$$

Again, since f is local and H is smooth, this quantity is of order $1/\mathrm{N}^2$. Indeed, in the expression $\nabla_{x,x+1}(\mathrm{Y}_x)$, there is a sum over $z\in\mathbb{Z}$, but in which only terms with $|z-x|\leqslant 2$ remain. The same holds for the third term of (III.54).

4.5 Proof of Theorem III.31

In this paragraph, we prove Theorem III.31 by using the central limit theorem variances given in Theorem III.6. First, we show how to relate (III.52) to such variances.

Proposition III.32. *Let $\psi\in\mathcal{C}_0$ such that $s_\psi\leqslant\mathrm{N}$. Then*

$$\left\langle\sup_{0\leqslant t\leqslant\mathrm{T}}\left[\int_0^t\psi(s)\,ds\right]^2\right\rangle_1 \leqslant \frac{24\mathrm{T}}{\mathrm{N}^2}\langle\psi,(-\mathcal{S}_\mathrm{N})^{-1}\psi\rangle_1. \qquad \text{(III.55)}$$

The previous result is proved for example in [52, Section 2, Lemma 2.4]. We are going to use this bound for functions of type $\sum_x \mathrm{G}(x/\mathrm{N})\tau_x\varphi$, where φ belongs to $\mathcal{Q}_0$. The main result of this subsection is the following.

Theorem III.33. *Let $\varphi\in\mathcal{Q}_0$, and G a smooth function on $\mathbb{T}$. Then,*

$$\limsup_{\mathrm{N}\longrightarrow\infty}\mathbb{E}\left\langle\sup_{0\leqslant t\leqslant\mathrm{T}}\left[\sqrt{\mathrm{N}}\int_0^t\sum_{x\in\mathbb{T}_\mathrm{N}}\mathrm{G}\left(\frac{x}{\mathrm{N}}\right)\tau_x\varphi(\mathbf{m},s)ds\right]^2\right\rangle_1 \leqslant \mathrm{CT}|||\varphi|||_1^2\int_\mathbb{T}\mathrm{G}^2(u)du. \qquad \text{(III.56)}$$

Proof. From Proposition III.32, the left-hand side of (III.56) is bounded by

$$24\mathrm{T}\,\mathbb{E}\left\langle\sqrt{\mathrm{N}}\sum_{x\in\mathbb{T}_\mathrm{N}}\mathrm{G}\left(\frac{x}{\mathrm{N}}\right)\tau_x\varphi(\mathbf{m}),(-\mathrm{N}^2\mathcal{S}_\mathrm{N})^{-1}\left(\sqrt{\mathrm{N}}\sum_{x\in\mathbb{T}_\mathrm{N}}\mathrm{G}\left(\frac{x}{\mathrm{N}}\right)\tau_x\varphi(\mathbf{m})\right)\right\rangle_1,$$

that can be written with the variational formula as

$$24\mathrm{T}\sup_{f\in\mathcal{C}}\left\{\sqrt{\mathrm{N}}\sum_{x\in\mathbb{T}_\mathrm{N}}\mathrm{G}\left(\frac{x}{\mathrm{N}}\right)\mathbb{E}\left[\langle f\,\tau_x\varphi\rangle_1\right]-\mathrm{N}^2\mathbb{E}\Big[\mathcal{D}_\mathrm{N}(\mu_1;f)\Big]\right\}.$$

Since $\varphi\in\mathcal{Q}_0$, from Proposition V.13 we can restrict the supremum over $f\in\mathcal{Q}$. Proposition III.4 gives

$$\big\langle f\,\tau_x\varphi\big\rangle_1\leqslant \mathrm{C}_\varphi\Big\langle\tau_{-x}f,(-\mathcal{S}_{\Lambda_\varphi})(\tau_{-x}f)\Big\rangle_1^{1/2}$$

and by Cauchy-Schwarz inequality,

$$\sqrt{N}\sum_{x\in\mathbb{T}_N} G\left(\frac{x}{N}\right)\langle f\,\tau_x\varphi\rangle_1 \leqslant \left(\frac{1}{N}\sum_{x\in\mathbb{T}_N} G\left(\frac{x}{N}\right)^2\right)^{1/2} N\,C_\varphi\,\langle f,(-\mathcal{S}_N)f\rangle_1^{1/2}.$$

The supremum on f can be explicitely computed, and gives the final bound

$$\mathbb{E}\left\langle \sup_{0\leqslant t\leqslant T}\left[\sqrt{N}\int_0^t\sum_{x\in\mathbb{T}_N} G\left(\frac{x}{N}\right)\tau_x\varphi(\mathbf{m},s)\mathrm{d}s\right]^2\right\rangle_1 \leqslant C'_\varphi T\left(\frac{1}{N}\sum_{x\in\mathbb{T}_N} G\left(\frac{x}{N}\right)^2\right). \tag{III.57}$$

We are now going to show that the constant on the right-hand side is proportional to $|||\varphi|||_1^2$. For that purpose, we average on microscopic boxes: for $k \ll N$, we denote

$$\overline{\varphi}_k = \sum_{y\in\Lambda_k}\tau_y\varphi,$$

and we want to substitute

$$\sqrt{N}\sum_{x\in\mathbb{T}_N} G\left(\frac{x}{N}\right)\tau_x\varphi \quad \text{with} \quad \frac{\sqrt{N}}{2k+1}\sum_{x\in\mathbb{T}_N} G\left(\frac{x}{N}\right)\tau_x\overline{\varphi}_k.$$

The error term that appears is estimated by

$$\mathbb{E}\left\langle \sup_{0\leqslant t\leqslant T}\left[\sqrt{N}\int_0^t\sum_{\substack{x,y\in\mathbb{T}_N\\|x-y|\leqslant k}}\frac{1}{2k+1}\left(G\left(\frac{x}{N}\right)-G\left(\frac{y}{N}\right)\right)\tau_x\varphi(\mathbf{m},s)\mathrm{d}s\right]^2\right\rangle_1.$$

From (III.57), the expression above is bounded by Ck/N, and then vanishes as $N\longrightarrow\infty$. We are reduced to estimate

$$\mathbb{E}\left\langle \sup_{0\leqslant t\leqslant T}\left[\frac{\sqrt{N}}{2k+1}\int_0^t\sum_{x\in\mathbb{T}_N} G\left(\frac{x}{N}\right)\tau_x\overline{\varphi}_k(\mathbf{m},s)\mathrm{d}s\right]^2\right\rangle_1.$$

By the same argument, this is bounded by

$$\begin{aligned}
&\frac{CT}{2k+1}\sum_{x\in\mathbb{T}_N}\sup_{f\in\mathcal{Q}}\left\{\sqrt{N}G\left(\frac{x}{N}\right)\mathbb{E}\left[\langle f\,\tau_x\overline{\varphi}_k\rangle_1\right]-\frac{N^2}{2k+1}\mathbb{E}\left[\left\langle\tau_{-x}f,\left(-\mathcal{S}_{\Lambda_k}\right)\tau_{-x}f\right\rangle_1\right]\right\}\\
&\leqslant\frac{CT}{2k+1}\sum_{x\in\mathbb{T}_N}\sup_{f\in\mathcal{Q}}\left\{C(\varphi)\sqrt{N}G\left(\frac{x}{N}\right)\mathbb{E}\left[\left\langle\tau_{-x}f,(-\mathcal{S}_{\Lambda_k})(\tau_{-x}f)\right\rangle_1\right]^{1/2}\right.\\
&\qquad\left.-\frac{N^2}{2k+1}\mathbb{E}\left[\left\langle\tau_{-x}f,\left(-\mathcal{S}_{\Lambda_k}\right)\tau_{-x}f\right\rangle_1\right]\right\}.
\end{aligned}$$

The supremum on f can be explicitely computed, and gives the final bound

$$C(\varphi)T\left(\frac{1}{N}\sum_{x\in\mathbb{T}_N} G^2\left(\frac{x}{N}\right)\right)\frac{1}{2k+1}\mathbb{E}\left\langle\overline{\varphi}_k,\left(-\mathcal{S}_{\Lambda_k}\right)^{-1}\overline{\varphi}_k\right\rangle_1.$$

Taking the limit as $N\longrightarrow\infty$ and then $k\longrightarrow\infty$, we obtain (III.56) from the central limit theorem for variances at equilibrium (Theorem III.6). □

We apply Theorem III.33 to $\mathfrak{I}^{1,\mathrm{N}}_{t,\mathbf{m},f}(\mathrm{H})$, and we get

$$\limsup_{\mathrm{N}\longrightarrow\infty} \mathbb{E}\left\langle \sup_{0\leqslant t\leqslant \mathrm{T}} \left(\mathfrak{I}^{1,\mathrm{N}}_{t,\mathbf{m},f}(\mathrm{H})\right)^2 \right\rangle_1 \leqslant \mathrm{CT}\|\!| j_{0,1} - \mathrm{D}(\omega_1^2 - \omega_0^2) - \mathcal{L}^{\mathbf{m}} f \|\!|_1^2 \int_{\mathbb{T}} \mathrm{H}'(u)^2 \mathrm{d}u.$$

In Section 2.2, we have shown that there exists a sequence of local functions $\{f_k\} \in \mathcal{Q}$ such that

$$\|\!| j_{0,1} - \mathrm{D}(\omega_1^2 - \omega_0^2) - \mathcal{L}^{\mathbf{m}} f_k \|\!|_1 \xrightarrow[k\longrightarrow\infty]{} 0.$$

Eventually, Proposition III.22 given in Section 2.3 proves the second statement of Theorem III.31.

5 Hydrodynamic Limits

In this last paragraph, we briefly enlighten the failure in the derivation of the hydrodynamic limits. Let us assume that the initial law for the Markov process $\{\omega(t)\}_{t\geqslant 0}$ (still generated by $\mathrm{N}^2\mathcal{L}^{\mathbf{m}}_{\mathrm{N}}$), is not the equilibrium measure μ^{N}_{β}, but a *local equilibrium measure* (defined in the same way as in Chapter II). The main goal would be to prove that this property of local equilibrium propagates in time: in other words hydrodynamics limits hold, with an energy profile solution of the diffusion equation with constant coefficient D.

5.1 Statement of the Hydrodynamic Limits Conjecture

The distribution at time t of the Markov chain on $\mathbb{T}_{\mathrm{N}}$ with the generator $\mathrm{N}^2\mathcal{L}^{\mathbf{m}}_{\mathrm{N}}$ and the initial probability measure μ_{N} is denoted by $\mathbb{P}^{\mathbf{m}}_{\mu_{\mathrm{N}},t}$. The measure induced by $\mathbb{P}^{\mathbf{m}}_{\mu_{\mathrm{N}},t}$ on $\mathcal{D}\left([0,\mathrm{T}],\Omega_{\mathrm{N}}\right)$ is denoted by $\mathbb{P}^{\mathbf{m}}_{\mathrm{N}}$.

Recall that we denote by $\mathcal{M}_1$ the set of probability measures on $\mathbb{T}$, endowed with the weak topology and by $\mathcal{D}\left([0,\mathrm{T}],\mathcal{M}_1\right)$ the Skorokhod space of trajectories in $\mathcal{M}_1$. The measure induced by $\mathbb{P}^{\mathbf{m}}_{\mathrm{N}}$ on $\mathcal{D}\left([0,\mathrm{T}],\mathcal{M}_1\right)$ is denoted by $\mathcal{Q}^{\mathbf{m}}_{\mathrm{N}} := \mathbb{P}^{\mathbf{m}}_{\mathrm{N}} \circ \left(\pi^{\mathrm{N}}\right)^{-1}$, where

$$\pi^{\mathrm{N}} := \frac{1}{\mathrm{N}} \sum_{x\in\mathbb{T}_{\mathrm{N}}} \omega_x^2 \delta_{\frac{x}{\mathrm{N}}}.$$

Conjecture III.34. *Let* $\mathrm{T}>0$ *be a time-horizon. Let* $\{\mu^{\mathrm{N}}\}_{\mathrm{N}}$ *be a sequence of probability measures on* Ω_{N}. *Under suitable conditions on the initial law* μ^{N}, *for almost every realization of the random environment* $\mathbf{m}$, *the measure* $\mathcal{Q}^{\mathbf{m}}_{\mathrm{N}}$ *weakly converges in* $\mathcal{D}\left([0,\mathrm{T}],\mathcal{M}_1\right)$ *to the probability measure concentrated on the path* $\{\mathbf{e}(t,u)\mathrm{d}u\}_{t\in[0,\mathrm{T}]}$, *where* $\mathbf{e}$ *is the unique weak solution of the system*

$$\begin{cases} \dfrac{\partial \mathbf{e}}{\partial t}(t,u) = \mathrm{D}\dfrac{\partial^2 \mathbf{e}}{\partial u^2}(t,u), & t>0,\ u\in\mathbb{T} \\ \mathbf{e}(0,u) = \mathbf{e}_0(u). \end{cases}$$

What we expect as for "suitable assumptions" on the initial law are the common ones in the literature of hydrodynamic limits, when dealing with non compact spaces. The first one is natural and related on the relative entropy:

Assumption III.35. *We suppose that there exists a positive constant* K_0 *such that the relative entropy* $H(\mu^N|\mu^N_\star)$ *of* μ^N *with respect to a reference measure* $\mu^N_\star$ *is bounded by* $K_0 N$*:*

$$H(\mu^N|\mu^N_\star) \leqslant K_0 N. \tag{III.58}$$

For instance, if μ^N is defined as a Gibbs local equilibrium state:

$$\prod_{x\in\mathbb{T}_N} \sqrt{\frac{2\pi}{\beta_0(x/N)}} \exp\left(-\frac{\beta_0(x/N)}{2}\omega_x^2\right) d\omega_x$$

for some continuous function $\beta_0 : \mathbb{T} \longrightarrow \mathbb{R}_+$, then (III.58) is satisfied. The second one is related to energy boundness, that has already been a major concern in Chapter II. More precisely,

Assumption III.36. *We assume there exists a positive constant* E_0 *such that*

$$\limsup_{N\longrightarrow\infty} \mu^N\left[\frac{1}{N}\sum_{x\in\mathbb{T}_N} \omega_x^4\right] \leqslant E_0. \tag{III.59}$$

In the derivation of hydrodynamic limits with the usual *entropy method*, we need the following two estimates: first, there exists a positive constant C such that, for any $t > 0$

$$\mathbb{E}_{\mathbb{P}^{\mathbf{m}}_N}\left[\frac{1}{N}\sum_{x\in\mathbb{T}_N} \omega_x^2(t)\right] \leqslant C. \tag{III.60}$$

This can be easily established using (III.59) and the Cauchy-Schwarz inequality. The second control that we need is

$$\lim_{N\longrightarrow\infty} \mathbb{E}_{\mathbb{P}^{\mathbf{m}}_N}\left[\int_0^t \frac{1}{N^2}\sum_{x\in\mathbb{T}_N} \omega_x^4(s)\, ds\right] = 0. \tag{III.61}$$

If μ^N is a convex combination of Gibbs local equilibrium states, then the same argument of Chapter II (Section 3) shows that the law of the process remains a convex combination of Gaussian measures, and that (III.61) holds.

Contrary to the velocity-flip model, we do not need to assume a good control of every energy moment if we expect the usual entropy method to work. This technical need was only due to the relative entropy method.

With Assumptions III.35 and III.36 we could try to prove Theorem III.34 by using the entropy method, which permits to consider more general initial profiles (for example, the profile β_0 can be assumed only bounded, not smooth). The usual technical points of this well-known procedure are the one and two-blocks estimates, as well as tightness. In this model, they are somehow easy to prove because the diffusion coefficient is constant, and there is no need to prove its regularity.

5.2 Replacement of the Current by a Gradient

In this subsection we recall the main steps of the usual entropy method, and explain which ones can be proved for our system. We fix the disorder $\mathbf{m} = \{m_x\}_{x\in\mathbb{T}_N}$ and $T > 0$. For $t \in [0, T]$, we denote by $\mathcal{Z}^N_{t,\mathbf{m}}$ the empirical energy field defined as

$$\mathcal{Z}^N_{t,\mathbf{m}}(H) = \frac{1}{N}\sum_{x\in\mathbb{T}_N} H\left(\frac{x}{N}\right)\omega_x^2(t),$$

where $\mathrm{H} : \mathbb{T} \longrightarrow \mathbb{R}$ is a smooth function. We rewrite $\mathcal{Z}^{\mathrm{N}}_{t,\mathbf{m}}(\mathrm{H})$ as

$$\mathcal{Z}^{\mathrm{N}}_{t,\mathbf{m}}(\mathrm{H}) = \mathcal{Z}^{\mathrm{N}}_{0,\mathbf{m}}(\mathrm{H}) + \int_0^t \sum_{x \in \mathbb{T}_{\mathrm{N}}} \nabla_{\mathrm{N}} \mathrm{H}\left(\frac{x}{\mathrm{N}}\right) j_{x,x+1}(\mathbf{m},\omega)(s)\mathrm{d}s + \mathfrak{M}^{\mathrm{N}}_{t,\mathbf{m}}(\mathrm{H}),$$

where $\mathfrak{M}^{\mathrm{N}}_{t,\mathbf{m}}(\mathrm{H})$ is a martingale. The strategy consists in replacing the current $j_{x,x+1}$ by the linear combination given in Theorem III.17. For that purpose, for any $f \in \mathcal{Q}$ we rewrite

$$\mathcal{Z}^{\mathrm{N}}_{t,\mathbf{m}}(\mathrm{H}) = \mathcal{Z}^{\mathrm{N}}_{0,\mathbf{m}}(\mathrm{H}) + \int_0^t \mathrm{D}\mathcal{Z}^{\mathrm{N}}_{s,\mathbf{m}}(\Delta_{\mathrm{N}}\mathrm{H})\mathrm{d}s + \mathfrak{I}^{1,\mathrm{N}}_{t,\mathbf{m},f}(\mathrm{H}) + \mathfrak{I}^{2,\mathrm{N}}_{t,\mathbf{m},f}(\mathrm{H}) + \mathfrak{M}^{\mathrm{N}}_{t,\mathbf{m}}(\mathrm{H}),$$

where

$$\mathfrak{I}^{1,\mathrm{N}}_{t,\mathbf{m},f}(\mathrm{H}) = \int_0^t \sum_{x \in \mathbb{T}_{\mathrm{N}}} \nabla_{\mathrm{N}} \mathrm{H}\left(\frac{x}{\mathrm{N}}\right) \Big[j_{x,x+1}(\mathbf{m},\omega)(s) - \mathrm{D}(\omega^2_{x+1} - \omega^2_x)(s) - \mathcal{L}^{\mathbf{m}}_{\mathrm{N}}(\tau_x f)(\mathbf{m},\omega)(s) \Big] \mathrm{d}s,$$

$$\mathfrak{I}^{2,\mathrm{N}}_{t,\mathbf{m},f}(\mathrm{H}) = \int_0^t \sum_{x \in \mathbb{T}_{\mathrm{N}}} \nabla_{\mathrm{N}} \mathrm{H}\left(\frac{x}{\mathrm{N}}\right) \mathcal{L}^{\mathbf{m}}_{\mathrm{N}}(\tau_x f)(\mathbf{m},\omega)(s)\mathrm{d}s.$$

Theorem III.34 would follow from the three lemmas below.

Lemma III.37. *For every smooth function* $\mathrm{H} : \mathbb{T} \longrightarrow \mathbb{R}$ *and every* $\delta > 0$*,*

$$\lim_{\mathrm{N}\longrightarrow\infty} \mathbb{P}^{\mathbf{m}}_{\mathrm{N}} \left[\sup_{[0,\mathrm{T}]} \left| \mathfrak{M}^{\mathrm{N}}_{t,\mathbf{m}}(\mathrm{H}) \right| > \delta \right] = 0.$$

Lemma III.38. *For every* $f \in \mathcal{Q}$ *and every smooth function* $\mathrm{H} : \mathbb{T} \longrightarrow \mathbb{R}$*,*

$$\limsup_{\mathrm{N}\longrightarrow\infty} \mathbb{E}_{\mathbb{P}^{\mathbf{m}}_{\mathrm{N}}} \left[\left| \mathfrak{I}^{2,\mathrm{N}}_{t,\mathbf{m},f}(\mathrm{H}) \right| \right] = 0.$$

Lemma III.39. *There exists a sequence of functions* $\{f_k\}_{k\in\mathbb{N}} \in \mathcal{Q}$ *such that, for every smooth function* $\mathrm{H} : \mathbb{T} \longrightarrow \mathbb{R}$*,*

$$\lim_{k\longrightarrow\infty} \lim_{\mathrm{N}\longrightarrow\infty} \mathbb{E}\left[\mathbb{E}_{\mathbb{P}^{\mathbf{m}}_{\mathrm{N}}} \left[\left| \mathfrak{I}^{1,\mathrm{N}}_{t,\mathbf{m},f_k}(\mathrm{H}) \right| \right] \right] = 0.$$

Lemma III.37 and Lemma III.38 can be proved, following the same standard arguments given for example in [49, Section 7]. We need the energy moment estimate (III.61) in Lemma III.37, in the computation of the quadratic variation of the martingale. The next subsection is devoted to highlight what fails in Lemma III.39, which should be related to the results of Sections 2.1, 2.3 and 2.2.

Remark *5.1.* Conditioned to proving Lemma III.39, Theorem III.34 would follow: recall that $\mathcal{Q}^{\mathbf{m}}_{\mathrm{N}}$ is the distribution on the path space $\mathcal{D}\left([0,\mathrm{T}],\mathcal{M}_1\right)$ of the process π^{N}_t. Following the same argument as for the generalized exclusion process in [49, Section 7.6], we can show that the sequence $\left\{\mathcal{Q}^{\mathbf{m}}_{\mathrm{N}}, \mathrm{N} \geqslant 1\right\}$ is weakly relatively compact. It remains to prove that every limit point $\mathcal{Q}^{\mathbf{m}}_{*}$ is concentrated on absolutely continuous paths $\mathbf{e}(t,\mathrm{d}u) = \mathbf{e}(t,u)\mathrm{d}u$ whose densities are solutions of the hydrodynamic equations given in Theorem III.34. It could be seen from Lemma III.39 by following the proof of [49, Theorem 7.0.1].

5.3 Failed Variance Estimate

In this paragraph we fix the disorder $\mathbf{m}$, and we erase it whenever no confusion arises. We are going to recall here the usual main steps of the entropy method. We rewrite $\mathfrak{I}^{1,N}_{t,\mathbf{m},f}(H)$ as

$$\mathfrak{I}^{1,N}_{t,\mathbf{m},f}(H) = \int_0^t \sum_{x\in\mathbb{T}_N} G\left(\frac{x}{N}\right) \tau_x \varphi(\mathbf{m},\omega)(s)ds,$$

where

$$\begin{cases} \varphi(\mathbf{m},\omega) := j_{0,1}(\mathbf{m},\omega) - D(\omega_1^2-\omega_0^2) - \mathcal{L}_N^{\mathbf{m}}(f)(\mathbf{m},\omega) \\ G\left(\frac{x}{N}\right) := \nabla_N H\left(\frac{x}{N}\right). \end{cases}$$

Entropy inequality – In Lemma III.39, note that the expectation with respect to the law of the process $\mathbb{P}_N^{\mathbf{m}}$ is taken. There is *a priori* no hope to get any estimate of this expectation, apart from the well-known entropy inequality. More precisely, let us denote by $X_N^f(\omega)$ the following quantity:

$$X_N^f(\omega) := \sum_{x\in\mathbb{T}_N} G\left(\frac{x}{N}\right)\tau_x\varphi(\omega).$$

From the entropy inequality, we obtain

$$\mathbb{E}_{\mathbb{P}_N^{\mathbf{m}}}\left[\left|\int_0^T X_N^f(\omega)(s)\,ds\right|\right] \leqslant \frac{1}{\alpha N} H(\mathbb{P}_N^{\mathbf{m}}|\mu_\beta^N) + \frac{1}{\alpha N}\log \mathbb{E}_{\mu_\beta^N}\left[\exp\left(\alpha N\left|\int_0^T X_N^f(\omega)(s)\,ds\right|\right)\right],$$

for all $\alpha > 0$. Since the entropy is decreasing in time, we know that, for all disorder field $\mathbf{m}$, $H(\mathbb{P}_N^{\mathbf{m}}|\mu_\beta^N)$ is bounded. From the arbitrariness of α, we are reduced to investigate the convergence of the second term in the previous right-hand side.

Feynman-Kac formula – Usually, the purpose is to reduce the dynamics problem to the study of the largest eigenvalue for a small perturbation of the generator $N^2\mathcal{S}_N$. This reduction relies on Feynman-Kac formula and on a variational formula for the largest eigenvalue of a symmetric operator. By Feynman-Kac formula,

$$\mathbb{E}_{\mu_\beta^N}\left[\exp\left\{N\int_0^T X_N^f(\omega)(s)\,ds\right\}\right] \leqslant \exp\left\{\int_0^T \lambda_N(s)\,ds\right\}$$

where $\lambda_N(s)$ is the largest eigenvalue of the symmetric operator $N^2\mathcal{S}_N(\cdot) + NX_N^f(\omega)$. From the variational formula for the largest eigenvalue of an operator in a Hilbert space, we also know that

$$\lambda_N(s) \leqslant \sup_g \left\{\left\langle NX_N^f(\cdot)\,g(\cdot)\right\rangle_\beta - N^2\mathcal{D}_N(\mu_\beta;\sqrt{g})\right\}$$

where the supremum is taken over all measurable functions g which are densities with respect to μ_β^N. In particular,

$$\frac{1}{N}\log \mathbb{E}_{\mu_\beta^N}\left[\exp\left\{\int_0^T NX_N^f(\omega)(s)\,ds\right\}\right] \leqslant \int_0^T \sup_g\left\{\left\langle X_N^f(\omega)\; g(\omega)\right\rangle_\beta - N\mathcal{D}_N(\mu_\beta;\sqrt{g})\right\}ds.$$

Reduction to microscopic blocks – With the same spirit of the one-block estimate presented in Chapter II, it is then crucial to replace microscopic quantities with their spatial averages. Here, with the same ideas of [49], we can replace

$$\begin{aligned} j_{0,1} &\quad \text{with} \quad \frac{1}{2\ell+1}\sum_{x\in\Lambda_\ell} j_{x,x+1} \\ \omega_0^2 &\quad \text{with} \quad \frac{1}{2\ell+1}\sum_{x\in\Lambda_\ell} \omega_x^2 \\ \mathcal{L}_{\mathrm{N}}^{\mathbf{m}}(f)(\omega) &\quad \text{with} \quad \frac{1}{2\ell_f+1}\sum_{x\in\Lambda_{\ell_f}} \mathcal{L}_{s_f+1}^{\mathbf{m}}(\tau_x f) \end{aligned}$$

where $\ell_f = \ell - s_f - 1$ so that $\mathcal{L}_{s_f+1}(\tau_y f)$ is $\mathcal{F}_{\Lambda_\ell}$-mesurable for every $y \in \Lambda_{\ell_f}$. Let us introduce the following notation

$$\mathrm{W}^{f,\ell} := \frac{1}{2\ell'+1}\sum_{y\in\Lambda_{\ell'}} j_{y,y+1} + \mathrm{D}\left[\frac{1}{2\ell+1}\sum_{|x|\leqslant\ell}\omega_x^2 - \frac{1}{2\ell+1}\sum_{|x-1|\leqslant\ell}\omega_x^2\right] - \frac{1}{2\ell_f+1}\sum_{y\in\Lambda_{\ell_f}}\mathcal{L}_{s_f+1}(\tau_y f) \tag{III.62}$$

with $\ell' = \ell - 1$. Finally, thanks to the regularity of the function G and the fact that D is constant, we are able to reduce Lemma III.39 to Lemma III.40 below. We also need to perform a cut-off in order to control high energy values, and this is valid thanks to (III.61).

Lemma III.40. *For all $\delta > 0$,*

$$\inf_{f\in\mathcal{Q}}\limsup_{\ell\longrightarrow\infty}\limsup_{\mathrm{N}\longrightarrow\infty}\sup_{g}\left\{\left\langle \mathrm{Y}_{\mathrm{N},\ell}^{f}(\omega)\, g(\omega)\right\rangle_\beta - \delta \mathrm{N}\mathcal{D}_{\mathrm{N}}(\mu_\beta;\sqrt{g})\right\} \leqslant 0, \tag{III.63}$$

where

$$\mathrm{Y}_{\mathrm{N},\ell}^{f}(\omega) := \sum_{x\in\mathbb{T}_{\mathrm{N}}} \mathrm{G}\left(\frac{x}{\mathrm{N}}\right)\tau_x \mathrm{W}^{f,\ell}(\omega).$$

Reduction to a variance estimate – Then, the challenge is to reduce the proof of Lemma III.40 to the following result:

$$\inf_{f\in\mathcal{Q}}\lim_{\ell\longrightarrow\infty} 2\ell \times \mathbb{E}\left[\left\langle \left(-\mathcal{S}_{\Lambda_\ell}\right)^{-1}\mathrm{W}^{f,\ell}, \mathrm{W}^{f,\ell}\right\rangle_\beta\right] = 0 \tag{III.64}$$

This convergence holds, since it is equivalent to the conclusion of Theorem III.17, where the diffusion coefficient D is defined through the non gradient approach. Here is the main obstacle. If we follow the strategy given in [49, Section 7.3], we can bound the supremum in (III.63) by the largest eigenvalue of $\mathcal{S}_{\Lambda_\ell} + \mathbf{b}\mathrm{W}^{f,\ell}$ where $\mathbf{b}$ is a small constant. In order to estimate this largest eigenvalue, we usually use a perturbation method which provides a bound on the largest eigenvalue in terms of the variance of $\mathrm{W}^{f,\ell}$. This can not be proved, and suggests that the entropy inequality together with the Feynman-Kac formula are not the good tools to prove the hydrodynamic limits for systems which do not have a spectral gap (see the last concluded section).

We conclude this section by explaining why the perturbation theory does not work. Let us try to prove Lemma III.40. Since μ_β is translation invariant, we may rewrite $\langle \mathrm{Y}_{\mathrm{N}}^{f,\ell}(\cdot)\, g(\cdot)\rangle_\beta$ as

$$\sum_{x\in\mathbb{T}_{\mathrm{N}}}\left\langle \mathrm{G}\left(\frac{x}{\mathrm{N}}\right)\mathrm{W}^{f,\ell}(\omega)\tau_{-x}g(\omega)\right\rangle_\beta .$$

Since the Dirichlet form is convex, the supremum in (III.63) is bounded from above by

$$\frac{\delta N}{2\ell}\sum_{x\in\mathbb{T}_N}\sup_g\left\{\mathbf{b}\left\langle W^{f,\ell}\, g\right\rangle_\beta-\mathcal{D}_\ell(\mu_\beta;\sqrt{g})\right\},\tag{III.65}$$

where the constant $\mathbf{b}=\mathbf{b}(x,\ell,\delta,N)$ satisfies

$$|\mathbf{b}|:=\left|G\left(\frac{x}{N}\right)\frac{2\ell}{\delta N}\right|\leqslant\|G\|_\infty\frac{2\ell}{\delta N}.$$

Let us denote by $\lambda_{N,\ell,f}$ this last supremum inside the sum (III.65), which does not depend on x. We consider a sequence $\{g_k\}_{k\in\mathbb{N}}$ that approaches this supremum, such that

$$\lim_{k\longrightarrow\infty}\left\langle\sqrt{g}_k,\left(\mathcal{S}_{\Lambda_\ell}+\mathbf{b}W^{f,\ell}\right)\sqrt{g}_k\right\rangle_\beta=\lambda_{N,\ell,f}.$$

The idea of the perturbation theory is to expand $\sqrt{g}_k$ around the constant value 1. We write

$$\left\langle\sqrt{g}_k,(\mathcal{S}_{\Lambda_\ell}+\mathbf{b}W^{f,\ell})\sqrt{g}_k\right\rangle_\beta=\mathbf{b}\Big(\left\langle W^{f,\ell}\right\rangle_\beta+2\left\langle W^{f,\ell}(\sqrt{g}_k-1)\right\rangle_\beta+\left\langle W^{f,l}(\sqrt{g}_k-1)^2\right\rangle_\beta\Big)-\mathcal{D}_\ell(\mu_\beta;\sqrt{g}_k).\tag{III.66}$$

We know that $\left\langle W^{f,\ell}\right\rangle_\beta=0$, and we use the Cauchy-Schwarz inequality for the scalar product $\langle\cdot,(-\mathcal{S}_{\Lambda_\ell})\cdot\rangle_\beta$ in the second term. We obtain that (III.66) is bounded, for every $A>0$, by

$$\mathbf{b}\left(\frac{\mathbf{b}}{A}\left\langle W^{f,\ell},(-\mathcal{S}_{\Lambda_\ell})^{-1}W^{f,\ell}\right\rangle_\beta+\frac{A}{\mathbf{b}}\mathcal{D}_\ell(\mu_\beta;\sqrt{g}_k)\right)+\mathbf{b}\left\langle W^{f,\ell}(\sqrt{g}_k-1)^2\right\rangle_\beta-\mathcal{D}_\ell(\mu_\beta;\sqrt{g}_k).$$

It remains to bound the third term in the expression above. This could be done if we had the following lemma.

Lemma III.41. *There exists a constant* $C:=C(\ell,f,\beta,\gamma,\lambda)$ *such that, for every* $g\geqslant 0$,

$$\left\langle W^{f,\ell}(\sqrt{g}-1)^2\right\rangle_\beta\leqslant C\mathcal{D}_\ell(\mu_\beta;\sqrt{g}).\tag{III.67}$$

As in Section 4, we could try to use the fact that $W^{f,\ell}$ is a quadratic function. Even this fact is not helpful, and we give now a counter-example to this last lemma. We denote by H_n the normalized one-variable Hermite polynomial of degree $n\geqslant 3$ (see Appendix 2.2.1). Let us consider

$$\begin{cases}\sqrt{g}(\omega)=|H_n(\omega_0)|\\ W^{f,\ell}(\omega)=H_2(\omega_0)=\omega_0^2-1.\end{cases}$$

Let us notice that $\langle H_n^2\rangle_\beta=1$, and $\langle H_2\rangle_\beta=0$, so that the two test functions g and $W^{f,\ell}$ satisfy all expected conditions. By using the recursive relation

$$H_{n+1}(\omega_0)=\omega_0H_n(\omega_0)-nH_{n-1}(\omega_0),$$

we get for the left-hand side of (III.67),

$$\begin{aligned}\left\langle H_2(|H_n|-1)^2\right\rangle_\beta&=\left\langle\omega_0^2H_n^2(\omega_0)\right\rangle_\beta-\left\langle H_n^2\right\rangle_\beta-2\left\langle H_2|H_n|\right\rangle_\beta+\left\langle H_2\right\rangle_\beta\\&=\left\langle H_{n+1}^2+2nH_{n+1}H_{n+1}+n^2H_{n-1}^2\right\rangle_\beta-1-2\left\langle H_2|H_n|\right\rangle_\beta\\&=1+n^2-1-2\left\langle H_2|H_n|\right\rangle_\beta\geqslant n^2-2.\end{aligned}$$

Above the last equality comes from the orthonormality of the polynomial basis, and the last inequality is a consequence of the Cauchy-Schwarz inequality $\langle H_2 | H_n | \rangle_\beta^2 \leqslant \langle H_2^2 \rangle_\beta \langle H_n^2 \rangle_\beta = 1$. Let us assume that there exists a constant $C > 0$ which does not depend on n such that

$$n^2 - 2 \leqslant \left\langle H_2(|H_n| - 1)^2 \right\rangle_\beta \leqslant C\mathcal{D}_\ell(\mu_\beta; |H_n|).$$

From the convexity of the Dirichlet form, we have

$$\mathcal{D}_\ell(\mu_\beta; |H_n|) \leqslant \mathcal{D}_\ell(\mu_\beta; H_n).$$

In the case where n is an even positive integer, the flip noise gives a zero contribution to the Dirichlet form, and then, for all n even, we have

$$\mathcal{D}_\ell(\mu_\beta; H_n) = \frac{\lambda}{2} \left\langle \big(H_n(\omega_1) - H_n(\omega_0)\big)^2 \right\rangle_\beta = \lambda \langle H_n^2 \rangle_\beta - \lambda \left\langle H_n(\omega_0) H_n(\omega_1) \right\rangle_\beta = \lambda.$$

In the last equality, we use the fact that H_n is unitary, and that $H_n(\omega_0)H_n(\omega_1)$ constitutes another element of the Hermite polynomial basis, then is orthogonal to the constant polynomial 1. Letting n go to infinity, we obtain a contradiction to (III.67).

Ergodic decomposition – Another idea would be to use the ergodic decomposition described in Subsection 2.1.2. The generator $\mathcal{S}_\ell$ restricted to finite boxes does not have a spectral gap, but it becomes ergodic when restricted to each orbit $\mathcal{G}_{\mathbf{x}}^{N,\beta}$. However, this approach fails, because the space is not compact, and we need to disintegrate the measure μ_β with respect to all energy levels in $(0, +\infty)$. This enforces us to introduce a cut-off in the variational formula giving the largest eigenvalue. In other words, an indicator function $\mathbf{1}\{|\omega_x| \leqslant E_0\}$ will appear in front of $W^{f,\ell}$. Finally, we will have to deal with functions of the configurations that are not quadratic any more, and we do not know how to prove the convergence result (III.64) for general functions.

5.4 Conclusion

Even if the non-gradient method can be applied in some cases when the spectral gap does not hold, (and then the diffusion coefficient is well-defined), this does not straightforwardly imply the hydrodynamic limits.

In order to derive the hydrodynamic theorem, we would need to bypass the entropy inequality together with the Feynman-Kac formula. The entropy inequality is however a convenient mean to transform the averages w.r.t. the unknown law μ_t^N into equilibrium averages w.r.t. μ_β^N, which are more easily tractable. The same problem would arise in the relative entropy method, because of the entropy inequality.

CHAPTER IV

Macroscopic Fluctuations: between a Diffusive Behavior and a Fractional Laplacian

Contents

We study the macroscopic fluctuations of an energy conserving chain of oscillators at equilibrium. The harmonic Hamiltonian dynamics is perturbed by two degenerate stochastic noises, one of them vanishing with the size of the chain. The limit of the energy fluctuation field depends on the evanescent speed of the random perturbation. In particular we obtain two very different regimes for the energy transport.

This chapter is based on a collaborative work with C. Bernardin, P. Gonçalves, M. Jara and M. Sasada.

1 The Homogeneous Harmonic Chain in the Evanescent Flip Noise Limit

1.1 Model and Notations

We consider an infinite chain of harmonic oscillators at equilibrium. There is no disorder (meaning that all masses are constant, equal 1 for simplicity). The velocities evolve according to the same Hamiltonian dynamics described in Chapter III, Section 1.4, namely the harmonic oscillators are perturbed by the exchange noise and the flip noise. We recall the following notations: the space of configurations is given by $\Omega = \mathbb{R}^{\mathbb{Z}}$, and we say that a function $f : \Omega \longrightarrow \mathbb{R}$ is *local* if there exists a finite subset Λ of $\mathbb{Z}$ such that the support of f is included in Λ. We define the generator

$$\mathcal{L}_n = \mathcal{A} + \gamma_n \mathcal{S}^{\text{flip}} + \lambda \mathcal{S}^{\text{exch}}$$

defined for all smooth local bounded functions $f : \Omega \longrightarrow \mathbb{R}$ by

$$\mathcal{A}f(\omega) = \sum_{x\in\mathbb{Z}} \big(\omega_{x+1} - \omega_{x-1}\big) \frac{\partial f}{\partial \omega_x}(\omega),$$

$$\mathcal{S}^{\text{flip}} f(\omega) = \sum_{x\in\mathbb{Z}} f(\omega^x) - f(\omega),$$
$$\mathcal{S}^{\text{exch}} f(\omega) = \sum_{x\in\mathbb{Z}} f(\omega^{x,x+1}) - f(\omega).$$

The configuration ω^x is the configuration obtained from ω by flipping the momentum of particle x:

$$(\omega^x)_z = \begin{cases} \omega_z & \text{if } z \neq x, \\ -\omega_x & \text{if } z = x. \end{cases}$$

The configuration $\omega^{x,x+1}$ is obtained from ω by exchanging the momenta of particles x and $x+1$:

$$(\omega^{x,x+1})_z = \begin{cases} \omega_z & \text{if } z \neq x, x+1, \\ \omega_{x+1} & \text{if } z = x, \\ \omega_x & \text{if } z = x+1. \end{cases}$$

We denote by $\mathcal{S}_n := \gamma_n \mathcal{S}^{\text{flip}} + \lambda \mathcal{S}^{\text{exch}}$ the total generator of the noise, where $\gamma_n, \lambda > 0$ are two positive parameters which regulate the respective strengths of noises. We assume that there exist two constants $c > 0$ and $b \geqslant 0$ such that

$$\gamma_n = \frac{c}{n^b}.$$

The Gibbs measures are given by the Gaussian product probability measures

$$\mu_\beta(\mathrm{d}\omega) = \prod_{x\in\mathbb{Z}} \sqrt{\frac{\beta}{2\pi}} \exp\Big(- \frac{\beta \omega_x^2}{2}\Big) \mathrm{d}\omega_x,$$

where $\beta > 0$ states for the inverse temperature. In the following, the expectation of a function f with respect to μ_β is denoted by $\langle f \rangle_\beta$. The current of energy satisfies $\mathcal{L}_n(\omega_x^2) = \nabla j_{x-1,x}$ and is explicitely given by

$$j_{x,x+1}(\omega) = j^{\text{A}}_{x,x+1}(\omega) + j^{\text{S}}_{x,x+1}(\omega) = 2\omega_x\omega_{x+1} + \lambda(\omega_{x+1}^2 - \omega_x^2). \tag{IV.1}$$

Let us notice that the current does not depend on n (since it does not involve the intensity γ_n of the flip noise).

We consider the dynamics starting with an equilibrium Gibbs measure at a fixed temperature β^{-1} in a subdiffusive time scale tn^a, $0 < a < 2$. The existence of the infinite dynamics under this initial distribution can be proved following by instance [40, 57]. We denote by $\mathcal{C}_c^\infty(\mathbb{R})$ the set of smooth functions with compact support. We define the energy fluctuation field $\{\mathcal{E}_t^n \, ; \, t \in [0,\mathrm{T}]\}$ as the $\mathcal{C}_c^\infty(\mathbb{R})$-valued process given by

$$\mathcal{E}_t^n(f) := \frac{1}{\sqrt{n}} \sum_{x\in\mathbb{Z}} f\Big(\frac{x}{n}\Big) \big\{\omega_x^2(tn^a) - \beta^{-1}\big\}.$$

Given two functions $f,h\in\mathcal{C}_c^\infty(\mathbb{R})$, we look at the evolution with t of the following quantity

$$\begin{aligned}\sigma_t^n(f,h) &:= \big\langle \mathcal{E}_t^n(f)\,;\,\mathcal{E}_0^n(h)\big\rangle_\beta\\ &= \frac{1}{n}\sum_{x,y\in\mathbb{Z}} f\Big(\frac{x}{n}\Big)h\Big(\frac{y}{n}\Big)\Big\langle\Big\{\omega_x^2(tn^a)-\beta^{-1}\Big\}\times\Big\{\omega_y^2(0)-\beta^{-1}\Big\}\Big\rangle_\beta\\ &= \frac{1}{n}\sum_{y,z\in\mathbb{Z}} f\Big(\frac{y+z}{n}\Big)h\Big(\frac{y}{n}\Big)\Big\langle\omega_z^2(tn^a)\times\Big\{\omega_0^2(0)-\beta^{-1}\Big\}\Big\rangle_\beta\end{aligned}$$

when n goes to infinity.

1.2 Statement of the Results

We briefly summarize the results of that chapter:

1) For any $b\geqslant 0$, the energy fluctuation field does not evolve up to the time scale $tn^{4/3}$. We are not going to write the proof here, since the complete argument is given in [11, Theorem 2].

2) If $0\leqslant b<2/3$, the fluctuation field does not evolve up to the time scale $tn^{2-b/2}$. In the time scale $tn^{2-b/2}$, the limit of the energy fluctuation field is given by a standard infinite dimensional Ornstein Uhlenbeck (OU) process independent of b.

   Precisely, a small value of b means that the velocity-flip does not vanish too fast, and then the energy behaves diffusively in the sense that energy fluctuations of the system at equilibrium evolve according to a linear heat equation, as expected from the results of Chapter III. The strategy for proving such a behavior is based on a fluctuation-dissipation decomposition of the microscopic energy currents $j_{x,x+1}$. More precisely, we are able to write explicitely the current in the form $\nabla(g)+\mathcal{L}(h)$, where g and h are two functions of the configuration ω. With such a decomposition it is possible to derive macroscopically the evolution of the energy and identify the thermal conductivity. Here, the fluctuation-dissipation decomposition is non-local, and convergence is proved thanks to accurate estimates.

3) If $b\in(1,+\infty]$, the energy fluctuation field does not evolve up to the time scale $tn^{3/2}$. In the time scale $tn^{3/2}$, the limit of the energy fluctuation field is given by an infinite dimensional fractional Ornstein-Uhlenbeck (fOU) process independent of b.

   Precisely, a big value of b means that the velocity-flip disappears quickly enough so as to recover the same behavior as the case $\gamma=0$, which is proved in [12]. The proof consists in adapting the argument in [12] to the case where an extra stochastic perturbation is added.

The case $b\in[2/3\,;1]$ remains open. The conjecture is not easy to guess. One possible behavior is the following: $b=1$ would be a field interpolating the standard OU process and the fOU process, and $b\in[2/3;1)$ would correspond to the same diffusive behavior as for $b\in[0;2/3)$. In any cases, by scaling considerations one can see that the limiting energy field

$$\mathcal{E}(t,x\,;\,c,b):=\lim_{n\longrightarrow\infty}\mathcal{E}_t^n$$

in the time scale tn^a shall satisfy the scaling relation (in law)

$$\mathcal{E}(t,x\,;\,c,b)=\varepsilon^{1/2}\mathcal{E}(t\varepsilon^a,\varepsilon x\,;\,c\varepsilon^{-b},b),\quad \varepsilon>0.$$

2 The Energy Fluctuation Field for $b < 2/3$

In this section we prove

THEOREM IV.1. *Let us assume that $a = 2 - b/2$ and $b < 2/3$. Let f and h be two functions in $\mathcal{C}_c^\infty(\mathbb{R})$ and let us fix $t > 0$. Then,*

$$\lim_{n\longrightarrow\infty} \sigma_t^n(f,h) = \frac{\chi(\beta)}{\sqrt{4\pi t\kappa}} \iint_{\mathbb{R}^2} \mathrm{d}u\mathrm{d}v\, f(u)h(v) \exp\Big(-\frac{(u-v)^2}{4t\kappa}\Big),$$

where $\chi(\beta)$ is the compressibility defined as $\chi(\beta) := \big\langle \omega_0^4\big\rangle_\beta - \big\langle \omega_0^2\big\rangle_\beta^2 = 2\beta^{-2}$ and

$$\kappa = \begin{cases} \dfrac{1}{\sqrt{2\lambda c}} & \text{if } b \neq 0, \\ \lambda + \dfrac{1}{\sqrt{2\lambda c}} & \text{if } b = 0. \end{cases}$$

With the same ideas of Chapter III, Section 4, one can also prove that the fluctuation field $\mathcal{E}_t^n$ converges in law to the infinite dimensional Ornstein Uhlenbeck process $\mathcal{E}_t$ solution of the linear stochastic partial differential equation

$$\partial_t \mathcal{E} = \kappa \partial_u^2 \mathcal{E}\,\mathrm{d}t + \sqrt{2\kappa\chi(\beta)}\,\partial_u \mathrm{B}(u,t),$$

where B is the standard normalized space-time white noise. This extension to Theorem IV.1 is standard, and we refer for instance to [49] for more details.

2.1 Fluctuation-dissipation Equation

In the sequel, we erase the dependence on the parameters n, b and c whenever no confusion arises. We consider a function u in the form

$$u = \sum_{x\in\mathbb{Z}} \sum_{k\geqslant 1} \rho_k(x)\omega_x\omega_{x+k}, \tag{IV.2}$$

where $\{\rho_k(x)\,;\, x \in \mathbb{Z}, k \geqslant 1\}$ is a real sequence that satisfies the condition

$$\sum_{x\in\mathbb{Z}} \sum_{k\geqslant 1} |\rho_k(x)|^2 < +\infty, \tag{IV.3}$$

so that u is a function in $\mathbf{L}^2(\mu_\beta)$. Observe first that $\mathcal{A}u$ is a sum of gradient terms. Indeed, we have

$$\mathcal{A}u = \sum_{x\in\mathbb{Z}} \sum_{k\geqslant 1} \rho_k(x)\,\nabla\big[\omega_{x-1}\omega_{x+k} + \omega_x\omega_{x+k-1}\big],$$

where the discrete gradient ∇ is defined for a function $u : \Omega \longrightarrow \mathbb{R}$ as

$$\nabla u(\omega) := \tau_1 u(\omega) - u(\omega).$$

Hereafter, τ_x denotes the translated operator that acts on u as $(\tau_x u)(\omega) := u(\tau_x\omega)$, and $\tau_x\omega$ is the configuration obtained from ω by shifting: $(\tau_x\omega)_y = \omega_{x+y}$. Our aim is now to solve the equation

$$(\gamma_n \mathcal{S}^{\text{flip}} + \lambda \mathcal{S}^{\text{exch}})u = 2\omega_0\omega_1 = j^{\text{A}}_{0,1}(\omega),$$

and then it will follow that

$$\mathcal{L}_n u - v = j^{\text{A}}_{0,1} \tag{IV.4}$$

where

$$v = \mathcal{A}u = \sum_{x\in\mathbb{Z}}\sum_{k\geqslant 1} \rho_k(x)\,\nabla\big[\omega_{x-1}\omega_{x+k} + \omega_x\omega_{x+k-1}\big]$$

is a sum of gradient functions. One can check that v and $\mathcal{L}_n u$ are also elements of $\mathbf{L}^2(\mu_\beta)$. Straightforward computations show that

$$(\gamma_n \mathcal{S}^{\text{flip}} + \lambda \mathcal{S}^{\text{exch}})u = \sum_{x\in\mathbb{Z}}\sum_{k\geqslant 1} \mathrm{F}_k(x)\omega_x\omega_{x+k},$$

where, for $x \in \mathbb{Z}$,

$$\begin{cases} \mathrm{F}_1(x) = -2(2\gamma_n+\lambda)\rho_1(x) + \lambda(\rho_2(x)+\rho_2(x-1)), \\ \mathrm{F}_k(x) = -4(\gamma_n+\lambda)\rho_k(x) + \lambda\Big(\rho_{k-1}(x)+\rho_{k-1}(x+1)+\rho_{k+1}(x)+\rho_{k+1}(x-1)\Big), \quad k\geqslant 2. \end{cases}$$

When identifying the coefficients in front of the different terms, we see that we need

$$\mathrm{F}_k(x) = 2\mathbf{1}_{\{k=1,x=0\}}. \tag{IV.5}$$

We use the Fourier transform (V.28) of square summable sequences defined in Appendix 2.3.1, and we reformulate the conditions (IV.5) for $\theta \in \mathbb{T}$ in an equivalent way:

$$\begin{cases} -2(2\gamma_n+\lambda)\widehat{\rho}_1(\theta) + \lambda(1+e^{2i\pi\theta})\widehat{\rho}_2(\theta) = 2, \\ -4(\gamma_n+\lambda)\widehat{\rho}_k(\theta) + \lambda(1+e^{-2i\pi\theta})\widehat{\rho}_{k-1}(\theta) + \lambda(1+e^{2i\pi\theta})\widehat{\rho}_{k+1}(\theta) = 0, \quad k\geqslant 2. \end{cases} \tag{IV.6}$$

By Parseval relation, condition (IV.3) is equivalent to

$$\sum_{k\geqslant 1}\int_{\mathbb{T}} |\widehat{\rho}_k(\theta)|^2\,\mathrm{d}\theta < +\infty.$$

It is then easy to show that (IV.6) and the above integrability condition lead to

$$\widehat{\rho}_k(\theta) = \widehat{\rho}_1(\theta)(\mathrm{X}(\theta))^{k-1},$$

with

$$\mathrm{X}(\theta) = \frac{2}{1+e^{2i\pi\theta}}\left\{1+\frac{\gamma_n}{\lambda} - \sqrt{\Big(1+\frac{\gamma_n}{\lambda}\Big)^2 - \cos^2(\pi\theta)}\right\}$$

and

$$\widehat{\rho}_1(\theta) = -\frac{1}{\gamma_n + \lambda\sqrt{\Big(1+\frac{\gamma_n}{\lambda}\Big)^2 - \cos^2(\pi\theta)}}.$$

In the following, we will need sharp estimates on $\widehat{\rho}_1$ and X, precisely:

Lemma IV.2. *For $\theta \in \mathbb{T}$, and for sufficiently large n, we have*

$$|X(\theta)| \leqslant \frac{|\cos(\pi\theta)|}{1+\sqrt{\frac{\gamma_n}{\lambda}}} \quad \text{and} \quad |\widehat{\rho}_1(\theta)| \leqslant \frac{1}{\lambda\sqrt{\frac{\gamma_n}{\lambda}+\sin^2(\pi\theta)}}.$$

Proof. We only prove the first estimate, the second one is straightforward. We define $C := \gamma_n/\lambda$. Then

$$|X(\theta)| = \frac{1}{|\cos(\pi\theta)|}\left\{1+C-\sqrt{(1+C)^2-\cos^2(\pi\theta)}\right\}.$$

For n large enough, we have $C<1$, and then $(1+C)^2 \leqslant (1+C)(1+\sqrt{C})$. This implies

$$1-\frac{\cos^2(\pi\theta)}{(1+C)(1+\sqrt{C})} \leqslant 1-\frac{\cos^2(\pi\theta)}{(1+C)^2} \leqslant \sqrt{1-\frac{\cos^2(\pi\theta)}{(1+C)^2}},$$

and the result follows straightforwardly. □

2.2 Sketch of the proof of Theorem IV.1

Let us write

$$\sigma_t^n(f,h) = \sigma_0^n(f,h) - n^{a-2}\int_0^t \sum_{y,z\in\mathbb{Z}} (\nabla_n f)\Big(\frac{y+z}{n}\Big)h\Big(\frac{y}{n}\Big)\Big\langle j_{z,z+1}(sn^a)\,,\,\omega_0^2(0)-\beta^{-1}\Big\rangle_\beta \mathrm{d}s$$

where ∇_n is the discretization of the derivative w.r.t. the lattice $n^{-1}\mathbb{Z}$, i.e.

$$(\nabla_n f)\left(\frac{y}{n}\right) = n\left[f\Big(\frac{y+1}{n}\Big) - f\Big(\frac{y}{n}\Big)\right].$$

The discretization Δ_n of the Laplacian is defined in a similar way. Let us recall that the current is decomposed as $j_{z,z+1} = j_{z,z+1}^{A} + j_{z,z+1}^{S}$.

If $a<2$, it is easy to see that the contribution coming from $j_{z,z+1}^{S}$ vanishes as $n \longrightarrow \infty$ since a second integration by parts can be performed and the time scale is subdiffusive. If $a=2$ and $b=0$, the symmetric part of the current gives a non trivial contribution. More precisely, after an integration by part we get the term

$$\int_0^t \sigma_s^n(\lambda f'',h)\,\mathrm{d}s,$$

and therefore the coefficient λ has to be added to the thermal conductivity κ.

We now assume that $a<2$. By using the fluctuation-dissipation equation (IV.4) for the contribution coming from $j_{0,1}^{A}$, we obtain that

$$\begin{aligned}\sigma_t^n(f,h) = \sigma_0^n(f,h) &+ n^{a-2}\int_0^t \sum_{y,z}(\nabla_n f)\Big(\frac{y+z}{n}\Big)h\Big(\frac{y}{n}\Big)\Big\langle\, (\tau_z v)(sn^a)\,,\,\omega_0^2(0)-\beta^{-1}\,\Big\rangle_\beta \mathrm{d}s\\ &- n^{a-2}\int_0^t \sum_{y,z}(\nabla_n f)\Big(\frac{y+z}{n}\Big)h\Big(\frac{y}{n}\Big)\Big\langle\, (\mathcal{L}_n\tau_z u)(sn^a)\,,\,\omega_0^2(0)-\beta^{-1}\,\Big\rangle_\beta \mathrm{d}s \;+\; o_n(1)\end{aligned}$$

where $o_n(1) \longrightarrow 0$ as n goes to ∞. We introduce the following notations:

$$\mathrm{V}_t^n(f,h) := n^{a-2}\int_0^t \sum_{y,z} (\nabla_n f)\Big(\frac{y+z}{n}\Big) h\Big(\frac{y}{n}\Big)\Big\langle\, (\tau_z v)(sn^a)\,,\ \omega_0^2(0) - \beta^{-1}\,\Big\rangle_\beta \mathrm{d}s,$$

$$\mathrm{U}_t^n(f,h) := n^{a-2}\int_0^t \sum_{y,z} (\nabla_n f)\Big(\frac{y+z}{n}\Big) h\Big(\frac{y}{n}\Big)\Big\langle\, (\mathcal{L}_n \tau_z u)(sn^a)\,,\ \omega_0^2(0) - \beta^{-1}\,\Big\rangle_\beta \mathrm{d}s.$$

Let us now focus on the term $\mathrm{V}_t^n(f,h)$. The function v can be rewritten as

$$v = \sum_{x\in\mathbb{Z}} \rho_1(x)\nabla(\omega_x^2) + \psi$$

where

$$\psi(\omega) = \sum_{x\in\mathbb{Z}}\sum_{k\geqslant 2} \rho_k(x)\nabla\Big[\omega_{x-1}\omega_{x+k} + \omega_x\omega_{x+k-1}\Big] + \sum_{x\in\mathbb{Z}} \rho_1(x)\Big\{\omega_x\omega_{x+2} - \omega_{x-1}\omega_{x+1}\Big\}. \qquad \text{(IV.7)}$$

Then, accordingly to this decomposition, we write the term $\mathrm{V}_t^n(f,h)$ as the sum of two terms

$$\mathrm{V}_t^n(f,h) = \mathrm{K}_t^n(f,h) + \Psi_t^n(f,h).$$

It turns out that

$$\mathrm{K}_t^n(f,h) = -n^{a-1}\int_0^t \sigma_s^n(\mathrm{F},h)\mathrm{d}s$$

where the function F is defined on $n^{-1}\mathbb{Z}$ by

$$\mathrm{F}\Big(\frac{w}{n}\Big) = \sum_{z\in\mathbb{Z}} \rho_1(z)\Big\{(\nabla_n f)\Big(\frac{w-z}{n}\Big) - (\nabla_n f)\Big(\frac{w-z-1}{n}\Big)\Big\}$$
$$= \frac{1}{n}\sum_{z\in\mathbb{Z}} \rho_1(z)(\Delta_n f)\Big(\frac{w-z}{n}\Big), \qquad w\in\mathbb{Z}.$$

In the sequel we prove the following convergences:

(i) If $b < 1$ then

$$\lim_{n\longrightarrow+\infty} |\mathrm{U}_t^n(f,h)| = 0.$$

(ii) If $a = 2 - b/2$ and $b < 2$, then

$$\lim_{n\longrightarrow\infty} \Big|\mathrm{K}_t^n(f,h) - \int_0^t \sigma_s^n(\kappa f'',h)\,\mathrm{d}s\Big| = 0.$$

(iii) If $b < 2/3$, then

$$\lim_{n\longrightarrow\infty} |\Psi_t^n(f,h)| = 0.$$

One can easily check that these three points imply Theorem IV.1. Besides, we shall see in the proof of (ii) that the case $a < 2 - b/2$ corresponds to $|\mathrm{V}_t^n(f,h)| \longrightarrow 0$. In other words, there is no evolution up to the time scale $a = 2 - b/2$.

REMARK *2.1.* If $b > 2$ and $a = 3/2$, we can adapt the argument in the proof of (ii) and show that the limit results in a constant times the 3/4-fractional Laplacian of f (instead of a constant times the second derivative of f). However, this is not sufficient to prove that for $b > 2$ the limit of the energy fluctuation field is given by a fractional heat equation, because we do not know how to control the other terms (U_t^n and Ψ_t^n) for $b > 2$. And in fact we know from the results of Section 3 that the contribution of these terms is not trivial, since a drift term should appear.

2.3 Proofs of Convergence Results

In this section we prove the above three convergence results.

LEMMA IV.3 (Fluctuation part). *If $b < 1$ then*

$$\lim_{n \longrightarrow +\infty} |\mathrm{U}_t^n(f,h)| = 0.$$

Proof. For each $z \in \mathbb{Z}$ we have that

$$n^a \int_0^t (\mathcal{L}_n \tau_z u)(sn^a) \mathrm{d}s = (\tau_z u)(tn^a) - (\tau_z u)(0) + \mathcal{N}_t^{z,n}$$

where $\mathcal{N}^{z,n}$ is a martingale equal to 0 at $t=0$, and then for any $t \geqslant 0$,

$$\left\langle \mathcal{N}_t^{z,n}, \omega_0^2(0) - \beta^{-1} \right\rangle_\beta = 0.$$

Notice that the expression for u only involves terms of the form $\omega_x \omega_y$ with $x \neq y$, and then

$$\left\langle \tau_z u(0) \left(\omega_0^2(0) - \beta^{-1}\right) \right\rangle_\beta = 0.$$

We use the translation invariance of the dynamics in order to write

$$\begin{aligned}
\mathrm{U}_t^n(f,h) &= \frac{1}{n^2} \sum_{y,z \in \mathbb{Z}} (\nabla_n f)\Big(\frac{y+z}{n}\Big) h\Big(\frac{y}{n}\Big) \Big\langle \left\{ (\tau_z u)(tn^a) - (\tau_z u)(0) \right\}, \omega_0^2(0) - \beta^{-1} \Big\rangle_\beta \\
&= \frac{1}{n} \left\langle \left\{ \frac{1}{\sqrt{n}} \sum_{y \in \mathbb{Z}} h\Big(\frac{y}{n}\Big) \left(\omega_y^2(0) - \beta^{-1}\right) \right\} \times \left\{ \frac{1}{\sqrt{n}} \sum_{z \in \mathbb{Z}} (\nabla_n f)\Big(\frac{z}{n}\Big) (\tau_z u)(tn^a) \right\} \right\rangle_\beta .
\end{aligned}$$

Then, from the Cauchy-Schwarz inequality and the stationarity of μ_β, there exist constants $\mathrm{C}', \mathrm{C} > 0$ which do not depend on n such that

$$\begin{aligned}
\left|\mathrm{U}_t^n(f,h)\right| &\leqslant \frac{\mathrm{C}'}{n} \left\| \frac{1}{\sqrt{n}} \sum_{y \in \mathbb{Z}} h\Big(\frac{y}{n}\Big) \left(\omega_y^2(0) - \beta^{-1}\right) \right\|_{\mathbf{L}^2(\mu_\beta)} \left\| \frac{1}{\sqrt{n}} \sum_{z \in \mathbb{Z}} (\nabla_n f)\Big(\frac{z}{n}\Big) \tau_z u \right\|_{\mathbf{L}^2(\mu_\beta)} \\
&\leqslant \frac{\mathrm{C}}{n} \left\| \frac{1}{\sqrt{n}} \sum_{z \in \mathbb{Z}} (\nabla_n f)\Big(\frac{z}{n}\Big) \tau_z u \right\|_{\mathbf{L}^2(\mu_\beta)} .
\end{aligned}$$

Using (IV.2) and the Parseval relation, a simple computation shows that

$$\begin{aligned}
\left\| \frac{1}{\sqrt{n}} \sum_{z \in \mathbb{Z}} (\nabla_n f)\Big(\frac{z}{n}\Big) \tau_z u \right\|^2_{\mathbf{L}^2(\mu_\beta)} &= \frac{1}{\beta^2 n} \sum_{k \geqslant 1} \sum_{y,x \in \mathbb{Z}} (\nabla_n f)\Big(\frac{y}{n}\Big) (\nabla_n f)\Big(\frac{y-x}{n}\Big) \left\{ \sum_{z \in \mathbb{Z}} \rho_k(z) \rho_k(z-x) \right\} \\
&= \frac{1}{\beta^2 n} \sum_{k \geqslant 1} \int_{\mathbb{T}} |\widehat{\rho}_k(\theta)|^2 \left\{ \sum_{y,x \in \mathbb{Z}} e^{-2i\pi\theta x} (\nabla_n f)\Big(\frac{y}{n}\Big) (\nabla_n f)\Big(\frac{y-x}{n}\Big) \right\} \mathrm{d}\theta \\
&= \frac{n}{\beta^2} \sum_{k \geqslant 1} \int_{\mathbb{T}} |\widehat{\rho}_k(\theta)|^2 |\mathcal{F}_n(\nabla_n f)|^2(n\theta)\, \mathrm{d}\theta \\
&= \frac{n}{\beta^2} \int_{\mathbb{T}} \frac{|\widehat{\rho}_1(\theta)|^2}{1 - |\mathrm{X}(\theta)|^2} |\mathcal{F}_n(\nabla_n f)|^2(n\theta)\, \mathrm{d}\theta.
\end{aligned}$$

In the last two equalities we use the Fourier transform $\mathcal{F}_n$ defined in (V.29), Appendix 2.3.1. According to Lemma IV.2, we know that there exists a constant $\mathrm{C} > 0$ such that

$$\frac{|\widehat{\rho}_1(\theta)|^2}{1 - |\mathrm{X}(\theta)|^2} \leqslant \frac{\mathrm{C}}{\sqrt{\gamma_n} \left[\frac{\gamma_n}{\lambda} + \sin^2(\pi\theta) \right]}.$$

By Lemma V.21 in Appendix 2.3.1, $|\mathcal{F}_n(\nabla_n f)|^2(n\theta)$ is bounded above by a constant $C > 0$ which does not depend on n, θ. We deduce that

$$\left\| \frac{1}{\sqrt{n}} \sum_{z\in\mathbb{Z}} (\nabla_n f)\Big(\frac{z}{n}\Big) \tau_z u \right\|^2_{L^2(\mu_\beta)} \leqslant \frac{Cn}{\sqrt{\gamma_n}} \int_{\mathbb{T}} \frac{1}{\frac{\gamma_n}{\lambda} + \sin^2(\pi\theta)} \, d\theta.$$

One can check that the right-hand side of the last inequality is of order n/γ_n. The lemma follows as soon as $\sqrt{n\gamma_n}$ diverges to ∞, which is equivalent to the condition $b < 1$. □

Now we deal with the term $K_t^n(f, h)$.

Lemma IV.4 (Diffusive behavior). *If $a = 2 - b/2$ and $b < 2$, then*

$$\lim_{n\longrightarrow\infty} \left| K_t^n(f,h) - \int_0^t \sigma_s^n(\kappa f'', h)\, ds \right| = 0.$$

Proof. First, let us write

$$\begin{aligned} &K_t^n(f,h) - \int_0^t \sigma_s^n(\kappa f'', h)\, ds \\ &= \int_0^t \frac{1}{n} \sum_{x,y\in\mathbb{Z}} \Big\{ - n^{a-1} F\Big(\frac{x}{n}\Big) - \kappa f''\Big(\frac{x}{n}\Big) \Big\} h\Big(\frac{y}{n}\Big) \Big\langle \Big\{ \omega_x^2(tn^a) - \beta^{-1} \Big\} \times \Big\{ \omega_y^2(0) - \beta^{-1} \Big\} \Big\rangle_\beta . \end{aligned}$$

Then, from the Cauchy-Schwarz inequality, we get that there exists a constant $C > 0$ such that

$$\left| K_t^n(f,h) - \int_0^t \sigma_s^n(\kappa f'', h)\, ds \right|^2 \leqslant \frac{C}{n} \sum_{w\in\mathbb{Z}} \Big[\big(n^{a-1} F\big)\Big(\frac{w}{n}\Big) + \kappa \big(f''\big)\Big(\frac{w}{n}\Big) \Big]^2 .$$

We are reduced to prove that the right-hand side vanishes as n goes to ∞. The proof relies on Fourier transform. The discrete Fourier transform of $n^{a-1}F$ is given by

$$\begin{aligned} n^{a-1}\mathcal{F}_n(F)(\xi) &= n^{a-2} \sum_y F\Big(\frac{y}{n}\Big) e^{2i\pi\xi y/n} = n^{a-2} \mathcal{F}_n(\Delta_n f)(\xi) \widehat{\rho}_1\Big(\frac{\xi}{n}\Big) \\ &= -n^a \frac{4\sin^2\big(\pi\frac{\xi}{n}\big)}{\gamma_n + \lambda\sqrt{(1+\frac{\gamma_n}{\lambda})^2 - \cos^2(\pi\frac{\xi}{n})}} \mathcal{F}_n(f)(\xi). \end{aligned}$$

We denote

$$q_n\big(\tfrac{\xi}{n}\big) := -n^a \frac{4\sin^2(\pi\frac{\xi}{n})}{\gamma_n + \lambda\sqrt{(1+\frac{\gamma_n}{\lambda})^2 - \cos^2(\pi\frac{\xi}{n})}}.$$

We now recall that $a = 2 - b/2$ and introduce the term $1/\sqrt{2\lambda c}$. By Plancherel relation it is equivalent to prove

$$\lim_{n\longrightarrow\infty} I_n := \lim_{n\longrightarrow\infty} \int_{-\frac{n}{2}}^{\frac{n}{2}} \left| q_n\Big(\frac{\xi}{n}\Big)\mathcal{F}_n(f)(\xi) - \frac{1}{\sqrt{2\lambda c}} \mathcal{F}_n(f'')(\xi) \right|^2 d\xi = 0.$$

By Corollary V.22 in Appendix 2.3.1 we know that, for any smooth and compactly supported function g,

$$\lim_{n\longrightarrow\infty} \int_{-\frac{n}{2}}^{\frac{n}{2}} |\mathcal{F}_n(g)(\xi) - (\mathcal{F}g)(\xi)|^2\, d\xi = 0.$$

Therefore, we can replace in I_n the term $\mathcal{F}_n(f'')(\xi)$ by $\mathcal{F}(f'')(\xi) = -4\pi^2|\xi|^2(\mathcal{F}f)(\xi)$, where $\mathcal{F}$ is the usual Fourier transform defined on the Schwartz space (see (V.27), Appendix 2.3.1). We write then

$$\begin{aligned}
&\int_{-\frac{n}{2}}^{\frac{n}{2}} \left| q_n\left(\frac{\xi}{n}\right)\mathcal{F}_n(f)(\xi) + \frac{4\pi^2\xi^2}{\sqrt{2\lambda c}}(\mathcal{F}f)(\xi)\right|^2 \mathrm{d}\xi \\
&\leqslant 2\int_{-\frac{n}{2}}^{\frac{n}{2}} \left| q_n\left(\frac{\xi}{n}\right) + \frac{4\pi^2\xi^2}{\sqrt{2\lambda c}}\right|^2 \left|\mathcal{F}_n(f)(\xi)\right|^2 \mathrm{d}\xi + \frac{16\pi^4}{\lambda c}\int_{-\frac{n}{2}}^{\frac{n}{2}} \xi^4 |\mathcal{F}_n(f)(\xi) - (\mathcal{F}f)(\xi)|^2 \mathrm{d}\xi.
\end{aligned}$$

The last term of the right-hand side of the previous inequality goes to 0 as $n \longrightarrow \infty$ since f is smooth and compactly supported. We are reduced to show that

$$\lim_{n\longrightarrow\infty} \int_{-\frac{n}{2}}^{\frac{n}{2}} \left| q_n\left(\frac{\xi}{n}\right) + \frac{4\pi^2\xi^2}{\sqrt{2\lambda c}}\right|^2 \left|\mathcal{F}_n(f)(\xi)\right|^2 \mathrm{d}\xi = 0.$$

A simple application of Lemma V.21 (Appendix 2.3.1) shows that it is equivalent to prove

$$\lim_{n\longrightarrow\infty} \int_{-\frac{n}{2}}^{\frac{n}{2}} \left| q_n\left(\frac{\xi}{n}\right) + \frac{4n^2}{\sqrt{2\lambda c}}\sin^2\left(\pi\frac{\xi}{n}\right)\right|^2 \left|\mathcal{F}_n(f)(\xi)\right|^2 \mathrm{d}\xi = 0.$$

Observe now that

$$\left| q_n\left(\frac{\xi}{n}\right) + \frac{4n^2}{\sqrt{2\lambda c}}\sin^2\left(\pi\frac{\xi}{n}\right)\right| = \frac{4n^2}{\sqrt{2\lambda c}}\sin^2\left(\pi\frac{\xi}{n}\right)\left| \left(\sqrt{1 + \frac{cn^{-b}}{2\lambda} + \frac{n^b\lambda}{2c}\sin^2\left(\pi\frac{\xi}{n}\right)} + \sqrt{\frac{cn^{-b}}{2\lambda}}\right)^{-1} - 1\right|. \tag{IV.8}$$

In particular, we have

$$\left| q_n\left(\frac{\xi}{n}\right) + \frac{4n^2}{\sqrt{2\lambda c}}\sin^2\left(\pi\frac{\xi}{n}\right)\right| \leqslant C|\xi|^2. \tag{IV.9}$$

By Lemma V.21 of Appendix 2.3.1 we know that

$$\limsup_{A\longrightarrow\infty}\ \limsup_{n\longrightarrow\infty} \int_{A\leqslant|\xi|\leqslant n/2} |\xi|^4 \left|\mathcal{F}_n(f)(\xi)\right|^2 \mathrm{d}\xi = 0.$$

Thus, by (IV.9), it is sufficient to prove that for any $A > 0$ fixed,

$$\lim_{n\longrightarrow\infty} \int_{|\xi|\leqslant A} \left| q_n\left(\frac{\xi}{n}\right) + \frac{4n^2}{\sqrt{2\lambda c}}\sin^2\left(\pi\frac{\xi}{n}\right)\right|^2 \left|\mathcal{F}_n(f)(\xi)\right|^2 \mathrm{d}\xi = 0.$$

By (IV.8) we have

$$\int_{|\xi|\leqslant A} \left| q_n\left(\frac{\xi}{n}\right) + \frac{4n^2}{\sqrt{2\lambda c}}\sin^2\left(\pi\frac{\xi}{n}\right)\right|^2 \left|\mathcal{F}_n(f)(\xi)\right|^2 \mathrm{d}\xi \leqslant \varepsilon_n(A)\int_{|\xi|\leqslant A} |\mathcal{F}_n(f)(\xi)|^2 \mathrm{d}\xi \leqslant \frac{\varepsilon_n(A)}{n}\sum_{x\in\mathbb{Z}} f^2\left(\frac{x}{n}\right)$$

where

$$\varepsilon_n(A) = \sup_{|\xi|\leqslant A}\left\{ \frac{4n^2}{\sqrt{2\lambda c}}\sin^2\left(\pi\frac{\xi}{n}\right)\left| \left(\sqrt{1 + \frac{cn^{-b}}{2\lambda} + \frac{n^b\lambda}{2c}\sin^2\left(\pi\frac{\xi}{n}\right)} + \sqrt{\frac{cn^{-b}}{2\lambda}}\right)^{-1} - 1\right|\right\}$$

vanishes as n goes to infinity since $b < 2$. The claim follows after noticing that

$$\sup_{n\geqslant 1} \frac{1}{n}\sum_{x\in\mathbb{Z}} f^2\left(\frac{x}{n}\right) < \infty.$$

Finally, let us remark that if $a < 2 - b/2$, the same computation using the Fourier transform shows that $V_t^n(f,h)$ vanishes. □

We conclude this section with the proof of the last convergence.

Lemma IV.5 (Boltzman-Gibbs principle). *If $b < 2/3$ then we have*

$$\lim_{n\longrightarrow\infty} \Psi_t^n(f,h) = 0.$$

Proof. Recall (IV.7). Performing a simple computation we can rewrite ψ as

$$\psi(\omega) = \sum_{x\in\mathbb{Z}}\sum_{k\geqslant 1}\big(\rho_{k-1}(x+1)+\rho_{k+1}(x)\big)\nabla\big[\omega_x\omega_{x+k}\big],$$

with the convention that $\rho_0(x) = 0$ for any $x \in \mathbb{Z}$. Let us introduce ψ_k defined on $\mathbb{Z}$ by

$$\psi_k(x) = \rho_{k-1}(x+1)+\rho_{k+1}(x).$$

By using the space invariance of μ_β, we can write

$$\Psi_t^n(f,h) = n^{a-2}\left\langle \left\{\sum_{y\in\mathbb{Z}} h\Big(\frac{y}{n}\Big)\Big(\omega_y^2(0)-\frac{1}{\beta}\Big)\right\}\times\left\{\int_0^t \varphi(\omega(sn^a))\,\mathrm{d}s\right\}\right\rangle_\beta$$

where the function φ is given by

$$\varphi(\omega) = \sum_{x,z\in\mathbb{Z}}\sum_{k\geqslant 1}(\nabla_n f)\Big(\frac{z}{n}\Big)\{\psi_k(x-1)-\psi_k(x)\}(\omega_{x+z}\omega_{x+z+k}). \tag{IV.10}$$

Thus, from the Cauchy-Schwarz inequality, it is sufficient to prove that the $\mathbf{L}^2(\mathbb{P}_{\mu_\beta})$ norm of

$$n^{a-3/2}\int_0^t \varphi(\omega(sn^a))\mathrm{d}s$$

vanishes with n, where $\mathbb{P}_{\mu_\beta}$ denotes the law of the Markov process $\{\omega(tn^a)\}_{t\geqslant 0}$ starting with μ_β. We denote by $\mathbb{E}_{\mu_\beta}$ the corresponding expectation. By a general inequality for variance of additive functionals of Markov processes (see [52, Lemma 2.4]), we have

$$\begin{aligned}\mathbb{E}_{\mu_\beta}\left[\left(\int_0^t \varphi(\omega(sn^a))\mathrm{d}s\right)^2\right] &\leqslant Ct\left\langle \varphi\,,\,\big(t^{-1}-n^a\mathcal{S}_n\big)^{-1}\varphi\right\rangle_\beta\\ &= Ctn^{-a}\left\langle \varphi\,,\,\big([tn^a]^{-1}-\mathcal{S}_n\big)^{-1}\varphi\right\rangle_\beta.\end{aligned} \tag{IV.11}$$

Now we can use some ideas from [11] in order to get a very sharp estimate of (IV.11). In Appendix 2.3.2, we prove that $\langle\varphi\,,\,([tn^a]^{-1}-\mathcal{S}_n)^{-1}\varphi\rangle_\beta$ is bounded from above by Cn^{2b}. As a consequence, the Boltzmann-Gibbs principle holds if $a-3+2b<0$. With the condition $a = 2-b/2$ we obtain $b < 2/3$. □

3 The Energy Fluctuation Field for $b > 1$

For the sake of simplicity, hereafter we assume $\lambda = 1$. The same computations for any $\lambda > 0$ could be done, but become significantly more technical. In this section we prove the following theorem.

Theorem IV.6. *Let $(\mathrm{P}_t)_{t\geqslant 0}$ be the semigroup generated by the infinitesimal generator*

$$\mathbb{L} := -\frac{1}{\sqrt{2}}\left((-\Delta)^{3/4} - \nabla(-\Delta)^{1/4}\right).$$

If $b > 1$ and $a = 3/2$ then

$$\lim_{n\longrightarrow+\infty} \sigma_t^n(f,h) = \chi(\beta)\iint_{\mathbb{R}^2} \mathrm{d}u\mathrm{d}v\, f(u)h(v)\mathrm{P}_t(u-v). \tag{IV.12}$$

As for Theorem IV.1, with a little more effort we could also prove that the energy fluctuation field $\mathcal{E}_t^n$ converges to an infinite dimensional 3/4-fractional Ornstein-Uhlenbeck process.

3.1 Weak Formulation

In this section we give the strategy of the proof, which is the same as in [12], so that we use the same notations. In the whole section, $a = 3/2$, and $b > 1$. We also assume $\beta = 1$, the general case follows after an easy change of variable into the Markov process.

Two coupled differential equations – Let g be a fixed function in $\mathcal{C}_c^\infty(\mathbb{R})$. We define the process $\{\mathcal{S}_t^n; t \geqslant 0\}$ acting on functions $f \in \mathcal{C}_c^\infty(\mathbb{R})$ as

$$\mathcal{S}_t^n(f) := \frac{1}{\chi(1)}\sigma_t^n(f,g) = \frac{1}{2}\sigma_t^n(f,g). \tag{IV.13}$$

for any $t \geqslant 0$, $n \in \mathbb{N}$. After arranging terms in a convenient way we have that

$$\mathcal{S}_t^n(f) = \frac{1}{2}\left\langle \left\{\frac{1}{\sqrt{n}}\sum_{x\in\mathbb{Z}} g\left(\frac{x}{n}\right)\left(\omega_x^2(0)-1\right)\right\} \times \left\{\frac{1}{\sqrt{n}}\sum_{y\in\mathbb{Z}} f\left(\frac{y}{n}\right)\left(\omega_y^2(tn^{3/2})-1\right)\right\}\right\rangle_1.$$

For a function $h \in \mathcal{C}_c^\infty(\mathbb{R}^2)$ we define $\{\mathrm{Q}_t^n(h); t \geqslant 0\}$ as

$$\mathrm{Q}_t^n(h) = \frac{1}{2}\left\langle \left\{\frac{1}{\sqrt{n}}\sum_{x\in\mathbb{Z}} g\left(\frac{x}{n}\right)\left(\omega_x^2(0)-1\right)\right\} \times \left\{\frac{1}{n}\sum_{\substack{y,z\in\mathbb{Z}\\ y\neq z}} h\left(\frac{y}{n},\frac{z}{n}\right)\omega_y(tn^{3/2})\omega_z(tn^{3/2})\right\}\right\rangle_1.$$

Notice that $\mathrm{Q}_t^n(h)$ depends only on the symmetric part of the function h. Therefore, we will always assume, without loss of generality, that $h(x,y) = h(y,x)$ for any $x, y \in \mathbb{Z}$. Notice as well that $\mathrm{Q}_t^n(h)$ does not depend on the values of h at the diagonal $\{x = y\}$. Let us write now the differential equations for $\mathcal{S}_t^n(f)$ and $\mathrm{Q}_t^n(h)$. We start with introducing some definitions.

Definition IV.1 (Discrete approximations). *For any function $f \in \mathcal{C}_c^\infty(\mathbb{R})$, and any function $h \in \mathcal{C}_c^\infty(\mathbb{R}^2)$, we define*

(i) the discrete approximation $\Delta_n f : \mathbb{R} \longrightarrow \mathbb{R}$ of the second derivative of f as

$$\Delta_n f\left(\frac{x}{n}\right) = n^2\left\{f\left(\frac{x+1}{n}\right) + f\left(\frac{x-1}{n}\right) - 2f\left(\frac{x}{n}\right)\right\}.$$

(ii) the discrete approximation $\nabla_n f \otimes \delta : n^{-1}\mathbb{Z}^2 \longrightarrow \mathbb{R}$ *of the distribution* $f'(x)\delta(x=y)$ *as*

$$\big(\nabla_n f \otimes \delta\big)\Big(\frac{x}{n},\frac{y}{n}\Big) = \begin{cases} \frac{n^2}{2}\Big\{f\left(\frac{x+1}{n}\right) - f\left(\frac{x}{n}\right)\Big\} & \text{if } y = x+1 \\ \frac{n^2}{2}\Big\{f\left(\frac{x}{n}\right) - f\left(\frac{x-1}{n}\right)\Big\} & \text{if } y = x-1 \\ 0 & \text{otherwise.} \end{cases} \tag{IV.14}$$

(iii) the discrete approximation $\Delta_n h : \mathbb{R}^2 \longrightarrow \mathbb{R}$ *of the Laplacian of* h *as*

$$\Delta_n h\Big(\frac{x}{n},\frac{y}{n}\Big) = n^2\Big\{h\Big(\frac{x+1}{n},\frac{y}{n}\Big)+h\Big(\frac{x-1}{n},\frac{y}{n}\Big)+h\Big(\frac{x}{n},\frac{y+1}{n}\Big)+h\Big(\frac{x}{n},\frac{y-1}{n}\Big)-4h\Big(\frac{x}{n},\frac{y}{n}\Big)\Big\},$$

(iv) the discrete approximation $\mathrm{A}_n h : \mathbb{R} \longrightarrow \mathbb{R}$ *of the directional derivative* $(-2,-2)\cdot\nabla h$ *as*

$$\mathrm{A}_n h\Big(\frac{x}{n},\frac{y}{n}\Big) = n\Big\{h\Big(\frac{x}{n},\frac{y-1}{n}\Big) + h\Big(\frac{x-1}{n},\frac{y}{n}\Big) - h\Big(\frac{x}{n},\frac{y+1}{n}\Big) - h\Big(\frac{x+1}{n},\frac{y}{n}\Big)\Big\},$$

(v) the discrete approximation $\mathcal{D}_n h : n^{-1}\mathbb{Z} \longrightarrow \mathbb{R}$ *of the directional derivative of* h *along the diagonal* $\{x=y\}$ *as*

$$\mathcal{D}_n h\Big(\frac{x}{n}\Big) = n\Big\{h\Big(\frac{x}{n},\frac{x+1}{n}\Big) - h\Big(\frac{x-1}{n},\frac{x}{n}\Big)\Big\},$$

(vi) the discrete approximation $\widetilde{\mathcal{D}}_n h : n^{-1}\mathbb{Z}^2 \longrightarrow \mathbb{R}$ *of the distribution* $\partial_y h(x,x)\otimes\delta(x=y)$ *as*

$$\widetilde{\mathcal{D}}_n h\Big(\frac{x}{n},\frac{y}{n}\Big) = \begin{cases} n^2\Big\{h\big(\frac{x}{n},\frac{x+1}{n}\big) - h\big(\frac{x}{n},\frac{x}{n}\big)\Big\} & \text{if } y = x+1 \\ n^2\Big\{h\big(\frac{x-1}{n},\frac{x}{n}\big) - h\big(\frac{x-1}{n},\frac{x-1}{n}\big)\Big\} & \text{if } y = x-1 \\ 0 & \text{otherwise.} \end{cases}$$

The following proposition can be deduced after straightforward computations, which are detailed in Appendix 2.3.3.

Proposition IV.7. *For any function* $f \in \mathcal{C}_c^\infty(\mathbb{R})$, *any function* $h \in \mathcal{C}_c^\infty(\mathbb{R}^2)$,

$$\frac{d}{dt}\mathcal{S}_t^n(f) = -2\mathrm{Q}_t^n(\nabla_n f\otimes\delta) + \mathcal{S}_t^n\left(n^{-1/2}\,\Delta_n f\right), \tag{IV.15}$$

$$\frac{d}{dt}\mathrm{Q}_t^n(h) = \mathrm{Q}_t^n\big(\mathrm{L}_n h\big) - 2\mathcal{S}_t^n\big(\mathcal{D}_n h\big) + 2\mathrm{Q}_t^n\big(n^{-1/2}\,\widetilde{\mathcal{D}}_n h\big), \tag{IV.16}$$

where the operator L_n *is defined by*

$$\mathrm{L}_n = \sqrt{n}\,\mathrm{A}_n + \frac{1}{\sqrt{n}}\,\Delta_n - 4n^{3/2}\gamma_n\mathrm{Id}. \tag{IV.17}$$

A priori bounds – For any function $f \in \mathcal{C}_c^\infty(\mathbb{R})$, define the weighted $\ell^2(\mathbb{Z})$-norm as

$$\|f\|_{2,n}^2 := \frac{1}{n}\sum_{x\in\mathbb{Z}} f^2\Big(\frac{x}{n}\Big).$$

By the Cauchy-Schwarz inequality we have the *a priori* bound

$$\left|\mathcal{S}_t^n(f)\right| \leqslant \|g\|_{2,n}\|f\|_{2,n} \tag{IV.18}$$

for any $t \geqslant 0$, any $n \in \mathbb{N}$ and any $f, g \in \mathcal{C}_c^\infty(\mathbb{R})$. Therefore, the term $\mathcal{S}_t^n(n^{-1/2}\Delta_n f)$ is negligible, as $n \longrightarrow \infty$. In (IV.15), the term $\mathrm{Q}_t^n(\nabla_n f \otimes \delta)$ is the relevant one. We also have the *a priori* bound

$$\left|\mathrm{Q}_t^n(h)\right| \leqslant 2\|g\|_{2,n}\|\overline{h}\|_{2,n}, \tag{IV.19}$$

where $\|\overline{h}\|_{2,n}$ is the weighted $\ell^2(\mathbb{Z}^2)$-norm of $\overline{h}$

$$\|\overline{h}\|_{2,n}^2 := \frac{1}{n^2}\sum_{x,y\in\mathbb{Z}} \overline{h}^2\Big(\frac{x}{n},\frac{y}{n}\Big)$$

and $\overline{h}$ is defined by

$$\overline{h}\Big(\frac{x}{n},\frac{y}{n}\Big) = h\Big(\frac{x}{n},\frac{y}{n}\Big)\,\mathbf{1}_{x\neq y}.$$

In Equation (IV.15), both fields $\mathcal{S}_t^n$ and Q_t^n appear with non-negligible terms. Moreover, the term involving Q_t^n is quite singular, since it involves an approximation of a distribution. Let us give the clever strategy explained in [12]: given $f \in \mathcal{C}_c^\infty(\mathbb{R})$, if we choose h such that $\mathrm{L}_n h = \nabla_n f \otimes \delta$, we can try to cancel the term $\mathrm{Q}_t^n(\nabla_n f \otimes \delta)$ and $\mathrm{Q}_t^n(\mathrm{L}_n h)$ out. Then the term $\mathcal{S}_t^n(\mathcal{D}_n h)$ provides a non-trivial drift for the differential equation (IV.15) and the term $\mathrm{Q}_t^n(n^{-1/2}\widetilde{\mathcal{D}}_n h)$ turns out to be negligible. We refer the reader to [12, Section 5.1] for an enlightening heuristic explanation of the proof.

3.2 Sketch of the Proof

After giving the topological setting needed for the theorem, we sketch the main steps of the argument, which are detailed in [12].

Topological setting – We fix a finite time-horizon $\mathrm{T} > 0$. Let us define the *Hermite polynomials* $\mathrm{H}_\ell : \mathbb{R} \longrightarrow \mathbb{R}$ as

$$\mathrm{H}_\ell(x) = (-1)^\ell e^{\frac{x^2}{2}}\frac{d^\ell}{dx^\ell}\Big[e^{-\frac{x^2}{2}}\Big]$$

for any $\ell \in \mathbb{N}_0$ and any $x \in \mathbb{R}$. We define the *Hermite functions* $f_\ell : \mathbb{R} \longrightarrow \mathbb{R}$ as

$$f_\ell(x) = \frac{1}{\sqrt{\ell!\sqrt{2\pi}}}\mathrm{H}_\ell(x)e^{-\frac{x^2}{4}}$$

For any $\ell \in \mathbb{N}_0$ and any $x \in \mathbb{R}$. The Hermite functions $\{f_\ell; \ell \in \mathbb{N}_0\}$ form an orthonormal basis of $\mathrm{L}^2(\mathbb{R})$. For each $k \in \mathbb{R}$, we define the *Sobolev space* $\mathcal{H}_k$ as the completion of $\mathcal{C}_c^\infty(\mathbb{R})$ with respect to the norm $\|\cdot\|_{\mathcal{H}_k}$ defined as

$$\|g\|_{\mathcal{H}_k}^2 := \sum_{\ell\in\mathbb{N}_0}(1+\ell)^{2k}\langle f_\ell, g\rangle^2$$

for any $g \in \mathcal{C}_c^\infty(\mathbb{R})$. Here we use the notation $\langle f_\ell, g\rangle = \int g(x)f_\ell(x)\mathrm{d}x$.

Main steps of the proof – First, we need to show tightness, and then to characterize the limit points of weakly converging subsequences.

1) TIGHTNESS. The same standard arguments exposed in [12] imply the following

   LEMMA IV.8. *For any $k > \frac{19}{24}$, the sequence $\{\mathcal{S}_t^n; t \in [0,\mathrm{T}]\}_{n\in\mathbb{N}}$ is weakly relatively compact in $\mathbf{L}^2([0,\mathrm{T}];\mathcal{H}_{-k})$. Moreover, for any $t \in [0,\mathrm{T}]$ fixed, the sequence $\{\mathcal{S}_t^n; n \in \mathbb{N}\}$ is sequentially, weakly relatively compact in $\mathcal{H}_{-k}$.*

2) CHARACTERIZATION OF LIMIT POINTS. Fix $k > \frac{19}{24}$ and let us consider a limit point of $\{\mathcal{S}_t^n; t \in [0,\mathrm{T}]\}_{n\in\mathbb{N}}$ with respect to the weak topology of $\mathbf{L}^2([0,\mathrm{T}];\mathcal{H}_{-k})$. The aim is to prove the following

   PROPOSITION IV.9. *Let $f : [0,\mathrm{T}] \times \mathbb{R} \longrightarrow \mathbb{R}$ be a smooth function of compact support (in $\mathcal{C}_c^\infty([0,\mathrm{T}] \times \mathbb{R})$). Then,*

$$\mathcal{S}_\mathrm{T}(f_\mathrm{T}) = \mathcal{S}_0(f_0) + \int_0^\mathrm{T} \mathcal{S}_t\big((\partial_t + \mathbb{L})f_t\big)\mathrm{d}t. \tag{IV.20}$$

   As a result, $\{\mathcal{S}_t; t \in [0,\mathrm{T}]\}$ is a *weak solution* of the fractional heat equation:

$$\partial_t u = -\frac{1}{\sqrt{2}}\{(-\Delta)^{3/4} + \nabla(-\Delta)^{1/4}\}u,$$

   as defined in (2.1) of [45, Section 8.1]. Precisely, it is shown in [45] that there is a unique solution of (IV.20) and therefore the limit process $\{\mathcal{S}_t; t \in [0,\mathrm{T}]\}$ is unique. Proposition IV.9 is the most challenging part of the proof, and the next section is devoted to it.

3) CONCLUSION. The proof of Theorem IV.6 is almost done: the first two points imply that the sequence $\{\mathcal{S}_t^n; t \in [0,\mathrm{T}]\}_{n\in\mathbb{N}}$ weakly converges in $\mathbf{L}^2([0,\mathrm{T}];\mathcal{H}_{-k})$ to a unique limit point, denoted by $\{\mathcal{S}_t; t \in [0,\mathrm{T}]\}$.

   It can be proved that the convergence also holds for fixed times $t \in [0,\mathrm{T}]_\mathbb{Q}$ with respect to the weak topology of $\mathcal{H}_{-k}$, where

$$[0,\mathrm{T}]_\mathbb{Q} := \left\{ t \in [0,\mathrm{T}]; \frac{t}{\mathrm{T}} \in \mathbb{Q} \right\}.$$

   Since T is arbitrary, this last convergence holds for any $t \in [0,\infty)$. In particular, $\mathcal{S}_t^n(f)$ converges to $\mathcal{S}_t(f)$ as $n \longrightarrow \infty$ for any $f \in \mathcal{C}_c^\infty(\mathbb{R})$.

The main differences between the model of [12] and ours rely on the velocity-flip noise, of intensity γ_n. This additional perturbation first appears in the definition of the operator L_n in (IV.17). Some technical details in the proof have to be slightly modified, but the main idea remains the same. More precisely, rigorous convergence estimates lead to the condition: $b > 1$.

3.3 Convergence estimates

We are going to give the proof of Proposition IV.9. Recall that the parameter b in the definition of γ_n is supposed to be strictly greater than 1. Let us assume that $\{\mathcal{S}_t^n; t \in [0,\mathrm{T}]\}_{n\in\mathbb{N}}$ converges to $\{\mathcal{S}_t; t \in [0,\mathrm{T}]\}$ with respect to the weak topology of $\mathbf{L}^2([0,\mathrm{T}];\mathcal{H}_{-k})$.

Let us fix a function $f \in \mathcal{C}_c^\infty(\mathbb{R})$ and let $h_n : n^{-1}\mathbb{Z} \times n^{-1}\mathbb{Z} \longrightarrow \mathbb{R}$ be the solution of the equation

$$\mathrm{L}_n h_n = \nabla_n f \otimes \delta. \tag{IV.21}$$

The following properties of h_n are shown in Appendix 2.3, following [12]:

Lemma IV.10. *Let $f \in \mathrm{C}_c^\infty(\mathbb{R})$. The solution of* (IV.21) *satisfies*

$$\lim_{n\longrightarrow\infty} \frac{1}{n^2} \sum_{x,y\in\mathbb{Z}} h_n^2\Big(\frac{x}{n},\frac{y}{n}\Big) = 0, \tag{IV.22}$$

$$\lim_{n\longrightarrow\infty} \frac{1}{n} \sum_{x\in\mathbb{Z}} \left| \mathcal{D}_n h_n\Big(\frac{x}{n}\Big) + \frac{1}{4}\mathbb{L} f\Big(\frac{x}{n}\Big)\right|^2 = 0. \tag{IV.23}$$

In other words, $\|h_n\|_{2,n}$ and $\big\|\mathcal{D}_n h_n + \frac{1}{4}\mathbb{L}f\big\|_{2,n}$ converge to 0 as $n \longrightarrow \infty$.

By (IV.15) and (IV.16), we see that

$$\mathcal{S}_{\mathrm{T}}^n(f) = \mathcal{S}_0^n(f) + \int_0^{\mathrm{T}} \mathcal{S}_t^n\big(-4\mathcal{D}_n h_n\big)\mathrm{d}t + 2\big[\mathrm{Q}_0^n(h_n) - \mathrm{Q}_{\mathrm{T}}^n(h_n)\big]$$
$$+ \int_0^{\mathrm{T}} \mathcal{S}_t^n\big(n^{-1/2}\Delta_n f\big)\mathrm{d}t + 4\int_0^{\mathrm{T}} \mathrm{Q}_t^n\big(n^{-1/2}\widetilde{\mathcal{D}}_n(h_n)\big)\mathrm{d}t.$$

Therefore, by the *a priori* bound (IV.19) and Lemma IV.10, we have that

$$\mathcal{S}_{\mathrm{T}}^n(f) = \mathcal{S}_0^n(f) + \int_0^{\mathrm{T}} \mathcal{S}_t^n(\mathbb{L}f)\mathrm{d}t + 4\int_0^{\mathrm{T}} \mathrm{Q}_t^n\big(n^{-1/2}\widetilde{\mathcal{D}}_n(h_n)\big)\mathrm{d}t \tag{IV.24}$$

plus an error term which goes to 0 as $n \longrightarrow \infty$. It turns out that the *a priori* bound (IV.19) is not sufficient to show that the last term on the right-hand side of (IV.24) goes to 0 with n since

$$\frac{1}{n^3}\sum_{x\in\mathbb{Z}} \big(\widetilde{\mathcal{D}}_n h_n\big)^2\Big(\frac{x}{n},\frac{x+1}{n}\Big) \tag{IV.25}$$

is of order one. Therefore we use again (IV.16) applied to $h = v_n$ where v_n is the solution of the Poisson equation

$$\mathrm{L}_n v_n = n^{-1/2}\widetilde{\mathcal{D}}_n h_n. \tag{IV.26}$$

Then we have

$$\int_0^{\mathrm{T}} \mathrm{Q}_t^n\Big(n^{-1/2}\widetilde{\mathcal{D}}_n h_n\Big)\mathrm{d}t = 2\int_0^{\mathrm{T}} \mathcal{S}_t^n(\mathcal{D}_n v_n)\mathrm{d}t - 2\int_0^{\mathrm{T}} \mathrm{Q}_t^n\Big(n^{-1/2}\widetilde{\mathcal{D}}_n v_n\Big)\mathrm{d}t + \mathrm{Q}_{\mathrm{T}}^n(v_n) - \mathrm{Q}_0^n(v_n).$$

Now, we can use the *a priori* bound (IV.18) and (IV.19). The following estimates on v_n are proved in Appendix 2.3.

Lemma IV.11. *The solution v_n of* (IV.26) *satisfies*

$$\lim_{n\longrightarrow\infty} \frac{1}{n^2} \sum_{x,y\in\mathbb{Z}} v_n^2\Big(\frac{x}{n},\frac{y}{n}\Big) = 0, \tag{IV.27}$$

$$\lim_{n\longrightarrow\infty} \frac{1}{n} \sum_{x\in\mathbb{Z}} \big(\mathcal{D}_n v_n\big)^2\Big(\frac{x}{n}\Big) = 0, \tag{IV.28}$$

$$\lim_{n\longrightarrow\infty} \frac{1}{n^3} \sum_{x\in\mathbb{Z}} \big(\widetilde{\mathcal{D}}_n v_n\big)^2\Big(\frac{x}{n},\frac{x+1}{n}\Big) = 0. \tag{IV.29}$$

In other words, $\|v_n\|_{2,n}$, $\|\mathcal{D}_n v_n\|_{2,n}$ and $\big\|\frac{1}{\sqrt{n}}\widetilde{\mathcal{D}}_n v_n\big\|_{2,n}$ converge to 0, as $n \longrightarrow \infty$.

It follows that

$$\mathcal{S}_{\mathrm{T}}^{n}(f) = \mathcal{S}_{0}^{n}(f) + \int_{0}^{\mathrm{T}} \mathcal{S}_{t}^{n}(\mathbb{L}f)\mathrm{d}t \tag{IV.30}$$

plus an error term which goes to 0 as $n \longrightarrow \infty$. Recall that $\{\mathcal{S}_t^n; t \in [0,\mathrm{T}]\}_{n\in\mathbb{N}}$ weakly converges to $\{\mathcal{S}_t; t \in [0,\mathrm{T}]\}$. The main difficulty is that the operator $\mathbb{L}$ is an integro-differential operator with heavy tails (in other words, even for $f \in \mathcal{C}_c^{\infty}(\mathbb{R})$ the function $\mathbb{L}f$ has heavy tails). As a result, we cannot take the limit $n \longrightarrow \infty$ in (IV.30). Bernardin et al. in [12] achieve to Proposition IV.9 after truncature considerations, and results about the Lipschitz property of the function $t \mapsto \mathcal{S}_t(f)$. We refer the reader to their paper, and also to [29,45] for useful properties of the fractional Laplacian.

In Appendix 2.3, Lemma IV.11 and Lemma IV.10 are proved. The computations are similar to [12], but they take into account the additional term due to the presence of the velocity-flip noise, and explain the needed assumption on the parameter b. The new technical estimate is given in Lemma V.26.

CHAPTER V

Appendices

Contents

1 Numerical Simulations

This section describes the numerical simulations we have performed for the models of Chapter II and Chapter III. The time-discretization of the dynamics is done with a standard splitting strategy, decomposing the generator as the sum of the deterministic part and the stochastic perturbation, and then integrating each part.

A simple numerical scheme for the deterministic part of the dynamics relies on the Hamiltonian interpretation of the system. Indeed, the longtime integration of Hamiltonian system is well understood. The most standard scheme used in practice is the so-called Störmer-Verlet scheme (Subsection 1.1). All the forthcoming theoretical results are detailed in [44, 74].

1.1 Symplectic Integration of Hamiltonian Systems

1.1.1 Symplecticity of Hamiltonian Flow

In this thesis we have studied interactions of oscillators that follow a Hamiltonian dynamics. Let us recall here the general context. The mechanical system evolves following Newton's equations:

$$\frac{d\omega}{dt} = \mathrm{J} \cdot \nabla \mathrm{H}(\omega), \tag{V.1}$$

where $\omega = (\mathbf{q}, \mathbf{p}) \in \mathbb{R}^{2\mathrm{N}}$ is the configuration of positions and momenta, and J is the real matrix of size 2N:

$$\mathrm{J} := \begin{pmatrix} 0 & \mathrm{I_N} \\ -\mathrm{I_N} & 0 \end{pmatrix}.$$

Let us remark that the matrix J is antisymmetric and orthogonal. The function $\mathrm{H}(\mathbf{q}, \mathbf{p})$ is called the *Hamiltonian* and remains constant along the trajectories.

Definition V.1. *Let* U *be an open set of* $\mathbb{R}^{2N}$. *A differentiable map* $g : U \longrightarrow \mathbb{R}^{2N}$ *is called* symplectic *if the Jacobian matrix* $g'(\mathbf{q},\mathbf{p})$ *satisfies: for all* $(\mathbf{q},\mathbf{p}) \in U$,

$$g'(\mathbf{q},\mathbf{p})^{T} \cdot J \cdot g'(\mathbf{q},\mathbf{p}) = J. \tag{V.2}$$

Equation (V.2) expresses that the map g preserves the area of sets in the $(\mathbf{q},\mathbf{p})$-plane. We recall that the flow $\phi_t : U \longrightarrow \mathbb{R}^{2N}$ of a Hamiltonian system is the mapping:

$$\phi_t(\mathbf{q}_0,\mathbf{p}_0) := (\mathbf{q}(t),\mathbf{p}(t)),$$

where $(\mathbf{q}(t),\mathbf{p}(t))$ is the solution of the system corresponding to initial values $\mathbf{q}(0) = \mathbf{q}_0$ and $\mathbf{p}(0) = \mathbf{p}_0$.

Theorem V.1. (Symplecticity of Hamiltonian flow, Poincaré 1899). *Let* $H(\mathbf{q},\mathbf{p})$ *be a twice continuously differentiable function on* $U \subset \mathbb{R}^{2N}$. *Then, for each fixed* t, *the flow* ϕ_t *is a symplectic transformation wherever it is defined.*

An important property of symplectic transformations, which goes back to Jacobi, is that they preserve the Hamiltonian character of the differential equation. More precisely, symplecticity is a characteristic property of Hamiltonian systems, as stated in the following theorem. We call a differential equation $\dot{\omega}(t) = F(\omega)$ *locally Hamiltonian* if for every $\omega_0 \in U$, there exists a neighbourhood where $F(\omega) = J \cdot \nabla H(\omega)$, for some function H.

Theorem V.2. [44]. *Let* $f : U \longrightarrow \mathbb{R}^{2N}$ *be continuously differentiable. Then,* $\dot{\omega}(t) = F(\omega)$ *is locally Hamiltonian if and only if its flow* $\phi_t(\omega_0)$ *is symplectic for all* $\omega_0 \in U$ *and for sufficiently small* t.

It is then natural to search for numerical methods that share this property. The Hamiltonian flow has another remarkable property: is is symmetric in time, and so could be the numerical scheme.

Definition V.2. *A numerical one-step method is called*

(i) symplectic *if the one-step map* $\Phi_{\Delta t} = y^0 \mapsto y^1 = \Phi_{\Delta t}(y^0)$ *is symplectic whenever the method is applied to a smooth Hamiltonian system.*

(ii) symmetric *if* $\Phi_{\Delta t} \circ \Phi_{-\Delta t} = \mathrm{Id}$.

Finally, it is known that a symplectic method preserves the total energy up to a small error term, for exponentially long times. We refer to [43, Chapter VI], or [44] for more details. Briefly speaking, a good control of the error term needs strong assumptions on the Hamiltonian (like analyticity), and weaker results can be obtained under weaker assumptions.

1.1.2 Numerical Schemes for the Deterministic Dynamics

Symmetrization of schemes – In general, the interactions between oscillators are described by the potential $V(\mathbf{q})$, and the total energy is given by the following Hamiltonian

$$H(\mathbf{q},\mathbf{p}) = V(\mathbf{q}) + \frac{1}{2}\mathbf{p}^{T}M^{-1}\mathbf{p},$$

where M is the matrix of masses, $\mathrm{M} := \mathrm{diag}(m_1, ..., m_{\mathrm{N}})$. As a result, the Hamiltonian can be written as $\mathrm{H}(\mathbf{q},\mathbf{p}) = \mathrm{H}_1(\mathbf{q},\mathbf{p}) + \mathrm{H}_2(\mathbf{q},\mathbf{p})$ with $\mathrm{H}_1(\mathbf{q},\mathbf{p}) := (1/2)\mathbf{p}^{\mathrm{T}}\mathrm{M}^{-1}\mathbf{p}$ and $\mathrm{H}_2(\mathbf{q},\mathbf{p}) = \mathrm{V}(\mathbf{q})$. The system of Newton's equations is then decomposed as

$$\begin{cases} \dot{\mathbf{q}} = \mathrm{M}^{-1}\mathbf{p} \\ \dot{\mathbf{p}} = 0 \end{cases}, \qquad \begin{cases} \dot{\mathbf{q}} = 0 \\ \dot{\mathbf{p}} = -\nabla \mathrm{V}(\mathbf{q}). \end{cases}$$

Each of these Hamiltonian systems has a flow which can be explicitely computed:

$$\phi_t^1(\mathbf{q},\mathbf{p}) = (\mathbf{q} + t\mathrm{M}^{-1}\mathbf{p}, \mathbf{p}), \qquad \phi_t^2(\mathbf{q},\mathbf{p}) = (\mathbf{q}, \mathbf{p} - t\nabla\mathrm{V}(\mathbf{q})).$$

The transformations ϕ_t^1 and ϕ_t^2 are symplectic for all t as they are flows of Hamiltonian systems. A numerical approximation of (V.65) can be obtained for instance by the following splitting (often named as *Lie-Trotter* splitting)

$$(\mathbf{q}^{n+1}, \mathbf{p}^{n+1}) = \phi_{\Delta t}^2 \circ \phi_{\Delta t}^1(\mathbf{q}^n, \mathbf{p}^n). \tag{V.3}$$

More explicitely,

$$\begin{cases} \mathbf{q}^{n+1} = \mathbf{q}^n + \Delta t \mathrm{M}^{-1}\mathbf{p}^n, \\ \mathbf{p}^{n+1} = \mathbf{p}^n - \Delta t \nabla \mathrm{V}(\mathbf{q}^{n+1}). \end{cases}$$

This numerical scheme is called the *symplectic Euler scheme*. It is explicit, and of order[1] 1, but non symmetric. We can obtain an other symplectic Euler scheme by interverting the transformations ϕ^1 and ϕ^2. The *Störmer-Verlet* scheme is more widespread. It symmetrises the decomposition (V.3) by doing the *Strang splitting*

$$\Phi_{\Delta t} = \phi_{\Delta t/2}^2 \circ \phi_{\Delta t}^1 \circ \phi_{\Delta t/2}^2.$$

This gives the following numerical scheme:

$$\begin{cases} \mathbf{p}^{n+1/2} = \mathbf{p}^n - \dfrac{\Delta t}{2}\nabla \mathrm{V}(\mathbf{q}^n), \\ \mathbf{q}^{n+1} = \mathbf{q}^n + \Delta t \mathrm{M}^{-1}\mathbf{p}^{n+1/2}, \\ \mathbf{p}^{n+1} = \mathbf{p}^{n+1/2} - \dfrac{\Delta t}{2}\nabla \mathrm{V}(\mathbf{q}^{n+1}). \end{cases} \tag{V.4}$$

This scheme is explicit, which is really comfortable in statistical physics: systems with large number of particles make indeed implicit algorithms not easily tractable. The numerical flow $\Phi_{\Delta t}$ shares three qualitative properties with the exact Hamiltonian flow: it is time reversible, symmetric, and symplectic [43], which are very important properties as far as the long time numerical integration of Hamiltonian dynamics is concerned. This algorithm also asks for a unique evaluation of the forces $-\nabla \mathrm{V}$ per time step. For all these reasons, it is the most commonly used algorithm in molecular dynamics.

Some elements of backward error analysis – The main motivation of this numerical scheme relies on a backward interpretation, which considers the numerical approximation as the exact

[1]The *order* of a numerical method quantifies the rate of convergence of the numerical approximation to the exact solution. A numerical solution is said to be of order n if the error is proportional to the step-size to the nth power.

solution of a modified problem. This backward analysis illustrates the preservation of invariant measures.

We consider the differential equation $\dot{y} = F(y)$, with its flow ϕ_t, and a numerical one-step method $y^{n+1} = \Phi_{\Delta t}(y^n)$ of order p. The idea consists in searching and studying a modified differential equation

$$\dot{z}(t) = F_{\Delta t}(z) \tag{V.5}$$

such that the exact flow ψ_t of (V.5) is a good approximation of the numerical flow $\Phi_{\Delta t}$, in the sense that $\Phi_{\Delta t}$ is a numerical approximation of order at least $p+1$ of ψ_t. More precisely, we compute the Taylor series expansion of $F_{\Delta t}$ and we identify the terms which appear in the related expansions of both flows (see [43, Chapter IX] for exact computations).

In other words, in our context the numerical scheme exactly conserves an approximate Hamiltonian $H_{\Delta t}$, and this implies an approximate conservation of the exact Hamiltonian. For the harmonic case (i.e. $V(\mathbf{q}) = (1/2)\mathbf{q}^T\mathbf{q}$) and the Störmer-Verlet scheme, the approximate Hamiltonian writes

$$H_{\Delta t}(\mathbf{p},\mathbf{q}) = H(\mathbf{p},\mathbf{q}) - \frac{(\Delta t)^2}{4}\mathbf{q}^T\mathbf{q}.$$

1.2 Sampling for the Initial Measure and Iterations

1.2.1 Heat Baths and Green-Kubo formula

In the framework of linear response theory, the dynamics should involve generalized Langevin equations, which are usually derived with the projection method (onto the conserved quantities), introduced independently by Mori [67] and Zwanzig [84].

Let us be more precise: the system of oscillators is brought into a non-equilibrium steady state, by introducing stochastic perturbations limited to the boundaries of the system. If we want to illustrate the thermal fluctuations of the system through its exchanges with its environment, we can model these exchanges by using a Langevin dynamics which acts at the boundaries.

Consider two heat baths that are coupled respectively to the first and the last particle of the chain. The initial conditions of the baths are distributed according to thermal equilibrium at inverse temperatures β_L and β_R. Integrating the variables of the heat baths leads to a system of random integro-differential equations: the generalized Langevin equations. They differ from the Newton equations of motion by the addition of two kinds of force: a (random) force exerted by the heat baths on the chain of oscillators and a dissipative force with memory which describes the genuine retroaction from the heat bath on the small system.

1.2.2 Sampling for the Initial Canonical Measure

An accurate numerical computation of the phase-space trajectories asks first for a good sampling of the starting points, for instance distributed according to the canonical μ_β defined as

$$d\mu_\beta(\mathbf{q},\mathbf{p}) = Z^{-1}\exp\left(-\beta H(\mathbf{q},\mathbf{p})\right) d\mathbf{q}d\mathbf{p}, \tag{V.6}$$

where β is the mean inverse $\beta = (\beta_L + \beta_R)/2$ in the non-equilibrium case, and $\beta = 1/T$ if the system starts at equilibrium with temperature T. As usual, Z is the normalization constant. In [25], Cancès et al. explain how to compute numerically an invariant distribution using a Langevin dynamics. Going further, [63] provides error estimates on the invariant distribution, and compares the sampling bias obtained for various choices of splitting method.

Indeed, the dynamics (V.65) cannot be used to generate points according to the canonical measure, because the energy H is preserved by the flow. The trajectory of the system remains indeed on the surface of constant energy

$$\left\{(\mathbf{q},\mathbf{p})\ ;\ H(\mathbf{q},\mathbf{p}) = H(\mathbf{q}(0),\mathbf{p}(0))\right\}.$$

In order to generate points according to the canonical measure, stochastic perturbations should ensure that different energy levels will be explored, and eventually all of them. These considerations straightforwardly extend to the numerical case since symplectic methods such as (V.4) almost preserve the energy over extremely long times.

Therefore, the idea consists in introducing some Brownian forces which model fluctuation, balanced with viscous damping forces which model dissipation and we obtain the so-called *Langevin dynamics*. More precisely, the equations of motion read

$$\begin{cases} d\mathbf{q}(t) = M^{-1}\mathbf{p}(t)\ dt \\ d\mathbf{p}(t) = -\nabla V(\mathbf{q}(t))\ dt - \xi M^{-1}\mathbf{p}(t)\ dt + \sigma dW(t) \end{cases} \tag{V.7}$$

where $(W(t))_{t\geqslant 0}$ is a N-dimensional Wiener process. The parameters ξ and σ stand for the magnitude of the dissipation and of the fluctuations respectively, and are linked by the fluctuation-dissipation relation:

$$\sigma = \left(\frac{2\xi}{\beta}\right)^{1/2}.$$

It is straightforward to show that the canonical probability measure (V.6) is a steady state of the Fokker-Planck equation associated with (V.7). In the harmonic case, these Brownian additional forces are not needed. In fact, the Gibbs equilibrium state turns out to be a product of independent Gaussian variables, and the initial configuration can be generated through standard Monte-Carlo simulations.

1.2.3 Final Numerical Scheme

Creating initial conditions –

1. *Initial measure.* First, we sample the canonical measure thanks to the previous Langevin dynamics, or the Monte-Carlo generation of Gaussian variables (in the harmonic case).
2. *Poissonian clocks and random masses.* If the deterministic dynamics is perturbed by the velocity-flip perturbation, then the velocity p_x is changed into p_x at exponentially distributed random times, with an average time γ^{-1}. Therefore, we generate one Poissonian clock τ_x^0 for each oscillator, with τ_x^0 drawn from an exponential law with parameter γ. We do the same for the exchange noise, and we also sample a sequence of random masses attributed to each oscillator if needed.

Iterations of the dynamics – We iterate the numerical scheme for the hybrid dynamics: the equations are governed by the usual Hamiltonian dynamics, to which the stochastic perturbation(s) is superposed.

1. *Verlet part.* We apply the Störmer-Verlet scheme (V.4).

2. *Stochastic noise.* The Poissonian time τ_x^m is updated as follows: if $\tau_x^m \geqslant \Delta t$, then $\tau_x^{m+1} = \tau_x^m - \Delta t$. Otherwise, p_x is flipped into $-p_x$ and τ_x^{m+1} is resampled from an exponential law of parameter γ.

1.3 Hydrodynamic Limits and Diffusion Coefficient

In this subsection we describe the numerical simulations we have implemented. For each one, the time-step Δt is chosen to ensure a good longtime preservation of energy for the deterministic dynamics in the absence of stochastic perturbation. In order to have a relative error in energy less than 10^{-5}, we use $\Delta t = 0.005$.

The velocity-flip model studied in Chapter II yields a system of coupled parabolic equations. Recall that the two profiles of deformation and energy, respectively $\mathbf{r}(t,q)$ and $\mathbf{e}(t,q)$, are defined on $\mathbb{R}_+ \times \mathbb{T}$ and are solutions of

$$\begin{cases} \partial_t \mathbf{r} = \dfrac{1}{\gamma}\partial_q^2 \mathbf{r} \\ \partial_t \mathbf{e} = \dfrac{1}{2\gamma}\partial_q^2\left(\mathbf{e} + \dfrac{\mathbf{r}^2}{2}\right) \end{cases} \qquad q \in \mathbb{T},\ t \in \mathbb{R}_+ \tag{V.8}$$

where γ stands for the intensity of the velocity-flip noise.

On the one hand, the two smooth solutions of (V.8) are simulated through classical finite difference schemes for scalar equations: first, we obtain the deformation $\mathbf{r}$, and then we plug the numerical solution for $\mathbf{r}$ into the second equation, so as to get a parabolic equation with a non trivial second member.

On the other hand, the hydrodynamic behavior of the molecular dynamics is obtained numerically through averaging over numerous replicas of the system. This provides us an efficient way to check the macroscopic behavior of our interacting particle system. Let us remind that the temperature for this model is defined as $\mathrm{T}(t,q) := \mathbf{e}(t,q) - \mathbf{r}^2(t,q)/2$, according to (II.1).

In the numerical simulation below, we used the following initial condition:

$$\mathbf{r}(0,q) = \begin{cases} 1 & \text{if } q \in [0,1/2) \\ 0.1 & \text{if } q \in [1/2,1] \end{cases} \qquad \text{and} \qquad \mathrm{T}(0,q) = \begin{cases} 0.5 & \text{if } q \in [0,1/2) \\ 1 & \text{if } q \in [1/2,1]. \end{cases}$$

These initial conditions correspond to *crenel* functions.

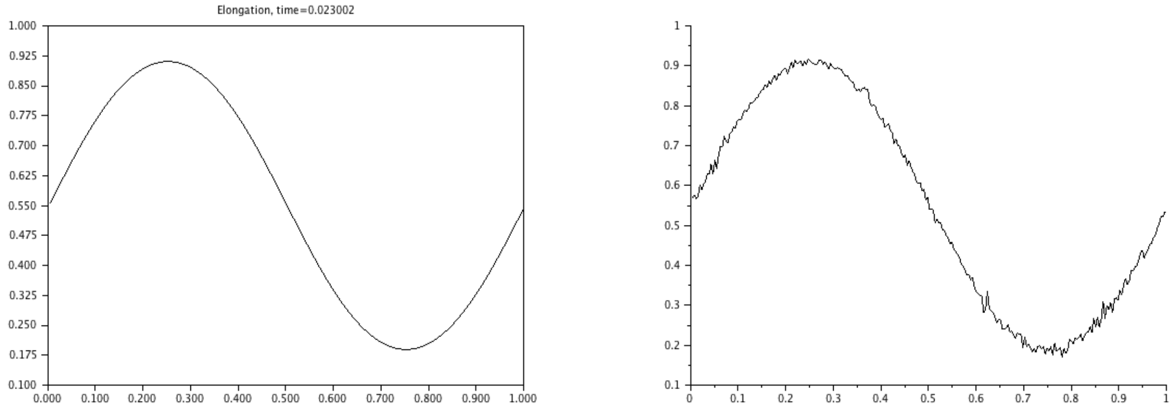

Figure V.1: Two pictures on the elongation profile at fixed time.
Left: Solution of the PDE. **Right:** Hydrodynamic profile with $N = 256$ particles.

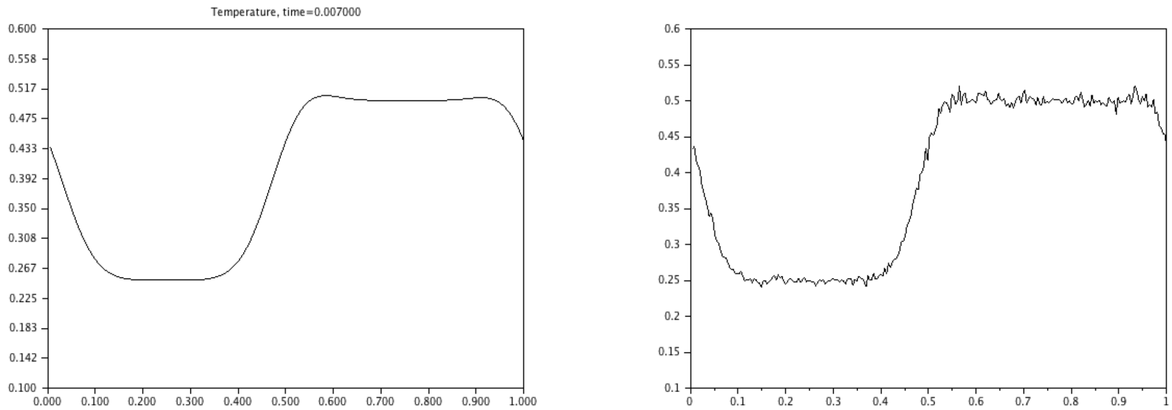

Figure V.2: Two pictures on the temperature profile at fixed time.
Left: Solution of the PDE. **Right:** Hydrodynamic profile with $N = 256$ particles.

In both models of Chapter II and Chapter III, the conservation of the energy gives rise to a diffusion coefficient, which can be defined either by the Green-Kubo formula, or through hydrodynamics.

The conservation law for the energy locally reads, for each atom x,

$$e_x(t) - e_x(0) = J_{x-1,x}(t) - J_{x,x+1}(t)$$

where $e_x(t)$ is the energy at site x, and $J_{x,x+1}(t)$ is energy current exchanged between particles x and $x+1$ up to time t. It can be written as:

$$J_{x,x+1}(t) = \int_0^t j_{x,x+1}(s)\, ds + M_{x,x+1}(t).$$

Here, $M_{x,x+1}(t)$ is a martingale term which can be explicitely written thanks to the stochastic calculus of Itô, and $j_{x,x+1}$ is the instantaneous current of energy between x and $x+1$. Hereafter, for the sake of simplicity, we denote by $Q_x(t)$ the integrated current between the particles x and $x+1$, and $Q(t)$ the total integrated current:

$$Q_x(t) := J_{x,x+1}(t), \qquad Q(t) := \sum_{x \in \mathbb{T}_N} Q_x(t).$$

The thermal conductivity κ of a system can be computed either at equilibrium, using a Green-Kubo formula, or in a non-equilibrium setting. The Green-Kubo method relies on the integration of the heat flux correlation function, and often requires long simulation times for the time integral to converge. The non-equilibrium approach assumes a linear response regime, so that the heat flux depends linearly on the temperature gradient $T_R - T_L$.

1. The *Green-Kubo formula* gives an expression for the thermal conductivity κ, which can be expressed in terms of $Q(t)$:

$$\kappa := \lim_{t\longrightarrow\infty}\lim_{N\longrightarrow\infty} \frac{1}{2T^2}\mathbb{E}_{\mu_\beta^N}\left[\left(\frac{Q(t)}{\sqrt{tN}}\right)^2\right] = \lim_{t\longrightarrow\infty}\lim_{N\longrightarrow\infty}\frac{1}{2T^2N}\frac{\mathbb{E}_{\mu_\beta^N}\left[Q(t)^2\right]}{t}.$$

2. The *Fourier law* provides an other way of simulating. When we add two heat baths in contact with the first and last particle at different temperatures T_R and T_L, the diffusion coefficient naturally appears. Let μ_{ss}^N be the non-equilibrium stationary state. According to the Fourier law,

$$\frac{N\mathbb{E}_{\mu_{ss}^N}\left[j_{x,x+1}\right]}{|T_R - T_L|} \xrightarrow[N\longrightarrow\infty]{} \kappa.$$

Let us recall a few results of Chapter III: we prove that homogenization effect occurs for the Green-Kubo formula: for almost every realization of the mass disorder, the thermal conductivity exists, is independent of the disorder, is positive and finite. When $\gamma > 0$ denotes the intensity of the flip noise, and $\lambda > 0$ the intensity of the exchange noise, we denote the diffusion coefficient by $D(\lambda,\gamma)$. Theorem III.26 states that $D(\lambda,\gamma)$ tends to $D(0,\gamma)$ as λ goes to 0, and that the speed of convergence is at most proportional to $\sqrt{\lambda}$.

This is about be checked by numerical simulations (but not available yet).

2 Technical Details and Proofs

2.1 Technical Proofs of Chapter II

2.1.1 Proof of the Taylor Expansions

Now we prove Proposition II.7. For the sake of simplicity, we define

$$\begin{cases} g_x(\mathbf{r},\mathbf{p}) := -\dfrac{r_x}{2\gamma}\left(p_{x+1}+p_x+\dfrac{\gamma}{2}r_x\right)\ , \\ f_x(\mathbf{r},\mathbf{p}) := -\dfrac{p_{x+1}}{\gamma}\ , \\ \delta_x(\mathbf{r},\mathbf{p}) := \beta_t'\left(\dfrac{x}{N}\right)\ g_x + \lambda_t'\left(\dfrac{x}{N}\right)\ f_x = F\left(t,\dfrac{x}{N}\right)\cdot\tau_x h(\mathbf{r},\mathbf{p})\ . \end{cases}$$

First we will compute the first part that appears in the integral $N^2\left(\phi_t^N\right)^{-1}\mathcal{L}_N^*\phi_t^N$, then we will compute the second part $-\partial_t\phi_t^N/\phi_t^N \times f_t^N$.

First, we compute the term involving the adjoint operator and prove a Taylor expansion.

Lemma V.3.

$$\mathcal{A}\phi_t^{\mathrm{N}} = \frac{\phi_t^{\mathrm{N}}}{\mathrm{N}^2} \sum_{x \in \mathbb{T}_{\mathrm{N}}} \beta_t''\left(\frac{x}{\mathrm{N}}\right) \left[p_{x+1} r_x + \frac{p_x^2 + r_x r_{x-1}}{2\gamma}\right] - \lambda_t''\left(\frac{x}{\mathrm{N}}\right)\left[p_{x+1} + \frac{r_{x+1}}{\gamma}\right]$$
$$+ \frac{\phi_t^{\mathrm{N}}}{\mathrm{N}^2} \sum_{x \in \mathbb{T}_{\mathrm{N}}} \left[\mathcal{L}^*(\delta_x) + \mathcal{A}(\delta_x)\right] + o\left(\frac{1}{\mathrm{N}}\right).$$

Proof. First, remind that the expression of ϕ_t^{N} is given by

$$\phi_t^{\mathrm{N}}(\mathbf{r}, \mathbf{p}) = \frac{(\mathrm{Z}(1,0))^n}{\mathrm{Z}(\chi_t(\cdot))} \prod_{x \in \mathbb{T}_{\mathrm{N}}} \exp\left(e_x\left(-\beta_t\left(\frac{x}{\mathrm{N}}\right) + 1\right) - \lambda_t\left(\frac{x}{\mathrm{N}}\right) r_x + \frac{1}{\mathrm{N}} \mathrm{F}\left(t, \frac{x}{\mathrm{N}}\right) \cdot \tau_x h(\mathbf{r}, \mathbf{p})\right).$$

By definition,

$$\mathcal{A}\phi_t^{\mathrm{N}} = \phi_t^{\mathrm{N}} \sum_{x \in \mathbb{T}_{\mathrm{N}}} \left[\left(1 - \beta_t\left(\frac{x}{\mathrm{N}}\right)\right) \mathcal{A}(e_x) - \lambda_t\left(\frac{x}{\mathrm{N}}\right) \mathcal{A}(r_x)\right] + \frac{\phi_t^{\mathrm{N}}}{\mathrm{N}} \sum_{x \in \mathbb{T}_{\mathrm{N}}} \mathcal{A}(\delta_x).$$

We write down the two conservation laws:

$$\mathcal{A}(e_x) = j_{x+1}^e - j_x^e \quad \text{where } j_x^e := p_x r_{x-1},$$
$$\mathcal{A}(r_x) = j_{x+1}^r - j_x^r \quad \text{where } j_x^r := p_x.$$

Hence,

$$\mathcal{A}\phi_t^{\mathrm{N}} = \phi_t^{\mathrm{N}} \sum_{x \in \mathbb{T}_{\mathrm{N}}} \left[\left(1 - \beta_t\left(\frac{x}{\mathrm{N}}\right)\right) \nabla(j_x^e)_x - \lambda_t\left(\frac{x}{\mathrm{N}}\right) \nabla(j_x^r)_x\right] + \frac{\phi_t^{\mathrm{N}}}{\mathrm{N}} \sum_{x \in \mathbb{T}_{\mathrm{N}}} \mathcal{A}(\delta_x).$$

where $\nabla(f)_x = f_{x+1} - f_x$. We are interested in the first two terms in the sum, and we compute a discrete summation by part. Indeed,

$$\sum_{y \in \mathbb{T}_{\mathrm{N}}} f_y \nabla(g)_y = -\sum_{y \in \mathbb{T}_{\mathrm{N}}} g_{y+1} \nabla(f)_y.$$

We obtain the following terms:

$$\beta_t\left(\frac{x+1}{\mathrm{N}}\right) - \beta_t\left(\frac{x}{\mathrm{N}}\right) = \beta_t'\left(\frac{x}{\mathrm{N}}\right)\frac{1}{\mathrm{N}} + \beta_t''\left(\frac{x}{\mathrm{N}}\right)\frac{1}{\mathrm{N}^2} + \mathrm{O}\left(\frac{1}{\mathrm{N}^3}\right),$$
$$\lambda_t\left(\frac{x+1}{\mathrm{N}}\right) - \lambda_t\left(\frac{x}{\mathrm{N}}\right) = \lambda_t'\left(\frac{x}{\mathrm{N}}\right)\frac{1}{\mathrm{N}} + \lambda_t''\left(\frac{x}{\mathrm{N}}\right)\frac{1}{\mathrm{N}^2} + \mathrm{O}\left(\frac{1}{\mathrm{N}^3}\right).$$

First of all, we look at the term obtained in the sum with $\mathrm{O}\left(\mathrm{N}^{-3}\right)$. We want to prove

$$\mathrm{N}^2 \int \sum_{x \in \mathbb{T}_{\mathrm{N}}} p_{x+1} r_x\, \mathrm{O}\left(\frac{1}{\mathrm{N}^3}\right) f_t^{\mathrm{N}} d\mu_{1,0}^{\mathrm{N}} \leqslant \mathrm{C}\, \mathrm{H}_{\mathrm{N}}(t) + o(\mathrm{N}).$$

We use the entropy inequality. Let $\varepsilon : \mathbb{N} \longrightarrow \mathbb{R}$ be a bounded function. We get

$$\frac{1}{\mathrm{N}} \int \sum_{x \in \mathbb{T}_{\mathrm{N}}} p_{x+1} r_x\, \varepsilon(\mathrm{N}) f_t^{\mathrm{N}} \mathrm{d}\mu_{1,0}^{\mathrm{N}} \leqslant \frac{\mathrm{H}_{\mathrm{N}}(t)}{\alpha} + \frac{1}{\alpha} \log \int \exp\left(\frac{\alpha}{\mathrm{N}} \sum_x p_{x+1} r_x\, \varepsilon(\mathrm{N})\right) \phi_t^{\mathrm{N}} \mathrm{d}\mu_{1,0}^{\mathrm{N}}.$$

But, let us recall the inequality $p_{x+1}r_x \leqslant (p_{x+1}^2 + r_x^2)/2$ and for N large enough, we have

$$\nu^{\mathrm{N}}_{\chi_t(\cdot)}\left[\exp\left(\frac{\alpha}{\mathrm{N}}p_x^2\varepsilon(\mathrm{N})\right)\right] \sim_{\mathrm{N}\longrightarrow\infty} \sqrt{\frac{2\pi\ 2\mathrm{N}}{\mathrm{N}\beta - 2\alpha\varepsilon(\mathrm{N})}} \times \sqrt{\frac{\beta}{2\pi}} = \mathrm{O}(1)\ .$$

We obtain a similar estimate for $\nu^{\mathrm{N}}_{\chi_t(\cdot)}\left[\exp\left(\alpha \mathrm{N}^{-1}r_x\varepsilon(\mathrm{N})\right)\right]$. Therefore, we have showed

$$\frac{1}{\mathrm{N}}\int \sum_{x\in\mathbb{T}_\mathrm{N}} p_{x+1}r_x^2\ \varepsilon(\mathrm{N})f_t^{\mathrm{N}}\mathrm{d}\mu_{1,0} \leqslant \frac{\mathrm{H}_\mathrm{N}(t)}{\alpha} + \mathrm{O}(1)\ .$$

Hence,

$$\begin{aligned}\mathcal{A}\phi_t^{\mathrm{N}} =& \frac{\phi_t^{\mathrm{N}}}{\mathrm{N}}\sum_{x\in\mathbb{T}_\mathrm{N}}\left[\beta_t'\left(\frac{x}{\mathrm{N}}\right)p_{x+1}r_x + \lambda_t'\left(\frac{x}{\mathrm{N}}\right)p_{x+1}\right] + \frac{\phi_t^{\mathrm{N}}}{\mathrm{N}^2}\sum_{x\in\mathbb{T}_\mathrm{N}}\left[\beta_t''\left(\frac{x}{\mathrm{N}}\right)p_{x+1}r_x + \lambda_t''\left(\frac{x}{\mathrm{N}}\right)p_{x+1}\right] \\ &+ \frac{\phi_t^{\mathrm{N}}}{\mathrm{N}}\sum_{x\in\mathbb{T}_\mathrm{N}}\mathcal{A}(\delta_x) + o\left(\frac{1}{\mathrm{N}}\right)\ .\end{aligned}$$

Moreover, we can compute two equations which are called “fluctuation-dissipation equations”. In other words, we decompose the current of energy and the current of deformation as the sum of a discrete gradient and a dissipative term:

$$p_{x+1} = \nabla\left(\frac{-r_x}{\gamma}\right)_x + \mathcal{L}^*(f_x)\ , \tag{V.9}$$

$$p_{x+1}r_x = \nabla\left(-\frac{p_x^2 + r_xr_{x-1}}{2\gamma}\right)_x + \mathcal{L}^*(g_x)\ . \tag{V.10}$$

We use the two equations (V.9) and (V.10), and we obtain

$$\begin{aligned}\mathcal{A}\phi_t^{\mathrm{N}} =& \frac{\phi_t^{\mathrm{N}}}{\mathrm{N}}\sum_{x\in\mathbb{T}_\mathrm{N}}\left\{\beta_t'\left(\frac{x}{\mathrm{N}}\right)\left[\nabla\left(-\frac{p_x^2 + r_xr_{x-1}}{2\gamma}\right)_x + \mathcal{L}^*(g_x)\right] + \lambda_t'\left(\frac{x}{\mathrm{N}}\right)\left[\nabla\left(\frac{-r_x}{\gamma}\right)_x + \mathcal{L}^*(f_x)\right]\right\} \\ &+ \frac{\phi_t^{\mathrm{N}}}{\mathrm{N}^2}\sum_{x\in\mathbb{T}_\mathrm{N}}\left[\beta_t''\left(\frac{x}{\mathrm{N}}\right)p_{x+1}r_x + \lambda_t''\left(\frac{x}{\mathrm{N}}\right)p_{x+1}\right] + \frac{\phi_t^{\mathrm{N}}}{\mathrm{N}}\sum_{x\in\mathbb{T}_\mathrm{N}}\mathcal{A}(\delta_x) + o\left(\frac{1}{\mathrm{N}}\right).\end{aligned}$$

We sum again by part, on the two terms with a gradient, and we obtain as before

$$\begin{aligned}\mathcal{A}\phi_t^{\mathrm{N}} =& \frac{\phi_t^{\mathrm{N}}}{\mathrm{N}^2}\sum_{x\in\mathbb{T}_\mathrm{N}}\left\{\beta_t''\left(\frac{x}{\mathrm{N}}\right)\left[\frac{p_{x+1}^2 + r_xr_{x+1}}{2\gamma} + p_{x+1}r_x\right] + \lambda_t''\left(\frac{x}{\mathrm{N}}\right)\left[\frac{r_{x+1}}{\gamma} + p_{x+1}\right]\right\} \\ &+ \frac{\phi_t^{\mathrm{N}}}{\mathrm{N}}\sum_{x\in\mathbb{T}_\mathrm{N}}\{\mathcal{A}(\delta_x) + \mathcal{L}^*(\delta_x)\} + o\left(\frac{1}{\mathrm{N}}\right).\end{aligned}$$

We get the result. □

LEMMA V.4.

$$\mathcal{S}\phi_t^{\mathrm{N}} = \frac{\phi_t^{\mathrm{N}}}{\mathrm{N}}\sum_{x\in\mathbb{T}_\mathrm{N}}\mathcal{S}(\delta_x) + \frac{\phi_t^{\mathrm{N}}}{4\mathrm{N}^2}\sum_{y\in\mathbb{T}_\mathrm{N}}\left(\sum_{x\in\mathbb{T}_\mathrm{N}}\delta_x(\mathbf{p}^y) - \delta_x(\mathbf{p})\right)^2 + \phi_t^{\mathrm{N}}\ \varepsilon(\mathrm{N})\ ,$$

where $\mu_t^{\mathrm{N}}\left[\mathrm{N}^2\varepsilon(\mathrm{N})\right] = o(\mathrm{N})$.

Proof. Thanks to the exponential term, we have

$$\mathcal{S}\phi_t^{\mathrm{N}} = \frac{\phi_t^{\mathrm{N}}}{2} \sum_{y\in\mathbb{T}_{\mathrm{N}}} \left\{ \exp\left[\frac{1}{\mathrm{N}} \sum_{x\in\mathbb{T}_{\mathrm{N}}} \delta_x(\mathbf{p}^y) - \delta_x(\mathbf{p}) \right] - 1 \right\} .$$

The main idea consists in noting that $e^x - 1 = x + x^2/2 + o(x^2)$. We are going to give a rigorous proof of this estimate in our context thanks to the hypothesis on the energy moments. More precisely, in view of (II.9) and Lemma II.6, we want to prove that

$$\mathrm{N}^2\mu_t^{\mathrm{N}} \left[\sum_{y\in\mathbb{T}_{\mathrm{N}}} \sum_{k\geqslant 3} \frac{\mathrm{F}_y^k}{k!\,\mathrm{N}^k} \right] = o(\mathrm{N}), \text{ where } \mathrm{F}_y = \sum_{x\in\mathbb{T}_{\mathrm{N}}} \big(\delta_x(\mathbf{p}^y) - \delta_x(\mathbf{p})\big) .$$

Let us compute F_y. We notice that in the following expression,

$$\sum_{x\in\mathbb{T}_{\mathrm{N}}} -\beta_t'\left(\frac{x}{\mathrm{N}}\right) \frac{r_x}{2\gamma}(p_{x+1} + p_x + \frac{\gamma}{2} r_x) - \lambda_t'\left(\frac{x}{\mathrm{N}}\right)\frac{p_{x+1}}{\gamma} ,$$

the only terms which are changing when we flip $\mathbf{p}$ into $\mathbf{p}^y$ are

- the term when $x = y$, and the difference is

$$\frac{r_y p_y}{\gamma}\beta_t'\left(\frac{y}{\mathrm{N}}\right) ,$$

- the term when $x = y-1$, and the difference is

$$\frac{r_{y-1}p_y}{\gamma}\beta_t'\left(\frac{y-1}{\mathrm{N}}\right) + \lambda_t'\left(\frac{y-1}{\mathrm{N}}\right)\frac{2p_y}{\gamma} .$$

In other words, we have to show that

$$\mathrm{N}\,\mu_t^{\mathrm{N}} \left[\sum_{y\in\mathbb{T}_{\mathrm{N}}} \sum_{k\geqslant 3} \frac{|\mathrm{F}_y|^k}{k!\,\mathrm{N}^k} \right] \xrightarrow[\mathrm{N}\to\infty]{} 0 .$$

with

$$\begin{aligned} |\mathrm{F}_y(t)| &= \left| \frac{r_y p_y}{\gamma}\beta_t'\left(\frac{y}{\mathrm{N}}\right) + \frac{r_{y-1}p_y}{\gamma}\beta_t'\left(\frac{y-1}{\mathrm{N}}\right) + \lambda_t'\left(\frac{y-1}{\mathrm{N}}\right)\frac{2p_y}{\gamma} \right| \\ &\leqslant \mathrm{C}_0\,|r_y p_y| + \mathrm{C}_1\,|r_{y-1}p_y| + \mathrm{C}_2\,|p_y| \\ &\leqslant \mathrm{C}_0\,\frac{r_y^2 + p_y^2}{2} + \mathrm{C}_1\,\frac{r_{y-1}^2 + p_y^2}{2} + \mathrm{C}_2\,(1 + p_y^2) \\ &\leqslant \mathrm{K}\,(1 + e_y + e_{y-1}) , \end{aligned}$$

where K is a constant which does not depend on N and t. First of all, we introduce the space $\mathrm{A}_y = \{e_y \leqslant 1,\ e_{y-1} \leqslant 1\}$.

$$\begin{aligned} \mathrm{N}\sum_{y\in\mathbb{T}_{\mathrm{N}}} \mu_t^{\mathrm{N}} \left[\sum_{k\geqslant 3} \frac{(e_y + e_{y-1} + 1)^k\,\mathrm{K}^k\,\mathbb{1}_{\{e_y\leqslant 1,\ e_{y-1}\leqslant 1\}}}{k!\,\mathrm{N}^k} \right] &\leqslant \mathrm{N}\sum_{y\in\mathbb{T}_{\mathrm{N}}} \sum_{k\geqslant 3} \frac{(3\mathrm{K})^k}{k!\,\mathrm{N}^k} \\ &= \mathrm{N}^2 \sum_{k\geqslant 3} \frac{(3\mathrm{K})^k}{k!\,\mathrm{N}^k} \xrightarrow[\mathrm{N}\to\infty]{} 0 \end{aligned}$$

Since we have $(e_y+e_{y-1})^k \mathbb{1}_{A_y^C} \leqslant (2e_y+e_{y-1})^k$, we deduce $(e_y+e_{y-1})^k \mathbb{1}_{A_y^C} \leqslant C_0^k\, e_y^k + C_1^k e_{y-1}^k$. Consequently,

$$\mathrm{N}\sum_{y\in\mathbb{T}_\mathrm{N}} \mu_t^\mathrm{N}\left[\sum_{k\geqslant 3}\frac{|\mathrm{F}_y|^k\ \mathrm{K}^k\ \mathbb{1}_{A_y^C}}{k!\ \mathrm{N}^k}\right] \leqslant \mathrm{N}\sum_{y\in\mathbb{T}_\mathrm{N}} \mu_t^\mathrm{N}\left[\sum_{k\geqslant 3}\frac{e_y^k\ \mathrm{K}'^k}{k!\ \mathrm{N}^k}\right] + \mathrm{N}\sum_{y\in\mathbb{T}_\mathrm{N}} \mu_t^\mathrm{N}\left[\sum_{k\geqslant 3}\frac{e_{y-1}^k\ \mathrm{K}'^k}{k!\ \mathrm{N}^k}\right].$$

Now we deal with $\mathrm{N}\sum_{y\in\mathbb{T}_\mathrm{N}} \mu_t^\mathrm{N}\left[\sum_{k\geqslant 3} e_y^k/(k!\mathrm{N}^k)\right]$. Remind that $e_y^k \leqslant 2\ (p_y^{2k}+r_y^{2k})$. We are reduced to prove that

$$\mathrm{N}\sum_{y\in\mathbb{T}_\mathrm{N}} \mu_t^\mathrm{N}\left[\sum_{k\geqslant 3}\frac{p_y^{2k}}{k!\ \mathrm{N}^k}\right] \xrightarrow[\mathrm{N}\longrightarrow\infty]{} 0 \quad \text{and} \quad \mathrm{N}\sum_{y\in\mathbb{T}_\mathrm{N}} \mu_t^\mathrm{N}\left[\sum_{k\geqslant 3}\frac{r_y^{2k}}{k!\ \mathrm{N}^k}\right] \xrightarrow[\mathrm{N}\longrightarrow\infty]{} 0\ .$$

We can flip the summations thanks to Fubini theorem. From the hypothesis on the moments bounds we get

$$\mathrm{N}\sum_{y\in\mathbb{T}_\mathrm{N}} \mu_t^\mathrm{N}\left[\sum_{k\geqslant 3}\frac{p_y^{2k}}{k!\ \mathrm{N}^k}\right] \leqslant \mathrm{N}^2\sum_{k\geqslant 3}\frac{(\mathrm{C}\ k)^k}{k!\ \mathrm{N}^k} \xrightarrow[\mathrm{N}\longrightarrow\infty]{} 0\ .$$

This last limit is deduced from the property of the series $\mathrm{S}(x) := \sum_{k\geqslant 3} k^k\ x^{k-2}/(k!)$. It is a power series which has a strictly positive radius and is continuous at 0. Then,

$$\mathrm{N}^2\sum_{k\geqslant 3}\frac{(\mathrm{C}\ k)^k}{k!\ \mathrm{N}^k} = \mathrm{C}^2\mathrm{S}\left(\frac{\mathrm{C}}{\mathrm{N}}\right) \xrightarrow[\mathrm{N}\longrightarrow\infty]{} 0\ .$$

The same happens for the second sum. It follows that

$$\mathrm{N}\sum_{y\in\mathbb{T}_\mathrm{N}} \mu_t^\mathrm{N}\left[\sum_{k\geqslant 3}\frac{\mathrm{F}_y^k}{k!\ \mathrm{N}^k}\right] \xrightarrow[\mathrm{N}\longrightarrow\infty]{} 0\ .$$

□

After adding the two terms and get some simplifications, we obtain this following final result.

Proposition V.5.

$$\frac{1}{\phi_t^\mathrm{N}}\mathrm{N}^2\mathcal{L}_\mathrm{N}^*\phi_t^\mathrm{N} = \sum_{x\in\mathbb{T}_\mathrm{N}}\left\{-\partial_q^2\beta\left(t,\frac{x}{\mathrm{N}}\right)\left[\frac{p_{x+1}^2+r_{x+1}r_x}{2\gamma}+p_{x+1}r_x\right]-\partial_q^2\lambda\left(t,\frac{x}{\mathrm{N}}\right)\left[\frac{r_{x+1}}{\gamma}+p_{x+1}\right]\right\}$$
$$+\frac{1}{4\gamma}\sum_{x\in\mathbb{T}_\mathrm{N}} p_x^2\left[r_x\partial_q\beta\left(t,\frac{x}{\mathrm{N}}\right)+r_{x-1}\partial_q\beta\left(t,\frac{x-1}{\mathrm{N}}\right)+2\partial_q\lambda\left(t,\frac{x-1}{\mathrm{N}}\right)\right]^2+o(\mathrm{N})\ .$$

Proof. There are simplifications when we write $(-\mathcal{A}+\gamma\mathcal{S})(\phi_t^\mathrm{N})$. Actually,

$$\frac{\phi_t^\mathrm{N}}{\mathrm{N}}\sum_{x\in\mathbb{T}_\mathrm{N}}\{-\mathcal{A}(\delta_x)+\gamma\mathcal{S}(\delta_x)-\mathcal{L}^*(\delta_x)\}=0\ .$$

The result follows. □

Now, we turn to the logarithmic derivative. First, we notice that $\partial_t \phi_t^N / \phi_t^N = \partial_t \{\log(\phi_t^N)\}$. Moreover,

$$\log(\phi_t^N) = C + \sum_{x \in \mathbb{T}_N} e_x \left(-\beta_t \left(\frac{x}{N}\right) + 1 \right) - \lambda_t \left(\frac{x}{N}\right) r_x - \beta_t' \left(\frac{x}{N}\right) \frac{r_x}{2\gamma N} (p_{x+1} + p_x + \frac{\gamma}{2} r_x) \\ + \lambda_t' \left(\frac{x}{N}\right) \frac{p_x}{\gamma N} - \log\left[Z\left(\beta_t(\cdot), \lambda_t(\cdot)\right)\right] .$$

We need to estimate the partition function $Z(\beta_t(\cdot), \lambda_t(\cdot))$. More precisely, in the following lemma we compare this new partition function to the exact partition function

$$\tilde{Z}(\beta_t(\cdot), \lambda_t(\cdot)) = \prod_{x \in \mathbb{T}_N} \frac{2\pi}{\beta_t(x/N)} \exp\left(\frac{\lambda_t^2(x/N)}{2\beta_t(x/N)} \right).$$

Lemma V.6.

$$\left| \partial_t \log Z(\beta_t(\cdot), \lambda_t(\cdot)) - \partial_t \log \tilde{Z}(\beta_t(\cdot), \lambda_t(\cdot)) \right| = O(1) \quad \textit{when } N \longrightarrow \infty.$$

Proof. First of all, remind that the exact expression of $Z_t := Z(\beta_t(\cdot), \lambda_t(\cdot))$ can be written as

$$\begin{aligned} Z_t = &\int_{\mathbb{R}^{2N}} \Bigg[\prod_{x \in \mathbb{T}_N} \exp\Bigg\{ -\beta_t \left(\frac{x}{N}\right) e_x - \lambda_t \left(\frac{x}{N}\right) r_x \\ &\qquad - \frac{1}{N} \beta_t' \left(\frac{x}{N}\right) \frac{r_x}{2\gamma} \left(p_{x+1} + p_x + \frac{\gamma}{2} r_x \right) - \frac{1}{N} \lambda_t' \left(\frac{x}{N}\right) \frac{p_{x+1}}{\gamma} \Bigg\} \Bigg] d\mathbf{p} d\mathbf{r} \\ = &\exp\left\{ \frac{1}{2} \|b_t\|^2 \right\} \int_{\mathbb{R}^{2N}} \exp\left\{ -\frac{1}{2} \langle X - b_t, C_t (X - b_t) \rangle \right\} dX = \exp\left\{ \frac{1}{2} \|b_t\|^2 \right\} (2\pi)^N |\det(C_t)|^{1/2}. \end{aligned}$$

where b_t is a vector and C_t is a symmetric positive matrix. More precisely, one can see that

$$\|b_t\|^2 = \sum_{x \in \mathbb{T}_N} \frac{\lambda_t^2}{\beta_t} \left(\frac{x}{N}\right) + \frac{1}{N} \sum_{x \in \mathbb{T}_N} h_t \left(\frac{x}{N}\right)$$

where h_t is a function that can be easily expressed with $\lambda_t, \beta_t, \lambda_t'$ and β_t'. Then, h_t is smooth. Moreover, C_t can be written as $C_t = D_t + N^{-1} H_t$ with D_t a diagonal matrix and H_t a symmetric matrix which has at most three non-zero components on each row and each column. More precisely,

$$D_t = \begin{pmatrix} \ddots & & (0) \\ & \beta_t(x/N) & \\ (0) & & \ddots \end{pmatrix},$$

$$H_t = \begin{pmatrix} \begin{pmatrix} \ddots & & (0) \\ & -(1/4)\beta_t'(x/N) & \\ (0) & & \ddots \end{pmatrix} & \begin{pmatrix} \ddots & -(2\gamma)^{-1}\beta_t'(x/N) & (0) \\ & -(2\gamma)^{-1}\beta_t'(x/N) & \ddots \\ (0) & & \ddots \end{pmatrix} \\ \begin{pmatrix} \ddots & & (0) \\ \ddots & -(2\gamma)^{-1}\beta_t'(x/N) & \\ (0) & -(2\gamma)^{-1}\beta_t'(x/N) & \ddots \end{pmatrix} & \Big(0\Big) \end{pmatrix}$$

Now we write

$$\partial_t \log Z_t = \frac{1}{2}\sum_x \partial_t \left(\frac{\lambda_t^2}{\beta_t}\left(\frac{x}{N}\right)\right) + \frac{1}{2}\partial_t \log\det(C_t) + \frac{1}{N}\sum_x \partial_t h_t\left(\frac{x}{N}\right),$$
$$\partial_t \log \tilde{Z}_t = \frac{1}{2}\sum_x \partial_t \left(\frac{\lambda_t^2}{\beta_t}\left(\frac{x}{N}\right)\right) + \frac{1}{2}\partial_t \log\det(D_t)\ .$$

But, $\left|N^{-2}\sum_x \partial_t h_t\left(x/N\right)\right| = O(1)$ since h_t is smooth. It remains to show that the following quantity is bounded above by a constant that does not depend on N:

$$\left|\partial_t\left(\log\frac{\det C_t}{\det D_t}\right)\right| = \left|\partial_t\left[\log\det\left(I + \frac{1}{N}D_t^{-1}H_t\right)\right]\right| = \left|\frac{\partial_t\{\det(I + D_t^{-1}H_t/N)\}}{\det(I + D_t^{-1}H_t/N)}\right|\ .$$

We denote by K_t the matrix $D_t^{-1}H_t$, which also has at most three non-zero components on each row and each column, and by K_t' the derivative of K_t with respect to t. We notice that for N large enough, the matrix $I + K_t/N$ is invertible, and we have

$$\left|\partial_t\left(\log\frac{\det C_t}{\det D_t}\right)\right| = \left|\frac{\mathrm{Tr}({}^t\mathrm{com}(I + K_t/N)\cdot(I + K_t'/N))}{\det(I + K_t/N)}\right| = \left|\mathrm{Tr}\left[\left(I + \frac{1}{N}K_t\right)^{-1}\left(I + K_t'\right)\right]\right|,$$

where com(A) is the comatrix of A. Now we deal with $(I + K_t/N)^{-1}$:

$$\left(I + \frac{1}{N}K_t\right)^{-1} = I - K_t + \sum_{k\geqslant 2}\frac{(-1)^k}{N^k}K_t^k\ .$$

But, the component (i,j) of K_t^k can be written as $\sum_{i_1,\dots,i_k} a_{i,i_1}\ a_{i_1,i_2}\cdots\ a_{i_k,j}$ where $a_{i,j}$ are the components of K_t. We know that there are at most three non-zero components on each row and each column, and that they are all bounded by a constant C that does not depend on N (since β_t and λ_t are smooth). Then, it implies that $|\mathrm{Tr}(K_t^k)| \leqslant N3^kC$. It follows that

$$\left|\mathrm{Tr}\left[\left(I + \frac{1}{N}K_t\right)^{-1}\right]\right| = \left|\mathrm{Tr}\left(I - K_t + \sum_{k\geqslant 2}\frac{(-1)^k}{N^k}K_t^k\right)\right| \leqslant 1 + |\mathrm{Tr}(K_t)| + C\sum_{k\geqslant 2}\frac{3^k}{N^{k-1}} = O(1)\ ,$$

because $\mathrm{Tr}(K_t) = O(1)$ (we can compute it and again use the smoothness of the profiles). In the same way, we show that

$$\left|\mathrm{Tr}\left[K_t'\left(I + \frac{1}{N}K_t\right)^{-1}\right]\right| = O(1)\ .$$

This ends the proof. □

We deduce from the previous result that

$$\partial_t \log\left[Z\left(\beta_t(\cdot), \lambda_t(\cdot)\right)\right] = \sum_{x\in\mathbb{T}_N} -\frac{\partial_t\beta_t(x/N)}{\beta_t(x/N)} + \partial_t\lambda_t(x/N)\frac{\lambda_t(x/N)}{\beta_t(x/N)} - \frac{\partial_t\beta_t(x/N)}{2}\frac{\lambda_t^2(x/N)}{\beta_t^2(x/N)} + O(1)\ .$$

Consequently, we have proved the following statement.

Proposition V.7.

$$\partial_t\{\log(\phi_t^{\mathrm{N}})\} = \sum_{x\in\mathbb{T}_{\mathrm{N}}} - e_x\partial_t\beta\left(t,\frac{x}{\mathrm{N}}\right) - r_x\partial_t\lambda\left(t,\frac{x}{\mathrm{N}}\right) - \frac{r_x}{2\gamma\mathrm{N}}\partial_t\partial_q\beta\left(t,\frac{x}{\mathrm{N}}\right)\left(p_{x+1}+p_x+\frac{\gamma}{2}r_x\right)$$
$$- \frac{p_x}{\gamma\mathrm{N}}\partial_t\partial_q\lambda\left(t,\frac{x}{\mathrm{N}}\right) + \frac{\partial_t\beta(t,x/\mathrm{N})}{\beta(t,x/\mathrm{N})}$$
$$- \partial_t\lambda(t,x/\mathrm{N})\frac{\lambda(t,x/\mathrm{N})}{\beta(t,x/\mathrm{N})} + \frac{\partial_t\beta(t,x/\mathrm{N})}{2}\frac{\lambda^2(t,x/\mathrm{N})}{\beta^2(t,x/\mathrm{N})},$$

$$\partial_t\{\log(\phi_t^{\mathrm{N}})\} = \sum_{x\in\mathbb{T}_{\mathrm{N}}} - \left[e_x - \mathbf{e}\left(t,\frac{x}{\mathrm{N}}\right)\right]\partial_t\beta\left(t,\frac{x}{\mathrm{N}}\right) + \left[r_x - \mathbf{r}\left(t,\frac{x}{\mathrm{N}}\right)\right]\partial_t\lambda\left(t,\frac{x}{\mathrm{N}}\right) + \mathrm{O}(1)\ .$$

We are now able to prove the Taylor expansion. According to the results above, we have

$$\frac{1}{\phi_t^{\mathrm{N}}}\mathrm{N}^2\mathcal{L}_{\mathrm{N}}^*\phi_t^{\mathrm{N}} - \partial_t\{\log(\phi_t^{\mathrm{N}})\} = \sum_{x\in\mathbb{T}_{\mathrm{N}}}\left\{-\partial_q^2\beta\left(t,\frac{x}{\mathrm{N}}\right)\left[\frac{p_x^2+r_{x-1}r_x}{2\gamma}+p_xr_{x-1}\right] - \partial_q^2\lambda\left(t,\frac{x}{\mathrm{N}}\right)\left[\frac{r_x}{\gamma}+p_x\right]\right.$$
$$+\frac{p_x^2}{4\gamma}\left[(r_x+r_{x-1})\partial_q\beta\left(t,\frac{x}{\mathrm{N}}\right)+2\partial_q\lambda\left(t,\frac{x}{\mathrm{N}}\right)\right]^2$$
$$\left.+\left[e_x-\mathbf{e}\left(t,\frac{x}{\mathrm{N}}\right)\right]\partial_t\beta\left(t,\frac{x}{\mathrm{N}}\right)+\left[r_x-\mathbf{r}\left(t,\frac{x}{\mathrm{N}}\right)\right]\partial_t\lambda\left(t,\frac{x}{\mathrm{N}}\right)\right\} + o(\mathrm{N})\ . \tag{V.11}$$

Using the notations introduced in Section 2 (Chapter II), this becomes:

$$\frac{1}{\phi_t^{\mathrm{N}}}\mathrm{N}^2\mathcal{L}_{\mathrm{N}}^*\phi_t^{\mathrm{N}} - \partial_t\{\log(\phi_t^{\mathrm{N}})\} = \sum_{x\in\mathbb{T}_{\mathrm{N}}}\left\{-\frac{1}{2\gamma}\partial_q^2\beta\left(t,\frac{x}{\mathrm{N}}\right)\mathrm{J}_x^1 - \frac{1}{\gamma}\partial_q^2\lambda\left(t,\frac{x}{\mathrm{N}}\right)\mathrm{J}_x^2\right.$$
$$+\frac{1}{4\gamma}\left[\partial_q\beta\left(t,\frac{x}{\mathrm{N}}\right)\right]^2\mathrm{J}_x^3 + \frac{1}{\gamma}\partial_q\beta\left(t,\frac{x}{\mathrm{N}}\right)\partial_q\lambda\left(t,\frac{x}{\mathrm{N}}\right)\mathrm{J}_x^4$$
$$+\frac{1}{\gamma}\left[\partial_q\lambda\left(t,\frac{x}{\mathrm{N}}\right)\right]^2\mathrm{J}_x^5$$
$$\left.+\left[e_x-\mathbf{e}\left(t,\frac{x}{\mathrm{N}}\right)\right]\partial_t\beta\left(t,\frac{x}{\mathrm{N}}\right)+\left[r_x-\mathbf{r}\left(t,\frac{x}{\mathrm{N}}\right)\right]\partial_t\lambda\left(t,\frac{x}{\mathrm{N}}\right)\right\} + o(\mathrm{N})\ .$$

We denote by H_k the function defined as follows:

$$\mathrm{H}_k\left(\eta\left(t,\frac{x}{\mathrm{N}}\right)\right) = \mu^{\mathrm{N}}_{\chi_t(x/\mathrm{N})}\left[\mathrm{J}_0^k\right].$$

The explicit formulations for H_k are given by Proposition II.7. The sum

$$\sum_{x\in\mathbb{T}_{\mathrm{N}}}\left\{-\frac{1}{2\gamma}\partial_q^2\beta\left(t,\frac{x}{\mathrm{N}}\right)\mathrm{H}_1\left(\eta\left(t,\frac{x}{\mathrm{N}}\right)\right) - \frac{1}{\gamma}\partial_q^2\lambda\left(t,\frac{x}{\mathrm{N}}\right)\mathrm{H}_2\left(\eta\left(t,\frac{x}{\mathrm{N}}\right)\right)\right.$$
$$+\frac{1}{4\gamma}\left[\partial_q\beta\left(t,\frac{x}{\mathrm{N}}\right)\right]^2\mathrm{H}_3\left(\eta\left(t,\frac{x}{\mathrm{N}}\right)\right)+\frac{1}{\gamma}\partial_q\beta\left(t,\frac{x}{\mathrm{N}}\right)\partial_q\lambda\left(t,\frac{x}{\mathrm{N}}\right)\mathrm{H}_4\left(\eta\left(t,\frac{x}{\mathrm{N}}\right)\right)$$
$$\left.+\frac{1}{\gamma}\left[\partial_q\lambda\left(t,\frac{x}{\mathrm{N}}\right)\right]^2\mathrm{H}_5\left(\eta\left(t,\frac{x}{\mathrm{N}}\right)\right)\right\}$$

is of order $o(\mathrm{N})$ (thanks to the regularity of the functions $\mathbf{e},\mathbf{r},\beta,\lambda$), so that we can introduce it in the right member of the equality (V.11). Then, we obtain after computations

$$-\frac{\partial_q^2\beta}{2\gamma}\,\partial_{\mathbf{e}}\mathrm{H}_1-\frac{\partial_q^2\lambda}{\gamma}\,\partial_{\mathbf{e}}\mathrm{H}_2+\frac{\left[\partial_q\beta\right]^2}{4\gamma}\,\partial_{\mathbf{e}}\mathrm{H}_3+\frac{\partial_q\beta\partial_q\lambda}{\gamma}\,\partial_{\mathbf{e}}\mathrm{H}_4+\frac{\left[\partial_q\lambda\right]^2}{\gamma}d_{\mathbf{e}}\mathrm{H}_5=-\partial_t\beta\ ,$$

and

$$-\frac{\partial_q^2\beta}{2\gamma}\,\partial_{\mathbf{r}}\mathrm{H}_1-\frac{\partial_q^2\lambda}{\gamma}\,\partial_{\mathbf{r}}\mathrm{H}_2+\frac{\left[\partial_q\beta\right]^2}{4\gamma}\,\partial_{\mathbf{r}}\mathrm{H}_3+\frac{\partial_q\beta\partial_q\lambda}{\gamma}\,\partial_{\mathbf{r}}\mathrm{H}_4+\frac{\left[\partial_q\lambda\right]^2}{\gamma}\,\partial_{\mathbf{r}}\mathrm{H}_5=\partial_t\lambda\ .$$

Indeed, these two quantities are respectively equal to

$$\frac{\partial_q^2\beta}{2\gamma}-\frac{\left[\partial_q\beta\right]^2}{\gamma}\left(\mathbf{e}+\frac{\mathbf{r}^2}{2}\right)-2\mathbf{r}\,\frac{\partial_q\beta\partial_q\lambda}{\gamma}-\frac{\left[\partial_q\lambda\right]^2}{\gamma}\ ,$$

and

$$\frac{\partial_q^2\beta}{2\gamma}\,\mathbf{r}+\frac{\partial_q^2\lambda}{\gamma}-\frac{\left[\partial_q\beta\right]^2}{2\gamma}\,\mathbf{r}\left(2\mathbf{e}-3\mathbf{r}^2\right)-\frac{\partial_q\beta\partial_q\lambda}{\gamma}\left(2\mathbf{e}-3\mathbf{r}^2\right)+\mathbf{r}\frac{\left[\partial_q\lambda\right]^2}{\gamma}\ .$$

This concludes the proof and gives Proposition II.7.

2.1.2 One-block Estimate and Large Deviations Replacement

We start with giving a sketch for the proof of the one-block estimate statement (II.15), which is completely done in [16, Section 3.4]. First, we define the space time average of distribution:

$$\bar{f}^{\mathrm{N}}=\frac{1}{t\mathrm{N}}\sum_{i=1}^{\mathrm{N}}\int_0^t\tau_i f_s^{\mathrm{N}}\mathrm{d}s\ ,$$

and $\bar{f}_k^{\mathrm{N}}$ its projection on $\{(r_i,p_i)\in\mathbb{R}^{2(k+1)}\ ;\ i\in\Lambda_k:=\{-[k/2]-1,\dots,[k/2]+1\}\}$.

We also denote $d\nu^{\mathrm{N}}=\bar{f}^{\mathrm{N}}\prod_{i\in\mathbb{T}_{\mathrm{N}}}\mathrm{d}r_i\mathrm{d}p_i$ and $\mathrm{d}\nu_k^{\mathrm{N}}=\bar{f}_k^{\mathrm{N}}\prod_{i\in\mathbb{T}_{\mathrm{N}}}\mathrm{d}r_i\mathrm{d}p_i$ the corresponding probability measures on $\mathbb{R}^{2\mathrm{N}}$ and $\mathbb{R}^{2(k+1)}$.

Observe first that (II.15) can be rewritten as

$$t\limsup_{\mathrm{M}\longrightarrow\infty}\limsup_{\ell\longrightarrow\infty}\limsup_{\mathrm{N}\longrightarrow\infty}\int\left\{\left|\frac{1}{\ell}\sum_{i\in\Lambda_\ell(0)}\mathrm{J}_{i,\mathrm{M}}-\mathrm{H}(\eta_{\ell,\mathrm{M}}(0))\right|\right\}\mathrm{d}\nu^{\mathrm{N}}=0\ ,$$

because

$$\frac{1}{\ell}\sum_{k=0}^{\ell-1}\frac{1}{p}\sum_{j=1}^{p}\tau_{x_j+k}=\frac{1}{\mathrm{N}}\sum_{x=1}^{\mathrm{N}}\tau_x.$$

We give the two main lemmas that can be proved following [16].

Lemma V.8. *For each fixed k, the sequence of probability measures $(\nu_k^{\mathrm{N}})_{\mathrm{N}\geqslant k}$ is tight.*

For any k let ν_k be a limit point of the sequence $(\nu_k^{\mathrm{N}})_{\mathrm{N}\geqslant 1}$. The sequence of probability measures $(\nu_k)_{k\geqslant 1}$ forms a consistent family and by Kolmogorov's theorem there exists a unique probability measure ν on $(\mathbb{R}\times\mathbb{R})^{\mathbb{Z}}$ such that the restriction of ν on $\{(r_i,p_i)\in\mathbb{R}^{2(k+1)}\ ;\ i\in\Lambda_k\}$ is ν_k. One has easily that ν is invariant by translations.

Lemma V.9. *For any bounded smooth local function* $F(\mathbf{r},\mathbf{p})$*, we have* $\int \mathcal{L}F d\nu = 0$.

Then, ν is a convex combination of grand canonical Gibbs measures $\mu_\chi = \mu_{\beta,\lambda}$, precisely we can write $\nu = \int d\rho(\chi)\mu_\chi$, with ρ a probability measure such that $\int d\rho(\chi)\mu_\chi[e_j] \leqslant C_0$ for any $j \in \mathbb{Z}$.

Hence, it results that

$$\begin{aligned}
&\limsup_{M\longrightarrow\infty}\limsup_{\ell\longrightarrow\infty}\limsup_{N\longrightarrow\infty}\int\left\{\left|\frac{1}{\ell}\sum_{i\in\Lambda_\ell(0)} J_{i,M} - H(\eta_{\ell,M}(0))\right|\right\} d\nu^N \\
&\quad = \limsup_{M\longrightarrow\infty}\limsup_{\ell\longrightarrow\infty}\int d\rho(\chi)\int\left\{\left|\frac{1}{\ell}\sum_{i\in\Lambda_\ell(0)} J_{i,M} - H(\eta_{\ell,M}(0))\right|\right\} d\mu_\chi \\
&\quad = \limsup_{M\longrightarrow\infty}\int d\rho(\chi)\left[\limsup_{\ell\longrightarrow\infty}\int\left\{\left|\frac{1}{\ell}\sum_{i\in\Lambda_\ell(0)} J_{i,M} - H(\eta_{\ell,M}(0))\right|\right\} d\mu_\chi\right],
\end{aligned}$$

where the last equality is a consequence of the dominated convergence theorem. Since μ_χ is ergodic with respect to $\{\tau_x \; ; \; x \in \mathbb{Z}\}$, the last term is equal to

$$\limsup_{M\longrightarrow\infty}\int d\rho(\chi)\left|\mu_\chi\left[J_{0,M}\right] - H(\mu_\chi[\eta_{0,M}])\right|.$$

As $M \longrightarrow \infty$, $\mu_\chi[J_{0,M}]$ converges to $\mu_\chi[J_0] = H\big(\mu_\chi[\xi_0]\big)$ and $\mu_\chi[\xi_{0,M}]$ to $\mu_\chi[\xi_0]$. By Fatou's lemma, the limit in M is equal to 0 and this concludes the proof of the one-block lemma.

Finally, we prove the large deviations estimate (Lemma II.8, Section 2.4), and we recall here the result we are going to prove.

Lemma V.10.

$$M_1(N,\ell,k,M) := \frac{1}{\alpha N}\sum_{j=1}^{p}\log\nu^N_{\chi_t(\cdot)}\left[e^{\alpha\ell\left|v\left(t,\frac{[x_j+k]}{N}\right)\Omega\left(\eta_{\ell,M}(x_j+k),\eta\left(t,\frac{[x_j+k]}{N}\right)\right)\right|}\right]$$

can be replaced by

$$M_2(N,\ell,k,M) := \frac{1}{\alpha N}\sum_{j=1}^{p}\log\mu^N_{\chi_t([x_j+k]/N)}\left[e^{\alpha\ell\left|v\left(t,\frac{[x_j+k]}{N}\right)\Omega\left(\eta_{\ell,M}(x_j+k),\eta\left(t,\frac{[x_j+k]}{N}\right)\right)\right|}\right].$$

The difference between these two terms is less than or equal to a small term which depends on ℓ *(but not on* k*) and vanishes in the* N *limit: there exists a constant* $C(\ell,M,N)$ *which does not depend on* k *such that*

$$M_1(N,\ell,k,M) - M_2(N,\ell,k,M) \leqslant C(\ell,M,N) \;\; \text{and} \;\; C(\ell,M,N) \xrightarrow[N\longrightarrow\infty]{} 0\,.$$

Proof. For each $j \in \{1,\dots,p\}$, the function

$$F_j := \exp\left\{\alpha\ell\left|v\left(t,\frac{[x_j+k]}{N}\right)\,\Omega\left(\eta_{\ell,M}(x_j+k),\eta\left(t,\frac{[x_j+k]}{N}\right)\right)\right|\right\}$$

is bounded above by $e^{C\ell}$, $C > 0$ (since $\eta_{\ell,M}$ is bounded and t belongs to a compact set), and depends on the configuration only through the coordinates in $\Lambda_\ell(x_j+k)$. Thus, each expectation appearing in the sum can be taken w.r.t the restriction to $\Lambda_\ell(x_j+k)$ of $\nu^{\mathrm{N}}_{\chi_t(\cdot)}$. These restrictions are inhomogeneous product measures but with slowly varying parameters and hence, each term $\log \nu^{\mathrm{N}}_{\chi_t(\cdot)}[\mathrm{F}_j]$ can be replaced by $\log \mu^{\mathrm{N}}_{\chi_t([x_j+k]/\mathrm{N})}[\mathrm{F}_j]$ with a small error.

Indeed, the difference between these two terms is equal to

$$\log \mu^{\mathrm{N}}_{\chi_t([x_j+k]/\mathrm{N})}\left[1+\frac{\mathrm{F}_j\,(h_j-1)}{\mu^{\mathrm{N}}_{\chi_t([x_j+k]/\mathrm{N})}[\mathrm{F}_j]}\right] = \log\left(1+\frac{\mu^{\mathrm{N}}_{\chi_t([x_j+k]/\mathrm{N})}[\mathrm{F}_j\,(h_j-1)]}{\mu^{\mathrm{N}}_{\chi_t([x_j+k]/\mathrm{N})}[\mathrm{F}_j]}\right)$$

with

$$h_j := \exp\left\{\sum_{i\in\Lambda_\ell(x_j+k)} \xi_{i,\mathrm{M}}\cdot\left[\chi_t\left(\frac{i}{\mathrm{N}}\right)-\chi_t\left(\frac{x_j+k}{\mathrm{N}}\right)\right]+\right.$$
$$\left.-\frac{1}{\mathrm{N}}\mathrm{F}\left(t,\frac{i}{\mathrm{N}}\right)\cdot\tau_i h+\left[\log \mathrm{Z}\left(\chi_t\left(\frac{i}{\mathrm{N}}\right)\right)-\log \mathrm{Z}\left(\chi_t\left(\frac{x_j+k}{\mathrm{N}}\right)\right)\right]\right\}. \quad \text{(V.12)}$$

The inequality $\log(1+x)\leqslant|x|$ (true for any real x) and the fact that $\mu^{\mathrm{N}}_{\chi_t([x_j+k]/\mathrm{N})}[\mathrm{F}_j]\geqslant 1$ reduces us to estimate

$$\mu^{\mathrm{N}}_{\chi_t([x_j+k]/\mathrm{N})}[|\mathrm{F}_j(h_j-1)|]\,.$$

By using the smoothness of χ_t and the inequality $|e^x-1|\leqslant|x|e^{|x|}$, one easily shows that there exist positive constants C_0, $\mathrm{C}(\ell)$, and $\bar\beta$ which do not depend on j such that

$$|\mathrm{F}_j(h_j-1)|\leqslant\frac{\mathrm{C}(\ell)\ell}{\mathrm{N}}\left(\sum_{i\in\Lambda_\ell(x_j+k)}[e_{i,\mathrm{M}}+e_{i+1,\mathrm{M}}+1]\right)\exp\left\{\frac{\mathrm{C}_0\ell}{\mathrm{N}}\sum_{i\in\Lambda_\ell(x_j+k)}[e_{i,\mathrm{M}}+e_{i+1,\mathrm{M}}+1]\right\},$$

$$\text{and}\qquad \left.\frac{d\mu^{\mathrm{N}}_{\chi_t([x_j+k]/\mathrm{N})}}{d\mu^{\mathrm{N}}_{\bar\beta,0}}\right|_{\Lambda_\ell(x_j+k)}\leqslant \mathrm{C}(\ell)\,.$$

Hence, the total error performing by these replacements is bounded above:

$$\mathrm{M}_1(\mathrm{N},\ell,k,\mathrm{M})-\mathrm{M}_2(\mathrm{N},\ell,k,\mathrm{M})\leqslant\frac{1}{\alpha\mathrm{N}}\mathrm{C}_1(\ell,\mathrm{M})\,\mu^{\mathrm{N}}_{\bar\beta,0}\left[\exp\left\{\frac{\mathrm{C}_0}{p}\sum_{i\in\Lambda_\ell(0)}[e_{i,\mathrm{M}}+e_{i+1,\mathrm{M}}+1]\right\}\right]$$

for some positive constant $\mathrm{C}_1(\ell,\mathrm{M})$, and goes to 0 as N goes to infinity for each given fixed ℓ. □

2.2 Technical Proofs of Chapter III

2.2.1 Hermite Polynomials and Quadratic Functions

In the whole subsection, we assume $\beta=1$. Every result can be restated for the general case after multiplying the process by $\beta^{-1/2}$.

Hermite polynomials on $\mathbb{R}^{\mathbb{Z}}$ – Let χ be the set of positive integer-valued functions $\xi : \mathbb{Z} \longrightarrow \mathbb{N}$, such that ξ_x vanish for all but a finite number of $x \in \mathbb{Z}$. The *length* of ξ, denoted by $|\xi|$, is defined as

$$|\xi| := \sum_{x\in\mathbb{Z}} \xi_x.$$

For $\xi \in \chi$, we define the polynomial function on Ω

$$\mathrm{H}_\xi(\omega) = \prod_{x\in\mathbb{Z}} h_{\xi_x}(\omega_x),$$

where $\{h_n\}_{n\in\mathbb{N}}$ are the normalized Hermite polynomials w.r.t. the centered one-dimensional Gaussian law with variance 1. The sequence $\{\mathrm{H}_\xi\}_{\xi\in\chi}$ forms an orthonormal basis of the Hilbert space $\mathbf{L}^2(\mu_1)$, where μ_1 is the infinite product Gibbs measure defined by (I.9). As a result, every function $f \in \mathbf{L}^2(\mu_1)$ can be decomposed in the form

$$f(\omega) = \sum_{\xi\in\chi} \mathrm{F}(\xi)\mathrm{H}_\xi(\omega).$$

Moreover, we can compute the scalar product $\langle f, g\rangle_1$ for $f = \sum_\xi \mathrm{F}(\xi)\mathrm{H}_\xi$ and $g = \sum_\xi \mathrm{G}(\xi)\mathrm{H}_\xi$ as

$$\langle f, g\rangle_1 = \sum_{\xi\in\chi} \mathrm{F}(\xi)\mathrm{G}(\xi).$$

Definition V.3. *We denote by $\chi_n \subset \chi$ the subset sequences of length n, i.e. $\chi_n := \{\xi \in \chi \ ; \ |\xi| = n\}$. A function $f \in \mathbf{L}^2(\mu_1)$ is* of degree n *if its decomposition*

$$f = \sum_{\xi\in\chi} \mathrm{F}(\xi)\mathrm{H}_\xi$$

satisfies: $\mathrm{F}(\xi) = 0$ *for all* $\xi \notin \chi_n$.

In the next paragraph we focus on degree 2 functions, which are by definition on the form

$$\sum_{x\in\mathbb{Z}} \varphi(x,x)(\omega_x^2 - 1) + \sum_{x\neq y} \varphi(x,y)\omega_x\omega_y \tag{V.13}$$

where $\varphi : \mathbb{Z}^2 \longrightarrow \mathbb{R}$ is a square summable symmetric function.

Local functions – On the set of n-tuples $\mathbf{x} := (x_1, \dots, x_n)$ of $\mathbb{Z}^n$, we introduce the equivalence relation $\mathbf{x} \sim \mathbf{y}$ if there exists a permutation σ on $\{1, \dots, n\}$ such that $x_{\sigma(i)} = y_i$ for all $i \in \{1, \dots, n\}$. The class of $\mathbf{x}$ for the relation $\sim$ is denoted by $[\mathbf{x}]$ and its cardinal by $c(\mathbf{x})$. Then the set of configurations of χ_n can be identified with the set of n-tuples classes for $\sim$ by the one-to-one application:

$$\begin{aligned} \mathbb{Z}^n/\sim \quad &\longrightarrow \chi_n \\ [\mathbf{x}] = [(x_1, \dots, x_n)] &\mapsto \quad \xi^{[\mathbf{x}]} \end{aligned}$$

where for any $y \in \mathbb{Z}$, $(\xi^{[\mathbf{x}]})_y = \sum_{i=1}^n \mathbf{1}_{y=x_i}$.

We identify $\xi \in \chi_n$ with the occupation numbers of a configuration with n particles, and $[\mathbf{x}]$ corresponds to the positions of those n particles. A function $\mathrm{F} : \chi_n \longrightarrow \mathbb{R}$ is nothing but a symmetric function $F : \mathbb{Z}^n \longrightarrow \mathbb{R}$ through the identification of ξ with $[\mathbf{x}]$. We denote (with some abuse of notations) by $\langle \cdot, \cdot \rangle$ the scalar product on $\oplus \mathbf{L}^2(\chi_n)$, each χ_n being equipped with the counting measure. Hence, for two functions $F, G : \chi \longrightarrow \mathbb{R}$, we have

$$\langle F, G \rangle = \sum_{n \geqslant 0} \sum_{\xi \in \chi_n} F_n(\xi) G_n(\xi) = \sum_{n \geqslant 0} \sum_{\mathbf{x} \in \mathbb{Z}^n} \frac{1}{c(\mathbf{x})} F_n(\mathbf{x}) G_n(\mathbf{x}),$$

with F_n, G_n the restrictions of F, G to χ_n.

Dirichlet form – It is not hard to check the following proposition, which is a direct consequence of the fact that h_n has the same parity of the integer n.

Proposition V.11. *If a local function $f \in \mathbf{L}^2(\mu_1)$ is written in the form $f = \sum_{\xi \in \chi} F(\xi) H_\xi$, then*

$$\mathcal{S} f(\omega) = \sum_{\xi \in \chi} (\mathfrak{S} F)(\xi) H_\xi(\omega),$$

where $\mathfrak{S}$ is the operator acting on functions $F : \chi \longrightarrow \mathbb{R}$ as

$$\mathfrak{S} F(\xi) = \lambda \sum_{x \in \mathbb{Z}} \left[F(\xi^{x,x+1}) - F(\xi) \right] + \gamma \sum_{x \in \mathbb{Z}} \left((-1)^{\xi_x} - 1 \right) F(\xi).$$

Here, $\xi^{x,y}$ is obtained from ξ by exchanging ξ_x and ξ_y.

From this result we deduce:

Corollary V.12. *For any $f = \sum_{\xi \in \chi} F(\xi) H_\xi \in \mathbf{L}^2(\mu_1)$, we have*

$$\mathcal{D}(f; \mu_1) = \left\langle f, -\mathcal{S} f \right\rangle_1 = \sum_{\xi \in \chi} \left\{ \frac{\lambda}{2} \sum_{x \in \mathbb{Z}} \left(F(\xi^{x,x+1}) - F(\xi) \right)^2 + \gamma \sum_{x \in \mathbb{Z}} \left((-1)^{\xi_x} - 1 \right) F^2(\xi) \right\}$$

Quadratic functions – In Chapter III, we deal with the set of *quadratic* functions f in $\mathbf{L}^2(\mu_1)$, namely degree two functions that are *homogeneous*, i.e. satisfies the algebraic relation

$$\forall \lambda \in \mathbb{R}, \quad f(\lambda \omega) = \lambda^2 f(\omega), \qquad \mu_1 - \text{a.s.} \tag{V.14}$$

We also assume that f has zero average with respect to μ_1. Therefore, we could also rewrite every f as

$$f(\omega) = \sum_{x \in \mathbb{Z}} \psi(x,x)(\omega_x^2 - \omega_{x+1}^2) + \sum_{x \neq y} \psi(x,y) \omega_x \omega_y,$$

for a suitable function $\psi : \mathbb{Z}^2 \longrightarrow \mathbb{R}$ square summable and symmetric, and we recover the form given in (III.1). We first restrict some variational formula to this class of functions, and then we study sequences of functions that weakly converge in $\mathbf{L}^2(\mu_1)$.

Proposition V.13. *If $f \in \mathbf{L}^2(\mu_1)$ is quadratic in the sense above with zero average w.r.t μ_1, then the following variational formula*

$$\sup_{g \in \mathbf{L}^2(\mu_1)} \left\{ 2 \left\langle f, g \right\rangle_1 - \mathcal{D}(g; \mu_1) \right\}$$

can be restricted over quadratic functions g of zero mean w.r.t μ_1.

Proof. This fact follows after decomposing g as $\sum_{\xi \in \chi} \mathrm{G}(\xi)\mathrm{H}_\xi$. Corollary V.12 and the orthogonality of Hermite polynomials imply that we can restrict the supremum over functions g of degree two (V.13). As a result, g writes as the sum of a quadratic function plus an additional constant term.

Then, notice that the constant term gives a zero contribution in the quantity to maximise: indeed, the Dirichlet form does not change if we add a constant, and the function f is supposed to be centered, so that $\langle f \rangle_1 = 0$. Therefore, we can assume that the supremum is taken over homogeneous functions of degree two, and the same argument shows that g can also be taken with zero average. □

Proposition V.14. *Let $\{f_n\}_n$ be a sequence of quadratic functions in $\mathbf{L}^2(\mu_1)$. Suppose that $\{f_n\}$ weakly converges to $f \in \mathbf{L}^2(\mu_1)$. Then, f is quadratic.*

Proof. For all $n \in \mathbb{N}$, and $\xi \notin \chi_2$, the scalar product $\langle f_n, \mathrm{H}_\xi \rangle_1$ vanishes (by definition). From the weak convergence, we know that

$$\langle f_n, \mathrm{H}_\xi \rangle_1 \longrightarrow \langle f, \mathrm{H}_\xi \rangle_1,$$

as n goes to infinity, for all $\xi \in \chi$. This implies: $\langle f, \mathrm{H}_\xi \rangle_1 = 0$ for all $\xi \notin \chi_2$.

Besides, the algebraic relation (V.14) is still valid after taking the weak limit in $\mathbf{L}^2(\mu_1)$, as well as the zero-average property (with respect to μ_1). This implies that the weak limit $f \in \mathbf{L}^2(\mu_1)$ is quadratic, and of zero mean if every f_n is centered. □

Remark *2.1.* In Chapter III, the set denoted by $\mathcal{Q}$ is restricted to *local* quadratic functions. The conclusions of Propositions V.13 and V.14 remain valid if we replace the quadratic functions in $\mathbf{L}^2(\mu_1)$ by elements of $\mathcal{Q}$.

2.2.2 A Weak Version of Closed Forms Results

In that section we prove a theorem that should be thought as a kind of closed forms results, as they are stated in [75] or in [49, Section A.3.4]. We give the link between Theorem V.15 below and closed forms at the end of this paragraph.

Decomposition of quadratic functions – For the sake of clarity, we erase the dependence on the disorder $\mathbf{m}$, and consider that the functions are defined on Ω, and square integrable w.r.t. the Gibbs measure μ_1. We explain how one can restate the same result for functions defined on $\Omega_{\mathcal{D}} \times \Omega$ in Remark 2.2.

Theorem V.15. *Let $\{f_n\}_{n \in \mathbb{N}}$ a sequence of quadratic functions in $\mathbf{L}^2(\mu_1)$. Let us define*

$$g_n := \nabla_0 \left(\Gamma_{f_n} \right) \quad \text{and} \quad h_n := \nabla_{0,1} \left(\Gamma_{f_n} \right).$$

If $\{g_n\}$, respectively $\{h_n\}$, weakly converges in $\mathbf{L}^2(\mu_1)$ towards g, respectively h, then there exist $a \in \mathbb{R}$ and $f \in \mathcal{Q}$ such that

$$g(\omega) = \nabla_0(\Gamma_f)(\omega), \tag{V.15}$$

$$h(\omega) = a(\omega_0^2 - \omega_1^2) + \nabla_{0,1}(\Gamma_f)(\omega), \tag{V.16}$$

where the above equalities are stated in $\mathbf{L}^2(\mu_1)$ sense. This result remains in force if μ_1 is replaced with the product measure $\mathbb{P}_1^\star = \mathbb{P} \otimes \mu_1$, where $\mathbb{P}$ is the law of the disorder (see Remark 2.2).

Proof. From Proposition V.14, we already know that g and h are quadratic functions in $\mathbf{L}^2(\mu_1)$. Hence, we look for g and h of the form

$$g(\omega) = \sum_{x,y\in\mathbb{Z}} \psi_1(x,y)\omega_x\omega_y \tag{V.17}$$

$$h(\omega) = \sum_{x,y\in\mathbb{Z}} \psi_2(x,y)\omega_x\omega_y \tag{V.18}$$

where $\psi_1, \psi_2 : \mathbb{Z}^2 \longrightarrow \mathbb{R}$ are square integrable symmetric functions. We are now going to give a list or equalities, being satisfied by the pair of sequences. Let us be more precise. We define, for a pair $(\mathbf{f}^1, \mathbf{f}^2)$ of two $\mathbf{L}^2(\mu_1)$ functions, the following identities, stated in $\mathbf{L}^2(\mu_1)$ sense:

(R1) $(\tau_x\mathbf{f}^1)(\omega) + (\tau_x\mathbf{f}^1)(\omega^x) = 0$, for all $x \in \mathbb{Z}$.

(R2) $(\tau_x\mathbf{f}^2)(\omega) + (\tau_x\mathbf{f}^2)(\omega^{x,x+1}) = 0$, for all $x \in \mathbb{Z}$.

(R3) $(\tau_x\mathbf{f}^1)(\omega) + (\tau_x\mathbf{f}^2)(\omega^x) = (\tau_x\mathbf{f}^2)(\omega) + (\tau_{x+1}\mathbf{f}^1)(\omega^{x,x+1})$, for all $x \in \mathbb{Z}$,

It is straightforward to check that, for all $n \in \mathbb{N}$, the pair (g_n, h_n) satisfy identities **(R1–R3)**. Easily, one can show that the latter always take place after passing to the weak limit in $\mathbf{L}^2(\mu_1)$. Precisely, the weak limit (g,h) of $\{g_n, h_n\}$ also satisfy **(R1–R3)**. This follows from the following easy lemma (which is a consequence of the translation invariance of μ_1):

Lemma V.16. *If $\{g_n\}_n$ weakly converges in $\mathbf{L}^2(\mu_1)$ towards g, then, for all $x \in \mathbb{Z}$,*

$$\big\{g_n(\omega^x)\big\}_n \textit{ weakly converges towards } g(\omega^x),$$
$$\big\{g_n(\omega^{x,x+1})\big\}_n \textit{ weakly converges towards } g(\omega^{x,x+1}).$$

Notice that all equalities **(R1–R3)** – now stated for (g,h) – turn into identities satisfied by ψ_1 and ψ_2, defined in (V.17) and (V.18). Namely, ψ_1 and ψ_2 have to satisfy

$$\textbf{(R1)} \begin{cases} \psi_1(x,y) = 0 & \text{if } x \neq 0 \text{ and } y \neq 0, \\ \psi_1(0,0) = 0. \end{cases}$$

$$\textbf{(R2)} \begin{cases} \psi_2(x,y) = 0 & \text{if } x \notin \{0,1\} \text{ and } y \notin \{0,1\}, \\ \psi_2(x,x) + \psi_2(x+1,x+1) = 0 & \text{for all } x \in \mathbb{Z}. \end{cases}$$

$$\textbf{(R3)} \begin{cases} 2\psi_2(x,0) = \psi_1(x-1,0) - \psi_1(x,0) & \text{if } x \notin \{0,1\}, \\ \psi_1(-1,0) = \psi_1(1,0). \end{cases}$$

The first two identities imply that g writes in $\mathbf{L}^2(\mu_1)$ on the form

$$g(\omega) = \sum_{x\neq 0} \psi_1(x,0)\omega_x\omega_0, \tag{V.19}$$

and h rewrites as

$$h(\omega) = \sum_{x\neq 0,1} \psi_2(x,0)\big[\omega_1\omega_x - \omega_0\omega_x\big] + \psi_2(0,0)(\omega_0^2 - \omega_1^2), \tag{V.20}$$

whereas the final equality makes a connection between g and h. In view of (V.15) and (V.16), we are going to need the following straightforward lemma:

LEMMA V.17. *Let $f \in \mathbf{L}^2(\mu_1)$ be on the form*

$$f(\omega) = \sum_{x,y\in\mathbb{Z}} \varphi(x,y)\omega_x\omega_y,$$

where $\varphi : \mathbb{Z}^2 \longrightarrow \mathbb{R}$ is a symmetric cylinder function. Then,

$$\nabla_0(\Gamma_f) = -4 \sum_{\substack{z\in\mathbb{Z} \\ x\neq 0}} \varphi(x+z,z)\omega_0\omega_x, \tag{V.21}$$

$$\nabla_{0,1}(\Gamma_f) = 2 \sum_{\substack{z\in\mathbb{Z} \\ x\neq 0,1}} \big[\varphi(x+z,z) - \varphi(x+z,z+1)\big](\omega_1\omega_x - \omega_0\omega_x). \tag{V.22}$$

Confronting (V.21)–(V.22) with (V.19)–(V.20), and keeping in mind the expected result of Theorem V.15, we are now looking for a symmetric function $\varphi : \mathbb{Z}^2 \longrightarrow \mathbb{R}$ which is square-summable on $\mathbb{Z}^2$ and satisfies

$$\begin{cases} \displaystyle\sum_{z\in\mathbb{Z}} \varphi(x+z,z) = -\frac{1}{4}\psi_1(x,0) & \text{for all } x \neq 0, \\ \displaystyle\sum_{z\in\mathbb{Z}} \big[\varphi(x+z,z) - \varphi(x+z,z+1)\big] = \frac{1}{2}\psi_2(x,0) & \text{for all } x \notin \{0,1\}. \end{cases}$$

Such a function φ exists if and only if, for all $x \notin \{0,1\}$,

$$2\psi_2(x,0) = \psi_1(x-1,0) - \psi_1(x,0).$$

This last equality is true according to **(R3)**, and the result is proved, with $a = \psi_2(0,0)$ and $f \in \mathcal{Q}$ defined as

$$f(\omega) = \sum_{x,y\in\mathbb{Z}} \varphi(x,y)\omega_x\omega_y.$$

□

REMARK *2.2.* In the whole section, every result that involves the Gibbs measure μ_1 can be translated into the same result involving the product measure $\mathbb{P}_1^\star$. By instance, the decomposition in the Hilbert space turns into the following: every $f \in \mathbf{L}^2(\mathbb{P}_1^\star)$ can be written as

$$f(\mathbf{m},\omega) = \sum_{\xi\in\chi} \mathrm{F}(\mathbf{m},\xi)\mathrm{H}_\xi(\omega),$$

and if f is quadratic, it rewrites

$$f(\mathbf{m},\omega) = \sum_{x,y\in\mathbb{Z}} \varphi(\mathbf{m},x,y)\omega_x\omega_y,$$

where, for all $\mathbf{m} \in \Omega_{\mathcal{D}}$, $\varphi(\mathbf{m},\cdot,\cdot)$ is a symmetric function on $\mathbb{Z}^2$, square summable and integrable w.r.t. $\mathbb{P}$. Moreover, the translation operator τ_x that is involved in identities **(R1-R3)** should translate also the disorder environment, as it is defined at the beginning of Subsection 1.3, Chapter III. The result follows since $\mathbb{P}_1^\star$ is space-translation invariant.

Connection with closed forms results – Let us briefly explain the connection between Theorem V.15 and the closed forms as they are defined for example in [75]. For that purpose, we are going to reformulate identities **(R1–R3)**. First, interprete $\mathbf{f}^1_x(\omega)$, respectively $\mathbf{f}^2_x(\omega)$, as the price to change the configuration $\omega \in \Omega$ into ω^x, respectively to change ω into $\omega^{x,x+1}$. In particular,

- the price to flip ω_x when the configuration is ω should be equal to $-\mathbf{f}^1_x(\omega^x)$: this is **(R1)**,
- the price to exchange ω_x and ω_{x+1} when the configuration is ω should also be equal to $-\mathbf{f}^2_x(\omega^{x,x+1})$: this is **(R2)**.

In the context of interacting particle systems, *closed forms* are expected to give the same price for any 2-step path with equal end points. In our setting, the last equality **(R3)** can be translated into: "The quantity at site x is flipped, and then exchanged with the quantity at site $x+1$. Equally, the quantities at site x and $x+1$ are exchanged first, and then the quantity at site $x+1$ is flipped." There are three other such paths, that we do not need to prove our statement:

- two quantities are exchanged at sites $x, x+1$, and also independently at sites $y, y+1$, with $\{x, x+1\} \cap \{y, y+1\} = \varnothing$,
- two quantities are flipped independently at sites x and y, with $x \neq y$,
- the quantity at site x is flipped, and then the quantities at sites y and $y+1$ are exchanged, for $y \notin \{x, x+1\}$, and the converse is also possible.

Recall that we have defined $\Omega := \mathbb{R}^{\mathbb{Z}}$. We denote by $\mathcal{B}$ the space of real-valued functions

$$\mathcal{B} := \{f : \Omega \longrightarrow \mathbb{R}\}.$$

We are now interested in the space of *forms*, which are defined as $(\mathbf{f}^1_x, \mathbf{f}^2_x)_{x\in\mathbb{Z}}$ where $\mathbf{f}^1_x \in \mathcal{B}$, and $\mathbf{f}^2_x \in \mathcal{B}$, for every $x \in \mathbb{Z}$. To each function $\mathrm{F} : \Omega \longrightarrow \mathbb{R}$ is associated a form:

Definition V.4. *A form* $\mathbf{f} = (\mathbf{f}^1_x, \mathbf{f}^2_x)_{x\in\mathbb{Z}}$ *is an* exact form *if there exists a continuous function* $\mathrm{F} : \Omega \longrightarrow \mathbb{R}$ *such that*

$$\forall\, x \in \mathbb{Z},\ \forall\, \omega \in \Omega,\ \begin{cases} \mathbf{f}^1_x(\omega) = \mathrm{F}(\omega^x) - \mathrm{F}(\omega), \\ \mathbf{f}^2_x(\omega) = \mathrm{F}(\omega^{x,x+1}) - \mathrm{F}(\omega). \end{cases}$$

Easily, one can prove that all exact forms are closed forms. We now present two examples of closed forms that play a central role.

Example *2.1.* We denote by $\mathfrak{a} = (\mathfrak{a}^1, \mathfrak{a}^1)$ the closed form defined by

$$\begin{cases} \mathfrak{a}^1_x(\omega) = 0, \\ \mathfrak{a}^2_x(\omega) = \omega_x^2 - \omega_{x+1}^2, \end{cases}$$

for all $x \in \mathbb{Z}$ and configurations $\omega \in \Omega$. This closed form corresponds to the formal function $\mathrm{F}(\omega) = \sum_x x\omega_x^2$, but this is not an exact form.

Example *2.2.* Let h be a cylinder function. Let us recall that we denote by Γ_h the formal sum $\sum_x \tau_x h$, and define $\mathfrak{u}_h = (\mathfrak{u}^1_h, \mathfrak{u}^2_h)$ as

$$\begin{cases} (\mathfrak{u}^1_h)_x(\omega) = \Gamma_h(\omega^x) - \Gamma_h(\omega), \\ (\mathfrak{u}^2_h)_x(\omega) = \Gamma_h(\omega^{x,x+1}) - \Gamma_h(\omega), \end{cases}$$

for all $x \in \mathbb{Z}$, and configurations $\omega \in \Omega$. Though $\sum_x \tau_x h$ is a formal sum, these two equalities are well defined. Let us notice that $\mathfrak{u}_h$ is a closed form that is not exact, unless h is constant.

These two examples show that closed forms on Ω are not always exact forms. Let us introduce the notion of a germ of a closed form.

DEFINITION V.5. *A pair of continuous functions $f = (f^1, f^2)$, where $f^i : \Omega \longrightarrow \mathbb{R}$, is a* germ of closed form *if $\mathbf{f} = (\tau_x f)_{x\in\mathbb{Z}}$ is a closed form.*

Examples 2.1 and 2.2 provide two types of germs of closed forms. Consider the cylinder function $\mathfrak{A}(\omega) = (0, \omega_0^2 - \omega_1^2)$. The collection $(\tau_x\mathfrak{A})_{x\in\mathbb{Z}}$ is the closed form $\mathfrak{a}$ of Example 2.1. For a cylinder function h, the collection $(\nabla_x\Gamma_h, \nabla_{x,x+1}\Gamma_h)_{x\in\mathbb{Z}}$ obtained through translations of the cylinder function $(\nabla_0\Gamma_h, \nabla_{0,1}\Gamma_h)$ is the closed from of Example 2.2. For a pair of $\mathbf{L}^2(\mathbb{P}_1^\star)$-functions $f = (f^1, f^2)$, we called it a *germ of closed form* if $\mathbf{f} = (\tau_x f)_{x\in\mathbb{Z}}$ satisfies all of conditions as a closed form in $\mathbf{L}^2(\mathbb{P}_1^\star)$-sense. Usually, Theorem V.15 is replaced with a similar result that concerns every germ of closed form in $\mathbf{L}^2(\mathbb{P}_1^\star)$. We refer the reader to [75, Theorem 5.1] or [49, Theorem A.3.4.14] for more details.

Proof of Lemma III.7 and Lemma III.9 – With Theorem V.15 we are able to prove the missing two lemmas of Chapter III, that we recall here:

LEMMA V.18. *Consider a quadratic cylinder function $\varphi \in \mathcal{Q}_0$. Then,*

$$\limsup_{\ell\longrightarrow\infty}(2\ell)^{-1}\mathbb{E}\left\langle \big(-\mathcal{S}_{\Lambda_\ell}\big)^{-1}\sum_{|x|\leqslant\ell_\varphi}\tau_x\varphi,\ \sum_{|x|\leqslant\ell_\varphi}\tau_x\varphi\right\rangle_1 \leqslant |||\varphi|||_1^2,$$

where ℓ_φ stands for $\ell - s_\varphi - 1$ so that the support of $\tau_x\varphi$ is included in Λ_ℓ for every $x \in \Lambda_{\ell_\varphi}$.

Proof. We follow the proof given in [69, Lemma 4.3] and we assume first that $\varphi = \nabla_0(\mathrm{F}) + \nabla_{0,1}(\mathrm{G})$, for two quadratic cylinder functions F, G. Then, the general case follows by linearity. We write the variational formula

$$(2\ell)^{-1}\mathbb{E}\left\langle \big(-\mathcal{S}_{\Lambda_\ell}\big)^{-1}\sum_{|x|\leqslant\ell_\varphi}\tau_x\varphi,\ \sum_{|x|\leqslant\ell_\varphi}\tau_x\varphi\right\rangle_1 = \sup_{h\in\mathcal{C}}\left\{2\mathbb{E}\left\langle\varphi, \frac{1}{2\ell}\sum_{|x|\leqslant\ell_\varphi}\tau_x h\right\rangle_1 - \frac{1}{2\ell}\mathbb{E}\Big[\mathcal{D}_\ell(\mu_1;h)\Big]\right\}$$

$$= \sup_{h\in\mathcal{C}}\left\{2\mathbb{E}\left\langle \mathrm{F}\nabla_0\left(\frac{1}{2\ell}\sum_{|x|\leqslant\ell_\varphi}\tau_x h\right) + \mathrm{G}\nabla_{0,1}\left(\frac{1}{2\ell}\sum_{|x|\leqslant\ell_\varphi}\tau_x h\right)\right\rangle_1 - \frac{1}{2\ell}\mathbb{E}\left[\mathcal{D}_\ell(\mu_1;h)\right]\right\}.$$

Since φ is quadratic, we can restrict the supremum in the class of quadratic functions h that are localized in Λ_ℓ (the proof of that statement is detailed in Proposition V.13). It turns out that we can also restrict the supremum to functions h such that $\mathbb{E}\left[\mathcal{D}_\ell(\mu_1;h)\right] \leqslant \mathrm{C}\ell$. This follows from the fact that the first term can be bounded as follows (according Proposition III.4 in addition to the convexity of the Dirichlet form):

$$\mathbb{E}\left\langle\varphi, \sum_{|x|\leqslant\ell_\varphi}\tau_x h\right\rangle_1 \leqslant \mathrm{C}_\varphi^{1/2}\left(\mathbb{E}\Big[\mathcal{D}_\ell(\mu_1;h)\Big]\right)^{1/2}.$$

Recall that C_φ is a constant that depends on φ. Next, we want to replace the sums over Λ_{ℓ_φ} with the same sums over Λ_ℓ (recall that $\ell_\varphi = \ell - s_\varphi - 1 \leqslant \ell$). For that purpose, we denote

$$\zeta_0^\ell(h) = \nabla_0\left(\frac{1}{2\ell}\sum_{|x|\leqslant\ell}\tau_x h\right), \qquad \zeta_1^\ell(h) = \nabla_{0,1}\left(\frac{1}{2\ell}\sum_{|x|\leqslant\ell}\tau_x h\right).$$

First of all, from Cauchy-Schwarz inequality, we have

$$\mathbb{E}\Big\langle \frac{\gamma}{2}\Big[\zeta_0^\ell(h)\Big]^2 + \frac{\lambda}{2}\Big[\zeta_1^\ell(h)\Big]^2\Big\rangle_1 \leqslant \frac{1}{2\ell}\mathbb{E}\Big[\mathcal{D}_\ell(\mu_1;h)\Big].$$

Then, we also can write as before

$$\left|\mathbb{E}\Big\langle \varphi, \frac{1}{2\ell}\sum_{\ell_\varphi\leqslant x\leqslant \ell}\tau_x h\Big\rangle_1\right| \leqslant \frac{1}{2\ell}\mathrm{C}_\varphi^{1/2}\Big(\mathbb{E}\Big[\mathcal{D}_\ell(\mu_1;h)\Big]\Big)^{1/2}.$$

These last two inequalities give the upper bound

$$\begin{aligned}(2\ell)^{-1}\mathbb{E}\Big\langle \big(-\mathcal{S}_{\Lambda_\ell}\big)^{-1}\sum_{|x|\leqslant\ell_\varphi}\tau_x\varphi, \sum_{|x|\leqslant\ell_\varphi}\tau_x\varphi\Big\rangle_1 \\ \leqslant \sup_h\Big\{2\mathbb{E}\Big\langle \mathrm{F}\,\zeta_0^\ell(h)+\mathrm{G}\,\zeta_1^\ell(h)\Big\rangle_1 - \mathbb{E}\Big\langle\frac{\gamma}{2}\Big[\zeta_0^\ell(h)\Big]^2+\frac{\lambda}{2}\Big[\zeta_1^\ell(h)\Big]^2\Big\rangle_1\Big\} + \frac{\mathrm{C}}{\sqrt{\ell}}.\end{aligned}$$

Let us choose a sequence $\{h_\ell\}$ satisfying $\mathbb{E}\big[\mathcal{D}_\ell(\mu_1;h_\ell)\big]\leqslant \mathrm{C}\ell$. Then, the sequence $\{\zeta_0^\ell(h_\ell),\zeta_1^\ell(h_\ell)\}$ is uniformly bounded in $\mathbf{L}^2(\mathbb{P}_1^\star)$, and this implies the existence of a weakly convergent subsequence. We denote by (ζ_0,ζ_1) a weak limit and assume that the sequence $\{\zeta_0^\ell(h_\ell),\zeta_1^\ell(h_\ell)\}$ weakly converges to (ζ_0,ζ_1). The conclusion is now based on the weak version of closed forms result that we proved before: the pair (ζ_0,ζ_1) can be written in $\mathbf{L}^2(\mathbb{P}_1^\star)$ as

$$(\nabla_0\Gamma_g, a(\omega_0^2-\omega_1^2)+\nabla_{0,1}\Gamma_g),$$

with $g\in\mathcal{Q}$ and $a\in\mathbb{R}$. We have obtained that

$$\begin{aligned}(2\ell)^{-1}\mathbb{E}\Big\langle\big(-\mathcal{S}_{\Lambda_\ell}\big)^{-1}\sum_{|x|\leqslant\ell_\varphi}\tau_x\varphi,\sum_{|x|\leqslant\ell_\varphi}\tau_x\varphi\Big\rangle_1 &\leqslant \sup_{\zeta_0,\zeta_1}\Big\{2\mathbb{E}\Big\langle \mathrm{F}\,\zeta_0+\mathrm{G}\,\zeta_1\Big\rangle_1 - \frac{\gamma}{2}\mathbb{E}_1^\star\big[\zeta_0^2\big]-\frac{\lambda}{2}\mathbb{E}_1^\star\big[\zeta_1^2\big]\Big\} \\ &= \sup_{\substack{g\in\mathcal{Q}\\ a\in\mathbb{R}}}\Big\{2\mathbb{E}\Big\langle \mathrm{F}\,\nabla_0\Gamma_g+\mathrm{G}\,\big(a(\omega_0^2-\omega_1^2)+\nabla_{0,1}\Gamma_g\big)\Big\rangle_1 \\ &\quad -\frac{\gamma}{2}\mathbb{E}_1^\star\Big[(\nabla_0\Gamma_g)^2\Big]-\frac{\lambda}{2}\mathbb{E}_1^\star\Big[\big(a(\omega_0^2-\omega_1^2)+\nabla_{0,1}\Gamma_g\big)^2\Big]\Big\}\end{aligned}$$

The inequality above is a consequence of the following fact: the $\mathbf{L}^2$-norm may only decrease along weakly convergent subsequences. The result follows, after recalling (III.15). □

The second inequality is more standard, we write down the proof for the sake of completeness:

Lemma V.19. *Under the assumptions of Theorem III.6,*

$$\limsup_{\ell\to\infty}(2\ell)^{-1}\mathbb{E}\Big\langle\big(-\mathcal{S}_{\Lambda_\ell}\big)^{-1}\sum_{|x|\leqslant\ell_\varphi}\tau_x\varphi,\sum_{|x|\leqslant\ell_\varphi}\tau_x\varphi\Big\rangle_1 \geqslant |\!|\!|\varphi|\!|\!|_1^2.$$

Proof. We define, for $f\in\mathcal{Q}$,

$$\mathrm{J}_\ell := \sum_{y,y+1\in\Lambda_\ell}\tau_y j_{0,1}^{\mathrm{S}}, \qquad \mathrm{H}_\ell^f = \sum_{|y|\leqslant \ell-s_f-1}\mathcal{S}(\tau_y f).$$

The following limits hold:

$$\lim_{\ell\longrightarrow\infty}(2\ell)^{-1}\mathbb{E}\left\langle\left(-\mathcal{S}_{\Lambda_\ell}\right)^{-1}\sum_{|x|\leqslant\ell_\varphi}\tau_x\varphi,\mathrm{J}_\ell\right\rangle_1 = \ll\varphi\gg_{1,\star\star}, \tag{V.23}$$

$$\lim_{\ell\longrightarrow\infty}(2\ell)^{-1}\mathbb{E}\left\langle\left(-\mathcal{S}_{\Lambda_\ell}\right)^{-1}\sum_{|x|\leqslant\ell_\varphi}\tau_x\varphi,\mathrm{H}_\ell^f\right\rangle_1 = \ll\varphi,f\gg_{1,\star},$$

$$\lim_{\ell\longrightarrow\infty}(2\ell)^{-1}\mathbb{E}\left\langle\left(-\mathcal{S}_{\Lambda_\ell}\right)^{-1}\left(a\mathrm{J}_\ell+\mathrm{H}_\ell^f\right),a\mathrm{J}_\ell+\mathrm{H}_\ell^f\right\rangle_1 = \frac{\lambda}{2}\mathbb{E}_1^\star\left[\left(a(\omega_0^2-\omega_1^2)+\nabla_{0,1}\Gamma_g\right)^2\right]+\frac{\gamma}{2}\mathbb{E}_1^\star\left[\left(\nabla_0\Gamma_g\right)^2\right].$$

We only prove (V.23), the other relations can be obtained in a similar way. As previously, we assume for the sake of simplicity that $\varphi=\nabla_0(\mathrm{F})+\nabla_{0,1}(\mathrm{G})$. We recall the elementary identity

$$\mathcal{S}_{\Lambda_\ell}\left(\sum_{x\in\Lambda_\ell}x\omega_x^2\right)=\mathrm{J}_\ell(\omega).$$

Therefore,

$$\begin{aligned}(2\ell)^{-1}\mathbb{E}\left\langle\left(-\mathcal{S}_{\Lambda_\ell}\right)^{-1}\sum_{|x|\leqslant\ell_\varphi}\tau_x\varphi,\mathrm{J}_\ell\right\rangle_1 &= -(2\ell)^{-1}\sum_{y,y+1\in\Lambda_\ell}\sum_{|x|\leqslant\ell_\varphi}y\,\mathbb{E}_1^\star\left[\varphi\,\omega_{y-x}^2\right]\\ &= -(2\ell)^{-1}\sum_{y,y+1\in\Lambda_\ell}\sum_{|x|\leqslant\ell_\varphi}y\,\mathbb{E}_1^\star\left[\mathrm{G}\,\nabla_{0,1}(\omega_{y-x}^2)\right]\\ &= -(2\ell)^{-1}\sum_{|x|\leqslant\ell_\varphi}x\,\mathbb{E}_1^\star\left[\mathrm{G}\,\nabla_{0,1}(\omega_0^2)\right]+(x+1)\mathbb{E}_1^\star\left[\mathrm{G}\,\nabla_{0,1}(\omega_1^2)\right]\\ &= (2\ell)^{-1}(2\ell_\varphi+1)\,\mathbb{E}_1^\star\left[\mathrm{G},\omega_0^2-\omega_1^2\right]\xrightarrow[\ell\longrightarrow\infty]{}\ll\varphi\gg_{1,\star\star}.\end{aligned}$$

The last limit comes from Proposition III.1 and the fact that $\ell_\varphi=\ell-s_\varphi-1$. Then, we obtain from the variational formula written with $h=(-\mathcal{S}_{\Lambda_\ell})^{-1}(a\mathrm{J}_\ell+\mathrm{H}_\ell^f)$:

$$\begin{aligned}&\liminf_{\ell\longrightarrow\infty}(2\ell)^{-1}\mathbb{E}\left\langle\left(-\mathcal{S}_{\Lambda_\ell}\right)^{-1}\sum_{|x|\leqslant\ell_\varphi}\tau_x\varphi,\sum_{|x|\leqslant\ell_\varphi}\tau_x\varphi\right\rangle_1\\ &\geqslant\liminf_{\ell\longrightarrow\infty}(2\ell)^{-1}\left\{2\mathbb{E}\left\langle\left(-\mathcal{S}_{\Lambda_\ell}\right)^{-1}\sum_{|x|\leqslant\ell_\varphi}\tau_x\varphi,a\mathrm{J}_\ell+\mathrm{H}_\ell^f\right\rangle_1-\mathbb{E}\left\langle\left(-\mathcal{S}_{\Lambda_\ell}\right)^{-1}\left(a\mathrm{J}_\ell+\mathrm{H}_\ell^f\right),a\mathrm{J}_\ell+\mathrm{H}_\ell^f\right\rangle_1\right\}\\ &=2\ll\varphi,f\gg_{1,\star}+2a\ll\varphi\gg_{1,\star\star}-\mathbb{E}\left[\mathcal{D}_0(\mu_1;a\omega_0^2+\Gamma_f)\right].\end{aligned}$$

The result follows after taking the supremum on $f\in\mathcal{Q}$, and recalling (III.15).

□

2.2.3 Proof of the Weak Sector Condition

In this section we prove Proposition III.15 (Chapter III) that we recall here for the sake of clarity. We write down the result for any $\beta>0$, even if the proof for $\beta=1$ would be sufficient for our purpose.

Proposition V.20 (Weak Sector condition). *(i) There exist two constants* $C_0(\gamma,\lambda)$ *and* $C_1(\gamma,\lambda)$ *such that the following inequality hold for all* $f, g \in \mathcal{Q}$*:*

$$\left| \ll \mathcal{A}^{\mathbf{m}} g, \mathcal{S} f \gg_\beta \right| \leqslant C_0 \|\|\mathcal{S} f\|\|_\beta \|\|\mathcal{S} g\|\|_\beta .$$
$$\left| \ll \mathcal{A}^{\mathbf{m}} g, \mathcal{S} f \gg_\beta \right| \leqslant C_1 \|\|\mathcal{S} g\|\|_\beta + \frac{1}{2} \|\|\mathcal{S} f\|\|_\beta .$$

(ii) There exists a positive constant $C(\beta)$ *such that, for all* $g \in \mathcal{Q}$*,*

$$\|\|\mathcal{A}^{\mathbf{m}} g\|\|_\beta \leqslant C(\beta) \|\|\mathcal{S} g\|\|_\beta .$$

Proof. We prove (i). We assume that

$$g(\mathbf{m},\omega) = \sum_{x\in\mathbb{Z}} \psi_{x,0}(\mathbf{m})(\omega_{x+1}^2 - \omega_x^2) + \sum_{\substack{x\in\mathbb{Z}\\ k\geqslant 1}} \psi_{x,k}(\mathbf{m})\omega_x\omega_{x+k}$$
$$f(\mathbf{m},\omega) = \sum_{x\in\mathbb{Z}} \varphi_{x,0}(\mathbf{m})(\omega_{x+1}^2 - \omega_x^2) + \sum_{\substack{x\in\mathbb{Z}\\ k\geqslant 1}} \varphi_{x,k}(\mathbf{m})\omega_x\omega_{x+k}.$$

We denote by $\nabla^{\mathbf{m}}\psi$ the discrete Laplacian in the variable $\mathbf{m}$, that is

$$\nabla^{\mathbf{m}}\psi(\mathbf{m}) = 2\psi(\mathbf{m}) - \psi(\tau_1\mathbf{m}) - \psi(\tau_{-1}\mathbf{m}),$$

and $\tau_x\nabla^{\mathbf{m}}$ is the operator defined as

$$(\tau_x\nabla^{\mathbf{m}})\psi(\mathbf{m}) := \nabla^{\mathbf{m}}\psi(\tau_x\mathbf{m}).$$

Straightforward computations show that

$$\begin{aligned}
\|\|\mathcal{S} g\|\|_\beta^2 &= \frac{\gamma}{2}\mathbb{E}_\beta^\star\left[\left(\nabla_0\Gamma_g\right)^2\right] + \frac{\lambda}{2}\mathbb{E}_\beta^\star\left[\left(\nabla_{0,1}\Gamma_g\right)^2\right] \\
&= \frac{4\gamma}{\beta^2}\sum_{\substack{x\in\mathbb{Z}\\ k\geqslant 1}} \mathbb{E}[\psi_{x,k}^2] + \frac{2\lambda}{\beta^2}\sum_{x\in\mathbb{Z}}\mathbb{E}\left[\left(\sum_{x\in\mathbb{Z}}\tau_x\left(\nabla^{\mathbf{m}}\psi_{x,0}\right)\right)^2\right] \\
&\quad + \frac{\lambda}{\beta^2}\sum_{k\geqslant 2}\mathbb{E}\left[\left(\sum_{x\in\mathbb{Z}}\left[\tau_{-x}(\psi_{x,k}) - \tau_{1-x}(\psi_{x,k})\right]\right)^2\right],
\end{aligned}$$

$$\|\|\mathcal{S} f\|\|_\beta^2 \geqslant \|\|\mathcal{S}^{\mathrm{flip}} f\|\|_\beta^2 = \frac{\gamma}{2}\mathbb{E}_\beta^\star\left[\left(2\sum_{\substack{z\in\mathbb{Z}\\ k\geqslant 1}}\varphi_{z,k}(\mathbf{m})\omega_0\omega_k\right)^2\right] = \frac{2\gamma}{\beta^2}\sum_{k\geqslant 1}\mathbb{E}\left[\left(\sum_{z\in\mathbb{Z}}\varphi_{z,k}(\mathbf{m})\right)^2\right]. \quad \text{(V.24)}$$

Now we deal with $\ll \mathcal{A}^{\mathbf{m}} g, \mathcal{S} f \gg_\beta$. From Proposition III.10 of Chapter III, and by definition,

$$\begin{aligned}
\ll \mathcal{A}^{\mathbf{m}} g, \mathcal{S} f \gg_\beta &= -\sum_{z\in\mathbb{Z}} \mathbb{E}^\star_\beta \left[f, \tau_z(\mathcal{A}^{\mathbf{m}} g)\right] \\
&= -\sum_{x,z\in\mathbb{Z}} \mathbb{E}\left[\varphi_{x,0}(\mathbf{m})\langle \omega_{x+1}^2 - \omega_x^2, \tau_z(\mathcal{A}^{\mathbf{m}} g)\rangle_\beta\right] - \sum_{\substack{x,z\in\mathbb{Z}\\ k\geqslant 1}} \mathbb{E}\left[\varphi_{x,k}(\mathbf{m})\langle \omega_x\omega_{x+k}, \tau_z(\mathcal{A}^{\mathbf{m}} g)\rangle_\beta\right] \\
&= \frac{2}{\beta^2}\sum_{x\in\mathbb{Z}} \mathbb{E}\left[\frac{\tau_x(\nabla^{\mathbf{m}}\psi_{x,0})}{\sqrt{m_x m_{x+1}}} \sum_{z\in\mathbb{Z}} \tau_{-z}(\varphi_{z,1})\right] \\
&\quad + \frac{1}{\beta^2}\sum_{x\in\mathbb{Z}} \mathbb{E}\left[\left(\frac{\tau_1\psi_{x,1}}{\sqrt{m_x m_{x+1}}} - \frac{\psi_{x,1}}{\sqrt{m_{x+1}m_{x+2}}}\right)\sum_{z\in\mathbb{Z}} \tau_{-z}(\varphi_{z,2})\right] \\
&\quad + \frac{1}{\beta^2}\sum_{k\geqslant 2}\sum_{x\in\mathbb{Z}} \mathbb{E}\left[\left(\frac{\tau_1\psi_{x,k}}{\sqrt{m_x m_{x+1}}} - \frac{\psi_{x,k}}{\sqrt{m_{x+k}m_{x+k+1}}}\right)\sum_{z\in\mathbb{Z}} \tau_{-z}(\varphi_{z,k+1})\right] \\
&\quad + \frac{1}{\beta^2}\sum_{k\geqslant 2}\sum_{x\in\mathbb{Z}} \mathbb{E}\left[\left(\frac{\tau_{-1}\psi_{x,k}}{\sqrt{m_x m_{x+1}}} - \frac{\psi_{x,k}}{\sqrt{m_{x+k}m_{x+k-1}}}\right)\sum_{z\in\mathbb{Z}} \tau_{-z}(\varphi_{z,k-1})\right].
\end{aligned}$$

From Cauchy-Schwarz inequality, and recalling $1/\sqrt{m_0 m_1} \leqslant \mathrm{C}$ ($\mathbb{P}$-a.s.), we obtain the following bound:

$$\begin{aligned}
|\ll \mathcal{A}^{\mathbf{m}} g, \mathcal{S} f \gg_\beta| &\leqslant \frac{2\mathrm{C}}{\beta^2}\mathbb{E}\left[\left(\sum_{x\in\mathbb{Z}} \tau_x(\nabla^{\mathbf{m}}\psi_{x,0})\right)^2\right]^{1/2} \mathbb{E}\left[\left(\sum_{z\in\mathbb{Z}}\tau_{-z}\varphi_{z,1}\right)^2\right]^{1/2} && \text{(V.25)}\\
&\quad + \frac{3\mathrm{C}}{\beta^2}\mathbb{E}\left[\left(\sum_{x\in\mathbb{Z}} \tau_1\psi_{x,1} - \psi_{x,1}\right)^2\right]^{1/2} \mathbb{E}\left[\left(\sum_{z\in\mathbb{Z}}\tau_{-z}\varphi_{z,2}\right)^2\right]^{1/2} && \text{(V.26)}\\
&\quad + \frac{3\mathrm{C}}{\beta^2}\sum_{k\geqslant 2}\mathbb{E}\left[\left(\sum_{x\in\mathbb{Z}} \tau_1\psi_{x,k} - \psi_{x,k}\right)^2\right]^{1/2} \mathbb{E}\left[\left(\sum_{z\in\mathbb{Z}}\tau_{-z}\varphi_{z,k+1}\right)^2\right]^{1/2} \\
&\quad + \frac{3\mathrm{C}}{\beta^2}\sum_{k\geqslant 2}\mathbb{E}\left[\left(\sum_{x\in\mathbb{Z}} \tau_{-1}\psi_{x,k} - \psi_{x,k}\right)^2\right]^{1/2} \mathbb{E}\left[\left(\sum_{z\in\mathbb{Z}}\tau_{-z}\varphi_{z,k-1}\right)^2\right]^{1/2}.
\end{aligned}$$

Now we are going to use two times the trivial inequality $\sqrt{ab} \leqslant a/\varepsilon + \varepsilon b/2$ for a particular choice of $\varepsilon > 0$. In (V.25) we take $\varepsilon = \gamma/\mathrm{C}$ and in (V.26) we take $\varepsilon = 2\gamma/(3\mathrm{C})$. This trick gives the final bound

$$\begin{aligned}
|\ll \mathcal{A}^{\mathbf{m}} g, \mathcal{S} f \gg_\beta| &\leqslant \frac{2\mathrm{C}^2}{\gamma\beta^2}\mathbb{E}\left[\left(\sum_{x\in\mathbb{Z}} \tau_x(\nabla^{\mathbf{m}}\psi_{x,0})\right)^2\right] + \frac{2\gamma}{\beta^2}\sum_{k\geqslant 1}\mathbb{E}\left[\left(\sum_{z\in\mathbb{Z}}\varphi_{z,k}(\tau_{-z}\mathbf{m})\right)^2\right] \\
&\quad + \frac{9\mathrm{C}^2}{\gamma\beta^2}\sum_{k\geqslant 2}\mathbb{E}\left[\left(\sum_{x\in\mathbb{Z}}\tau_1\psi_{x,k} - \psi_{x,k}\right)^2\right].
\end{aligned}$$

Recalling (V.24), we obtain

$$|\ll \mathcal{A}^{\mathbf{m}} g, \mathcal{S} f \gg_\beta| \leqslant \frac{9\mathrm{C}^2}{\gamma\lambda} |||\mathcal{S} g|||_\beta^2 + \frac{1}{2}|||\mathcal{S} f|||_\beta^2.$$

If we use the Cauchy-Schwarz inequality, we get:

$$\ll \mathcal{A}^{\mathrm{m}} g, \mathcal{S} f \gg_{\beta}^{2} \leqslant \frac{18C^2}{\gamma\lambda} |||\mathcal{S} g|||_{\beta}^{2}\ |||\mathcal{S} f|||_{\beta}^{2}.$$

We have proved (i) with $C_0 = \sqrt{18C^2/(\gamma\lambda)}$ and $C_1 = 9C^2/(\gamma\lambda)$. Now we turn to (ii). From Lemma III.13 of Chapter III and Statement (i),

$$\ll \mathcal{A}^{\mathrm{m}} g, j_{0,1}^{\mathrm{S}} \gg_{\beta} = \ll \mathcal{S} g, j_{0,1}^{\mathrm{A}} \gg_{\beta} \leqslant |||\mathcal{S} g|||_{\beta} |||j_{0,1}^{\mathrm{A}}|||_{\beta}.$$

Moreover, from Statement (i), we also get, for all $f \in \mathcal{Q}_0$,

$$-2 \ll \mathcal{A}^{\mathrm{m}} g, \mathcal{S} f \gg_{\beta} \leqslant\ |||\mathcal{S} f|||_{\beta}^{2} + \frac{2C}{\gamma\lambda} |||\mathcal{S} g|||_{\beta}^{2}.$$

As a result, the variational formula (III.19) for $|||\mathcal{A}^{\mathrm{m}} g|||_{\beta}^{2}$ gives:

$$|||\mathcal{A}^{\mathrm{m}} g|||_{\beta}^{2}\ \leqslant\ \frac{1}{\lambda\chi(\beta)} \ll \mathcal{A}^{\mathrm{m}} g, j_{0,1}^{\mathrm{S}} \gg_{\beta}^{2} + \frac{9C^2}{\gamma\lambda} |||\mathcal{S} g|||_{\beta}^{2} \leqslant \left(\frac{|||j_{0,1}^{\mathrm{A}}|||_{\beta}^{2}}{\lambda\chi(\beta)} + \frac{9C^2}{\gamma\lambda} \right) |||\mathcal{S} g|||_{\beta}^{2}.$$

The result is proved. □

2.3 Technical Proofs of Chapter IV

2.3.1 Tools on Fourier Analysis

In Chapter IV, Fourier analysis is one of the most important tools. Actually, the Fourier transform is very useful, since it is reversible, being able to transform from either domain to the other. In the case of a periodic function, the Fourier transform can be simplified to the calculation of series coefficients. Also, when the domain is a lattice, it is still possible to recreate a version of the original Fourier transform according to the Poisson summation formula, also known as discrete-time Fourier transform. In Chapter IV we need to introduce three different Fourier transforms.

1. **Fourier transform of integrable functions –** If $f : \mathbb{R} \longrightarrow \mathbb{R}$ is an integrable function, we define its Fourier transform $\mathcal{F} f : \mathbb{R} \longrightarrow \mathbb{C}$ as

$$\mathcal{F} f(\xi) := \int_{\mathbb{R}} f(x) e^{2i\pi\xi x}\, \mathrm{d}x, \qquad \xi \in \mathbb{R}. \tag{V.27}$$

2. **Fourier transform of square summable sequences –** If $h : \mathbb{Z} \longrightarrow \mathbb{R}$ is square summable, we define its Fourier transform $\widehat{h} : \mathbb{T} \longrightarrow \mathbb{C}$ in $\mathbf{L}^2(\mathbb{T})$ as

$$\widehat{h}(\theta) := \sum_{x\in\mathbb{Z}} h(x) e^{2i\pi\theta x}, \qquad \theta \in \mathbb{T}. \tag{V.28}$$

3. **Discrete Fourier transform of integrable functions –** If $g : \mathbb{R} \longrightarrow \mathbb{R}$ is an integrable function, we define its Fourier transform $\mathcal{F}_n(g) : \mathbb{R} \longrightarrow \mathbb{C}$ as

$$\mathcal{F}_n(g)(\xi) = \frac{1}{n} \sum_{x\in\mathbb{Z}} g\left(\frac{x}{n}\right) e^{2i\pi x\xi/n}, \qquad \xi \in \mathbb{R}. \tag{V.29}$$

These definitions can easily be extended for d-dimensional spaces, $d \geqslant 1$. For each Fourier transform, we have the *Parseval-Plancherel identity* between suitable norms of the involved spaces, and we also can recover the initial functions for the knowledge of their Fourier transforms by the *inverse Fourier transform*.

For example, for the Fourier transform (3), the Parseval-Plancherel identity reads

$$\frac{1}{n}\sum_{x\in\mathbb{Z}}\Big|g\Big(\frac{x}{n}\Big)\Big|^2 = \int_{\left[-\frac{n}{2},\frac{n}{2}\right]} \left|\mathcal{F}_n(g)(\xi)\right|^2 \mathrm{d}\xi.$$

The function g can be recovered from the knowledge of its Fourier transform by the inverse Fourier transform of $\mathcal{F}_n(g)$:

$$g\Big(\frac{x}{n}\Big) = \int_{\left[-\frac{n}{2},\frac{n}{2}\right]} \mathcal{F}_n(g)(\xi)\, e^{-2i\pi x\xi/n}\,\mathrm{d}\xi.$$

Now we give the properties that we need in Chapter IV.

Lemma V.21. *If $g \in \mathcal{S}(\mathbb{R})$ is in the Schwartz space then for any $p \geqslant 1$, there exists a constant* $\mathrm{C} := \mathrm{C}(p,f)$ *such that for any $|y| \leqslant 1/2$,*

$$|\mathcal{F}_n(g)(ny)| \leqslant \frac{\mathrm{C}}{1+(n|y|)^p}.$$

Proof. This lemma is entirely proved in [12]. □

The following result is an easy corollary of the previous lemma.

Corollary V.22. *If $g \in \mathcal{S}(\mathbb{R})$ is in the Schwartz space, then, for any $p \geqslant 0$,*

$$\lim_{n\longrightarrow\infty}\int_{\left[-\frac{n}{2},\frac{n}{2}\right]} |\xi|^p \left|\mathcal{F}_n(g)(\xi)-(\mathcal{F}g)(\xi)\right|^2 \mathrm{d}\xi = 0,$$

and there exists a constant $\mathrm{C} > 0$ *such that*

$$\int_{\left[-\frac{n}{2},\frac{n}{2}\right]} |\xi|^p\, |\mathcal{F}_n(g)(\xi)|^2 \mathrm{d}\xi \leqslant \mathrm{C}.$$

2.3.2 Sharp Estimate of the Resolvent Norm and Boltzmann-Gibbs Principle

Recall the definition of the Hermite polynomials given in Section 2.2.1. Hereafter we consider the orthonormal basis of $\mathbf{L}^2(\mu_\beta)$, for some value of $\beta > 0$. For any $z > 0$ and any $f \in \mathbf{L}^2(\mu_\beta)$ we define the $\mathrm{H}_{\pm 1,z}$ norm of f by

$$\|f\|_{\pm 1,z} = \big\langle f\,,\,(z-\mathcal{S}_n)^{\pm 1} f\big\rangle_\beta^{1/2}.$$

Let us notice that

$$\|f\|_{1,z}^2 = z\langle f, f,\rangle_\beta + \mathcal{D}(\mu_\beta; f)$$

where $\mathcal{D}(\mu_\beta; f) := \langle f, (-\mathcal{S}_n) f\rangle_\beta$ is the Dirichlet form of f. We have seen in Section 2.2.1 that, if f has the decomposition $f = \sum_{\xi\in\chi} \mathrm{F}(\xi)\mathrm{H}_\xi$, then

$$\mathcal{D}(\mu_\beta; f) = \sum_{\xi\in\chi}\left\{\frac{\lambda}{2}\sum_{x\in\mathbb{Z}}\left(\mathrm{F}(\xi^{x,x+1})-\mathrm{F}(\xi)\right)^2 + \gamma_n\sum_{x\in\mathbb{Z}}\left((-1)^{\xi_x}-1\right)\mathrm{F}^2(\xi)\right\}. \qquad \text{(V.30)}$$

We recall some tools presented in [11], which permit to compare the Dirichlet form associated to the symmetric operator $\mathcal{S}_n$ with the Dirichlet form associated to a simple symmetric random walk on $\mathbb{Z}^2$. Let us introduce a few notations. We define

$$\begin{aligned}\Delta_+ &= \left\{(x,y)\in\mathbb{Z}^2\,;\, y\geqslant x+1\right\}\\ \Delta_- &= \left\{(x,y)\in\mathbb{Z}^2\,;\, y\leqslant x-1\right\}\\ \Delta_0 &= \left\{(x,x)\,;\, x\in\mathbb{Z}\right\}.\end{aligned}$$

We denote by $\mathbb{D}$ the Dirichlet form associated to a symmetric simple random walk on $\mathbb{Z}^2$, which satisfies the following two rules: first, jumps from $\Delta_\pm$ to Δ_0 and from Δ_0 to $\Delta_\pm$ have been suppressed, and second, jumps from $(x,x)\in\Delta_0$ to $(x\pm1,x\pm1)\in\Delta_0$ have been added, i.e.

$$\mathbb{D}(f)=\frac{1}{2}\sum_{|\mathbf{e}|=1}\sum_{\substack{\mathbf{x}\in\Delta_\pm\\ \mathbf{x}+\mathbf{e}\in\Delta_\pm}}\big(f(\mathbf{x}+\mathbf{e})-f(\mathbf{x})\big)^2+\frac{1}{2}\sum_{\mathbf{x}\in\Delta_0}\big(f(\mathbf{x}\pm(1,1))-f(\mathbf{x})\big)^2,$$

where $f:\mathbb{Z}^2\longrightarrow\mathbb{R}$ is a square summable symmetric function. The proof of the following lemma is straightforward.

Lemma V.23. *Let $f=\sum_{\xi\in\chi_2}\mathrm{F}(\xi)\mathrm{H}_\xi$ be a local function of degree 2.*

There exists a positive constant C, that does not depend on f and n, such that

$$\mathrm{C}^{-1}\left[\mathbb{D}(f)+\gamma_n\sum_{\mathbf{x}\notin\Delta_0}\mathrm{F}^2(\mathbf{x})\right]\leqslant\mathcal{D}(\mu_\beta;f)\leqslant\mathrm{C}\left[\mathbb{D}(f)+\gamma_n\sum_{\mathbf{x}\notin\Delta_0}\mathrm{F}^2(\mathbf{x})\right].$$

Now we turn to the proof of the Boltzmann-Gibbs principle (Lemma IV.5). Observe that the function φ defined by (IV.10) is a function of degree 2 with a decomposition in the form $\varphi=\sum_{\xi\in\chi_2}\Phi(\xi)\mathrm{H}_\xi$ which satisfies $\Phi(\xi)=0$ if $\xi=2\delta_x$, for some $x\in\mathbb{Z}$. We have that

$$\left\langle\varphi\,,(z-\mathcal{S}_n)^{-1}\varphi\right\rangle_\beta=\sup_g\left\{2\langle\varphi,g\rangle_\beta-z\langle g\,,g\rangle_\beta-\mathcal{D}(\mu_\beta;g)\right\}$$

where the supremum is taken over local functions $g\in\mathbf{L}^2(\mu_\beta)$. From Proposition V.13, we can restrict this supremum over degree 2 functions g, and in addition we can impose that $\mathrm{G}(\xi)=0$ if ξ writes $2\delta_x$ for some $x\in\mathbb{Z}$. Then, by Lemma V.23,

$$\begin{aligned}\left\langle\varphi,(z-\mathcal{S}_n)^{-1}\varphi\right\rangle_\beta\leqslant\mathrm{C}\sup_{\mathrm{G}}\Bigg\{&\sum_{x\neq y}\Phi(x,y)\mathrm{G}(x,y)-(z+\gamma_n)\sum_{\substack{(x,y)\in\mathbb{Z}^2\\ x\neq y}}\mathrm{G}^2(x,y)\\ &-\mathrm{C}'\sum_{|\mathbf{e}|=1}\sum_{\substack{(x,y)\in\Delta^{\neq}\\ (x,y)+\mathbf{e}\in\Delta^{\neq}}}\Big(\mathrm{G}((x,y)+\mathbf{e})-\mathrm{G}(x,y)\Big)^2\Bigg\}\end{aligned}$$

where C,C' are positive constants, $\Delta^{\neq}=\{(x,y)\in\mathbb{Z}^2\,;\,x\neq y\}$ and as usual we identify the functions defined on χ_n with symmetric functions defined on $\mathbb{Z}^n$. In order to get rid of the geometric constraints appearing in the last term of the variational formula, for any symmetric function G defined on the set $\Delta^{\neq}$, we denote by $\tilde{\mathrm{G}}$ its extension to $\mathbb{Z}^2$ defined by

$$\tilde{\mathrm{G}}(x,y)=\mathrm{G}(x,y)\ \text{ if }\ x\neq y,\quad\text{ and }\quad\tilde{\mathrm{G}}(x,x)=\frac{1}{4}\sum_{|\mathbf{e}|=1}\mathrm{G}((x,x)+\mathbf{e}).$$

It is trivial that there exists a constant $C > 0$ such that

$$\sum_{(x,y)\in\mathbb{Z}^2} \tilde{G}^2(x,y) \leqslant C \sum_{\substack{(x,y)\in\mathbb{Z}^2\\ x\neq y}} G^2(x,y),$$

and

$$\sum_{|\mathbf{e}|=1}\sum_{(x,y)\in\mathbb{Z}^2} \Big(\tilde{G}((x,y)+\mathbf{e}) - \tilde{G}(x,y)\Big)^2 \leqslant C \sum_{|\mathbf{e}|=1} \sum_{\substack{(x,y)\in\Delta^{\neq}\\ (x,y)+\mathbf{e}\in\Delta^{\neq}}} \Big(G((x,y)+\mathbf{e}) - G(x,y)\Big)^2.$$

Thus, we have

$$\Big\langle \varphi, (z-\mathcal{S}_n)^{-1}\varphi\Big\rangle_\beta \leqslant C_0 \sup_G \Bigg\{ \sum_{(x,y)\in\mathbb{Z}^2} \Phi(x,y)G(x,y) - C_1(z+\gamma_n)\sum_{(x,y)\in\mathbb{Z}^2} G^2(x,y)$$
$$-C_2 \sum_{|\mathbf{e}|=1}\sum_{(x,y)\in\mathbb{Z}^2} \Big(G((x,y)+\mathbf{e}) - G(x,y)\Big)^2 \Bigg\}$$

where the supremum is now taken over all symmetric local functions $G : \mathbb{Z}^2 \longrightarrow \mathbb{R}$. Notice that the last variational formula is equal to the resolvent norm, for a simple symmetric two dimensional random walk, of the function Φ.

Then by using Fourier transform, it is proved in [11] that the last supremum is equal to

$$\frac{C_0}{4}\int_{[0,1]^2} \frac{|\widehat{\Phi}(\mathbf{k})|^2}{C_1[z+\gamma_n] + 4C_2\sum_{i=1}^2 \sin^2(\pi k_i)} d\mathbf{k}, \tag{V.31}$$

where C_0, C_1, C_2 are three positive constants, and the Fourier transform $\widehat{\Phi}$ of Φ is given by

$$\widehat{\Phi}(\mathbf{k}) = \sum_{(x,y)\in\mathbb{Z}^2} \Phi(x,y) e^{2i\pi(k_1x+k_2y)}, \quad \mathbf{k} = (k_1,k_2)\in[0,1]^2.$$

Thus we have reduced the problem to estimate the behavior w.r.t. n of the integral (V.31) with $z = 1/(tn^a)$. Since the constants t, C_0, C_1, C_2 do not play any role, we fix them equal to 1. The function φ can be rewritten as

$$\varphi(\omega) = \sum_{v>u}\Bigg\{\sum_{z\in\mathbb{Z}} (\nabla_n f)\Big(\frac{z}{n}\Big)\big[\psi_{|v-u|}(u-z-1) - \psi_{|v-u|}(u-z)\big]\Bigg\}\ \omega_u\omega_v = \sum_{u,v}\Phi(u,v)\omega_u\omega_v$$

with the symmetric function Φ given by

$$\Phi(u,v) = \frac{\mathbf{1}_{u\neq v}}{2}\sum_{z\in\mathbb{Z}}(\nabla_n f)\Big(\frac{z}{n}\Big)\big[\psi_{|v-u|}(u\wedge v - z - 1) - \psi_{|v-u|}(u\wedge v - z)\big].$$

Its Fourier transform is given by

$$\widehat{\Phi}(\mathbf{k}) = \sum_{u\in\mathbb{Z}}\sum_{j\geqslant1}\Phi(u,u+j)e^{2i\pi(k_1u+k_2(u+j))} + \sum_{u\in\mathbb{Z}}\sum_{j\geqslant1}\Phi(u+j,u)e^{2i\pi(k_1(u+j)+k_2u)}$$
$$= -\frac{1}{2}\mathcal{F}_n(\Delta_n f)(n(k_1+k_2)) \sum_{j=1}^{\infty}\big(e^{2i\pi k_1 j} + e^{2i\pi k_2 j}\big)\widehat{\psi}_j(k_1+k_2).$$

Since $|\mathcal{F}_n(\Delta_n f)(\xi)| \leqslant C_0$ for a suitable constant $C_0 > 0$ independent of n and ξ, it follows that there exist constants $C, C' > 0$ such that

$$
\begin{aligned}
|\widehat{\Phi}(\mathbf{k})|^2 &\leqslant C\left|\sum_{j=1}^{\infty}\big(e^{2i\pi k_1 j}+e^{2i\pi k_2 j}\big)\widehat{\psi}_j(k_1+k_2)\right|^2 \\
&= C\left|\sum_{j=1}^{\infty}\big(e^{2i\pi k_1 j}+e^{2i\pi k_2 j}+e^{2i\pi k_1 (j-1)}+e^{2i\pi k_2 (j-1)}\big)\widehat{\rho}_j(k_1+k_2)\right|^2 \\
&\leqslant C'\frac{|\widehat{\rho}_1(k_1+k_2)|^2}{(1-|\mathrm{X}(k_1+k_2)|)^2}.
\end{aligned}
$$

To get the last inequality, we used the explicit form of $\widehat{\rho}_j$ and the fact that

$$|1-\mathrm{X}(k_1+k_2)w| \geqslant 1-|\mathrm{X}(k_1+k_2)| > 0$$

for any complex number w of modulus one. Then, from Lemma IV.2 it follows that

$$\frac{|\widehat{\rho}_1(\theta)|^2}{(1-|\mathrm{X}(\theta)|)^2} \leqslant \frac{C}{\gamma_n\big[\gamma_n+\sin^2(\pi\theta)\big]}.$$

It remains to study the behavior of the integral

$$\mathrm{I}_n := \int_{[0,1]^2} \mathrm{d}\mathbf{k}\left\{\frac{1}{(n^{-a}+\gamma_n)+\sin^2(\pi k_1)+\sin^2(\pi k_2)} \times \frac{1}{\gamma_n\left[\gamma_n+\sin^2(\pi(k_1+k_2))\right]}\right\}.$$

The leading term in this integral is provided when

(1) either $\mathbf{k}$ is an extremal point of $[0,1]^2$, i.e. $(0,0),(0,1),(1,0),(1,1)$,
(2) or $\mathbf{k}$ belongs to the diagonal $\{k_1+k_2=1\}$, and $\mathbf{k}$ is not one of the previous four points.

We first consider the first case (1). By periodicity, we can assume that the extremal point is $(0,0)$. We also have that $a > b$, and then $\gamma_n \gg n^{-a}$. We perform a Taylor expansion and forget about the constants. We are reduced to compute the order as n goes to ∞ of

$$\int_{[0,1]^2}\frac{\mathrm{d}\mathbf{k}}{\gamma_n\left[\gamma_n+k_1^2+k_2^2\right]\left[\gamma_n+(k_1+k_2)^2\right]} \approx \int_0^1\frac{r\,\mathrm{d}r}{\gamma_n\big[\gamma_n+r^2\big]^2} \approx n^{2b}.$$

The first estimate comes after a change into polar coordinates, and the last one is deduced from another change of variables:

$$\int_0^1\frac{r\,\mathrm{d}r}{\gamma_n\big[\gamma_n+r^2\big]^2} = \int_0^{1/\sqrt{\gamma_n}}\frac{\mathrm{d}u}{\gamma_n^2\big[1+u^2\big]^2} \approx n^{2b}.$$

In the second case (2), with the same argument we are reduced to investigate the behavior of

$$\int_0^1\frac{r\,\mathrm{d}r}{\gamma_n^2\big[\gamma_n+r^2\big]}$$

which is of the same order n^{2b}.

When $\mathbf{k}$ is not close to one of these points, we can bound by below $\sin^2(\pi k_1)+\sin^2(\pi k_2)$ and $\sin^2(\pi(k_1+k_2))$ by a strictly positive constant independent of n and then show that the corresponding integral gives a smaller contribution. Finally, I_n is of order n^{2b}.

2.3.3 Computations Involving the Generator

In this subsection, we explain how to obtain the differential equations of Proposition IV.7. Let $f : \mathbb{Z} \longrightarrow \mathbb{R}$ be a function of finite support, and let $\mathcal{E}(f) : \Omega \longrightarrow \mathbb{R}$ be defined as

$$\mathcal{E}(f) = \sum_{x \in \mathbb{Z}} f(x)\omega_x^2.$$

A simple computation shows that

$$\mathcal{S}_n \mathcal{E}(f) = \sum_{x \in \mathbb{Z}} \Delta f(x)\omega_x^2,$$

where $\Delta f(x) = f(x+1) + f(x-1) - 2f(x)$ is the discrete Laplacian on $\mathbb{Z}$. On the other hand

$$\mathcal{A}\mathcal{E}(f) = -2\sum_{x \in \mathbb{Z}} \nabla f(x)\omega_x \omega_{x+1},$$

where $\nabla f(x) = f(x+1) - f(x)$ is the discrete right-derivative in $\mathbb{Z}$. Let $f : \mathbb{Z}^2 \longrightarrow \mathbb{R}$ be a symmetric function of finite support, and let $\mathrm{Q}(f) : \Omega \longrightarrow \mathbb{R}$ be defined as

$$\mathrm{Q}(f) = \sum_{\substack{x,y \in \mathbb{Z} \\ x \neq y}} f(x,y)\omega_x \omega_y.$$

Define $\Delta f : \mathbb{Z}^2 \longrightarrow \mathbb{R}$ as

$$\Delta f(x,y) = f(x+1,y) + f(x-1,y) + f(x,y+1) + f(x,y-1) - 4f(x,y)$$

for any $x, y \in \mathbb{Z}$ and $\mathrm{A}f : \mathbb{Z}^2 \longrightarrow \mathbb{R}$ by

$$\mathrm{A}f(x,y) = f(x-1,y) + f(x,y-1) - f(x+1,y) - f(x,y+1)$$

for any $x, y \in \mathbb{Z}$. Notice that Δf is the discrete Laplacian on the lattice $\mathbb{Z}^2$ and $\mathcal{A}f$ is a possible definition of the discrete derivative of f in the direction $(-2,-2)$. Notice that we are using the same symbol Δ for the one-dimensional and two-dimensional, discrete Laplacian. From the context it will be clear which operator is used. We have that

$$\begin{aligned}
\mathcal{S}_n \mathrm{Q}(f) &= \sum_{\substack{x,y \in \mathbb{Z} \\ x \neq y}} \big[(\Delta f)(x,y) - 4\gamma_n f(x,y)\big]\omega_x \omega_y \\
&\quad + 2\sum_{x \in \mathbb{Z}} \Big\{\big[f(x,x+1) - f(x,x)\big] + \big[f(x,x+1) - f(x+1,x+1)\big]\Big\}\omega_x \omega_{x+1} \\
&= \mathrm{Q}(\Delta f - 2\gamma_n \mathrm{Id}) \\
&\quad + 2\sum_{x \in \mathbb{Z}} \Big\{\big[f(x,x+1) - f(x,x)\big] + \big[f(x,x+1) - f(x+1,x+1)\big]\Big\}\omega_x \omega_{x+1}.
\end{aligned}$$

Similarly, we have that

$$\mathcal{A}\mathrm{Q}(f) = \mathrm{Q}(\mathrm{A}f) + 2\sum_{x \in \mathbb{Z}} \Big\{\big[f(x-1,x) - f(x,x+1)\big]\omega_x^2 - \big[f(x,x) - f(x+1,x+1)\big]\omega_x \omega_{x+1}\Big\}.$$

It follows that

$$\mathcal{L}_n \mathrm{Q}(f) = \mathrm{Q}\big((\Delta + \mathrm{A} - 4\gamma_n \mathrm{Id})f\big) + \mathrm{D}(f), \tag{V.32}$$

where the diagonal term $\mathrm{D}(f)$ is given by

$$\mathrm{D}(f)=2\sum_{x\in\mathbb{Z}}\big(\omega_x^2-\beta^{-1}\big)\big(f(x-1,x)-f(x,x+1)\big)+4\sum_{x\in\mathbb{Z}}\big(f(x,x+1)-f(x,x)\big)\omega_x\omega_{x+1}.$$

The normalization constant β^{-1} can be added for free because $f(x,x+1)-f(x-1,x)$ is a mean-zero function. Notice that the operators $f\mapsto \mathrm{Q}(f)$, $f\mapsto \mathcal{L}_n\mathrm{Q}(f)$ are continuous maps from $\ell^2(\mathbb{Z}^2)$ to $\mathbf{L}^2(\mu_\beta)$. Therefore, an approximation procedure shows that the identities above hold true for any $f\in\ell^2(\mathbb{Z}^2)$. Recalling the definition of $\mathcal{S}_t^n$, we deduce (IV.15), that is

$$\frac{d}{dt}\mathcal{S}_t^n=\frac{1}{n}\frac{\beta^2}{2}\mathbb{E}_{\mathbb{P}_1}\Big[\sum_{x\in\mathbb{Z}}g\left(\frac{x}{n}\right)\big(\omega_x^2(0)-\beta^{-1}\big)\times n^{3/2}\mathcal{L}_n\big(\mathcal{E}(f)\big)\Big]=-2\mathrm{Q}_t^n(\nabla_n f\otimes\delta)+\mathcal{S}_t^n\big(n^{-1/2}\Delta_n f\big).$$

2.3.4 Proof of Lemma IV.10

Let us define the following functions, for $x,y\in\mathbb{Z}$

$$\Lambda(x,y)=4\big[\sin^2(\pi x)+\sin^2(\pi y)\big],\quad \Omega(x,y)=2\big[\sin(2\pi x)+\sin(2\pi y)\big]. \tag{V.33}$$

Several times we will use the following elementary change of variable property proved in [12].

Lemma V.24. *Let $f:\mathbb{R}^2\longrightarrow\mathbb{C}$ be a n-periodic function in each direction of $\mathbb{R}^2$. Then we have*

$$\iint_{[-\frac{n}{2},\frac{n}{2}]^2}f(k,\ell)\,\mathrm{d}k\mathrm{d}\ell=\iint_{[-\frac{n}{2},\frac{n}{2}]^2}f(\xi-\ell,\ell)\,\mathrm{d}\xi\mathrm{d}\ell.$$

The proof is similar to the proof given in [12]. The Fourier transform of h_n is given by

$$\mathcal{F}_n(h)(k,\ell)=\frac{1}{2\sqrt{n}}\frac{i\Omega\big(\frac{k}{n},\frac{\ell}{n}\big)\mathcal{F}_n(f)(k+\ell)}{\big(\Lambda+4\gamma_n-i\Omega\big)\big(\frac{k}{n},\frac{\ell}{n}\big)}, \tag{V.34}$$

where Λ and Γ are defined in (V.33). Observe first that

$$i\Omega\big(\tfrac{\xi-\ell}{n},\tfrac{\ell}{n}\big)=e^{\frac{2i\pi\ell}{n}}\Big(1-e^{-\frac{2i\pi\xi}{n}}\Big)-e^{-\frac{2i\pi\ell}{n}}\Big(1-e^{\frac{2i\pi\xi}{n}}\Big)$$

so that

$$\Big|i\Omega\big(\tfrac{\xi-\ell}{n},\tfrac{\ell}{n}\big)\Big|^2\leqslant 4\Big|1-e^{\frac{2i\pi\xi}{n}}\Big|^2=16\sin^2\Big(\frac{\pi\xi}{n}\Big).$$

Then, by Plancherel-Parseval relation and Lemma V.24 we have that

$$\begin{aligned}\|h_n\|_{2,n}^2&=\iint_{[-\frac{n}{2},\frac{n}{2}]^2}|\mathcal{F}_n(h)(k,\ell)|^2\,\mathrm{d}k\mathrm{d}\ell=\frac{1}{4n}\iint_{[-\frac{n}{2},\frac{n}{2}]^2}\frac{\Omega^2\big(\frac{k}{n},\frac{\ell}{n}\big)\,|\mathcal{F}_n(f)(k+\ell)|^2}{\Big(\Lambda\big(\frac{k}{n},\frac{\ell}{n}\big)+4\gamma_n\Big)^2+\Omega^2\big(\frac{k}{n},\frac{\ell}{n}\big)}\,\mathrm{d}k\mathrm{d}\ell\\&\leqslant\frac{1}{n}\int_{[-\frac{n}{2},\frac{n}{2}]}\Big|1-e^{\frac{2i\pi\xi}{n}}\Big|^2\,|\mathcal{F}_n(f)(\xi)|^2\left\{\int_{[-\frac{n}{2},\frac{n}{2}]}\frac{\mathrm{d}\ell}{\Lambda^2\big(\frac{\xi-\ell}{n},\frac{\ell}{n}\big)+\Omega^2\big(\frac{\xi-\ell}{n},\frac{\ell}{n}\big)}\right\}\mathrm{d}\xi\\&=4n\int_{[-\frac{n}{2},\frac{n}{2}]}\sin^2(\pi y)|\mathcal{F}_n(f)(ny)|^2\,\mathrm{W}(y)\,\mathrm{d}y,\end{aligned}$$

where for the last equality we perform the changes of variables $y = \frac{\xi}{n}$ and $x = \frac{\ell}{n}$ and forget the positive term $4\gamma_n$. The function W is defined by

$$\mathrm{W}(y) = \int_{\left[-\frac{1}{2},\frac{1}{2}\right]} \frac{\mathrm{d}x}{\Lambda^2(y-x,x)+\Omega^2(y-x,x)}. \tag{V.35}$$

It is proved in [12, Lemma F.5] that $\mathrm{W}(y) \leqslant \mathrm{C}|y|^{-3/2}$ for $|y| \leqslant 1/2$. Hence, we get, by using the second part of Lemma V.21 with $p = 3$ and the elementary inequality $\sin^2(\pi y) \leqslant (\pi y)^2$, that

$$\iint_{\left[-\frac{n}{2},\frac{n}{2}\right]^2} |\mathcal{F}_n(h)(k,\ell)|^2 \,\mathrm{d}k\mathrm{d}\ell \leqslant \mathrm{C}' n \int_{-1/2}^{1/2} \frac{|y|^{1/2}}{1+(n|y|)^3}\mathrm{d}y = \mathrm{O}(n^{-1/2}).$$

We have proved the first part of Lemma IV.10, that is (IV.22). We turn now to (IV.23). We denote by G_n the 1-periodic function defined by

$$\mathrm{G}_n(y) = \frac{1}{4}\int_{\left[-\frac{n}{2},\frac{n}{2}\right]} \frac{\Omega^2(y-z,z)}{4\gamma_n + \Lambda(y-z,z) - i\,\Omega(y-z,z)}\mathrm{d}z. \tag{V.36}$$

As $y \longrightarrow 0$, the function G_n is close (in a sense defined below) to the function G_0 given by

$$\mathrm{G}_0(y) = \frac{1}{2}|\pi y|^{3/2}(1 + i\,\mathrm{sgn}(y)). \tag{V.37}$$

In fact we show in Lemma V.26 that there exists one constant $\mathrm{C} > 0$ such that for any $|y| \leqslant 1/2$ and for all positive integer n,

$$|\mathrm{G}_n(y) - \mathrm{G}_0(y)| \leqslant \mathrm{C}\left[\sin^2(\pi y) + \gamma_n^2\,|\sin(\pi y)|^{-1/2} + \gamma_n\,|\sin(\pi y)|^{1/2}\right]. \tag{V.38}$$

We denote by $q := q(f) : \mathbb{R} \longrightarrow \mathbb{R}$ the function defined by

$$q(x) = \int_{\mathbb{R}} e^{-2i\pi x y}\mathrm{G}_0(y)\mathcal{F}f(y)\mathrm{d}y$$

which coincides with $-\frac{1}{4}\mathbb{L}f(x)$. Let $q_n : n^{-1}\mathbb{Z} \longrightarrow \mathbb{R}$ the function defined by

$$q_n\left(\frac{x}{n}\right) = \mathcal{D}_n h_n\left(\frac{x}{n}\right).$$

Then, the proof of (IV.23) reduces to the following

Lemma V.25. *We have*

$$\lim_{n\longrightarrow+\infty} \frac{1}{n}\sum_{x\in\mathbb{Z}}\left[q\left(\frac{x}{n}\right) - q_n\left(\frac{x}{n}\right)\right]^2 = 0.$$

Proof. Since $\mathcal{F}_n(h)$ is a symmetric function we can easily see that

$$\mathcal{F}_n(q)(\xi) = -\frac{i}{2}\sum_{x\in\mathbb{Z}} e^{\frac{2i\pi\xi x}{n}} \iint_{\left[-\frac{n}{2},\frac{n}{2}\right]^2} e^{-\frac{2i\pi(k+\ell)x}{n}}\,\Omega\left(\frac{k}{n},\frac{\ell}{n}\right)\mathcal{F}_n(h)(k,\ell)\,\mathrm{d}k\mathrm{d}\ell.$$

We use now Lemma V.24 and the inverse Fourier transform relation to get

$$\mathcal{F}_n(q)(\xi) = -\frac{in}{2}\int_{\left[-\frac{n}{2},\frac{n}{2}\right]} \Omega\left(\frac{\xi-\ell}{n},\frac{\ell}{n}\right)\mathcal{F}_n(h)(\xi-\ell,\ell)\,\mathrm{d}\ell.$$

By the explicit expression (V.34) of $\mathcal{F}_n(h)$ we obtain that

$$\mathcal{F}_n(q)(\xi) = \frac{\sqrt{n}}{4}\left[\int_{\left[-\frac{n}{2},\frac{n}{2}\right]} \frac{\Omega^2\left(\frac{\xi-\ell}{n},\frac{\ell}{n}\right)}{4\gamma_n + \Lambda\left(\frac{\xi-\ell}{n},\frac{\ell}{n}\right) - i\Omega\left(\frac{\xi-\ell}{n},\frac{\ell}{n}\right)}\,\mathrm{d}\ell\right] \mathcal{F}_n(f)(\xi).$$

Again by the inverse Fourier transform we get that

$$q_n\left(\frac{x}{n}\right) = \int_{\left[-\frac{n}{2},\frac{n}{2}\right]} e^{-\frac{2i\pi\xi x}{n}} n^{3/2}\,\mathrm{G}_n\left(\frac{\xi}{n}\right)\mathcal{F}_n(f)(\xi)\,\mathrm{d}\xi.$$

Then we have

$$q\left(\frac{x}{n}\right) - q_n\left(\tfrac{x}{n}\right) = \int_{|\xi|\geqslant n/2} e^{-\frac{2i\pi\xi x}{n}}\,\mathrm{G}_0(\xi)\,\mathcal{F}f(\xi)\,\mathrm{d}\xi$$

$$+\int_{|\xi|\leqslant n/2} e^{-\frac{2i\pi\xi x}{n}}\,\mathrm{G}_0(\xi)\left[\mathcal{F}f(\xi)-\mathcal{F}_n(f)(\xi)\right]\mathrm{d}\xi + n^{3/2}\int_{|\xi|\leqslant n/2} e^{-\frac{2i\pi\xi x}{n}}(\mathrm{G}_0-\mathrm{G}_n)\left(\frac{\xi}{n}\right)\mathcal{F}_n(f)(\xi)\,\mathrm{d}\xi.$$

Above we have used the fact that $n^{3/2}\mathrm{G}_0\left(\frac{\xi}{n}\right) = \mathrm{G}_0(\xi)$. Then we use the triangular inequality and Plancherel's theorem in the two last terms of the RHS to write

$$\begin{aligned}\frac{1}{n}\sum_{x\in\mathbb{Z}}\left[q\left(\frac{x}{n}\right) - q_n\left(\frac{x}{n}\right)\right]^2 \leqslant\ & \frac{1}{n}\sum_{x\in\mathbb{Z}}\left|\int_{|\xi|\geqslant n/2} e^{-\frac{2i\pi\xi x}{n}}\,\mathrm{G}_0(\xi)\,(\mathcal{F}f)(\xi)\,\mathrm{d}\xi\right|^2\\ &+\int_{|\xi|\leqslant n/2}\left|\mathrm{G}_0(\xi)\left[\mathcal{F}f(\xi)-\mathcal{F}_n(f)(\xi)\right]\right|^2\mathrm{d}\xi\\ &+n^3\int_{|\xi|\leqslant n/2}\left|(\mathrm{G}_0-\mathrm{G}_n)\left(\frac{\xi}{n}\right)\mathcal{F}_n(f)(\xi)\right|^2\mathrm{d}\xi\\ &=: (\mathrm{I}) + (\mathrm{II}) + (\mathrm{III}).\end{aligned} \tag{V.39}$$

We refer to [12] for a proof of the following fact: both terms (I) and (II) give a trivial contribution in (V.39). The first one is estimated by performing an integration by parts and using the fact that the Fourier transform $\mathcal{F}f$ of f is in the Schwartz space and that G_0 and G_0' grow polynomially. For the second one, a change of variables $\xi = yn$ and the fact that f is in the Schwartz space together with Lemma V.21 permit to conclude.

The contribution of (III) is estimated by using (V.45) and is different from [12]. Recall the trivial inequality $|\sin(\pi y)| \leqslant |\pi y|$, for $|y| \leqslant 1/2$. The first term of the RHS gives the upper bound

$$\frac{\mathrm{C}}{n}\int_{|\xi|\leqslant n/2} |\xi|^4\,|\mathcal{F}_n(f)(\xi)|^2\,\mathrm{d}\xi = \mathrm{C}\int_{\left[-\frac{1}{2},\frac{1}{2}\right]} n^4|z|^4|\mathcal{F}_n(f)(nz)|^2\mathrm{d}z$$

which goes to 0, as $n \longrightarrow \infty$, by Lemma V.21 applied with $p = 2$. We now deal with the last term of the RHS of (V.45), which gives the upper bound

$$\mathrm{C}n^2\gamma_n^2\int_{|\xi|\leqslant n/2} |\xi|\,|\mathcal{F}_n(f)(\xi)|^2\,\mathrm{d}\xi = \mathrm{C}\,(\gamma_n^2 n^3)\int_{\left[-\frac{1}{2},\frac{1}{2}\right]} n|z|\,|\mathcal{F}_n(f)(nz)|^2\mathrm{d}z,$$

which goes to 0, as $n \longrightarrow \infty$. Indeed, this is a consequence of Lemma V.21, and of the fact that $\gamma_n^2 n^2$ goes to 0 (as long as $b > 1$). The second part gives

$$\mathrm{C}n^3\gamma_n^4\int_{|\xi|\leqslant n/2} \frac{|\mathcal{F}_n(f)(\xi)|^2}{\left|\sin\left(\frac{\pi\xi}{n}\right)\right|}\mathrm{d}\xi = \mathrm{C}n^4\gamma_n^4\int_{\left[-\frac{1}{2},\frac{1}{2}\right]} \frac{|\mathcal{F}_n(f)(nz)|^2}{|\sin(\pi z)|}\mathrm{d}z.$$

Again, since $z \mapsto |\sin(\pi z)|^{-1}$ is integrable on $\{|z| \leqslant 1/2\}$, and thanks to Lemma V.21, this bound goes to 0 as soon as $\gamma_n^4 n^4$ goes to 0, which is automatically satisfied if $b > 1$.

2.3.5 Proof of Lemma IV.11

The proof is similar to the proof given in [12]. Let $w_n : n^{-1}\mathbb{Z} \longrightarrow \mathbb{R}$ be defined by

$$w_n\left(\frac{x}{n}\right) = h_n\left(\frac{x}{n}, \frac{x+1}{n}\right) - h_n\left(\frac{x}{n}, \frac{x}{n}\right)$$

and observe that

$$\frac{1}{\sqrt{n}}\tilde{\mathcal{D}}_n h_n\left(\frac{x}{n}, \frac{y}{n}\right) = n^{3/2}\begin{cases} w_n\left(\frac{x}{n}\right), & y = x+1, \\ w_n\left(\frac{x-1}{n}\right), & y = x-1, \\ 0, & \text{otherwise.} \end{cases}$$

The Fourier transform $\mathcal{F}_n(v_n)$ is thus given by

$$\mathcal{F}_n(v_n)(k,\ell) = -\frac{1}{n}\,\frac{e^{2i\pi\frac{k}{n}} + e^{2i\pi\frac{\ell}{n}}}{\left(\Lambda + 4\gamma_n - i\Omega\right)\left(\frac{k}{n}, \frac{\ell}{n}\right)}\,\mathcal{F}_n(w_n)(k+\ell). \tag{V.40}$$

By using Lemma V.24, we can write that the Fourier transform of w_n is given by

$$\mathcal{F}_n(w_n)(\xi) = \int_{\left[-\frac{n}{2},\frac{n}{2}\right]} \mathcal{F}_n(h_n)(\xi-\ell,\ell)\left\{e^{-\frac{2i\pi\ell}{n}} - 1\right\}\mathrm{d}\ell$$

By (V.34) we get

$$\mathcal{F}_n(w_n)(\xi) = -\frac{\sqrt{n}}{2}\mathrm{I}_n\left(\frac{\xi}{n}\right)\mathcal{F}_n(f)(\xi) \tag{V.41}$$

where the function I_n is defined by

$$\mathrm{I}_n(y) = \int_{\left[-\frac{1}{2},\frac{1}{2}\right]} \left(\frac{i\,\Omega\mathrm{R}}{\Lambda + 4\gamma_n - i\Omega}\right)(y-x,x)\mathrm{d}x. \tag{V.42}$$

Proof of (IV.27) **–** As in [12], we can easily get

$$\|v_n\|_{2,n}^2 \leqslant \mathrm{C}n\int_{\left[-\frac{1}{2},\frac{1}{2}\right]} \left|\mathcal{F}_n(f)(ny)\right|^2 \left|\mathrm{I}_n(y)\right|^2 \mathrm{W}(y)\mathrm{d}y$$

by using Lemma V.21. Then, from Lemma V.27 and since $\mathrm{W}(y) \leqslant \mathrm{C}|y|^{-3/2}$ (see [12, Lemma F.5]), we get that

$$\|v_n\|_{2,n}^2 \leqslant \mathrm{C}n\int_{\left[-\frac{1}{2},\frac{1}{2}\right]} |\mathcal{F}_n(f)(ny)|^2|\sin(\pi y)|^{3/2}\mathrm{d}y \leqslant \mathrm{C}\int_{\left[-\frac{1}{2},\frac{1}{2}\right]} \frac{|y|^{3/2}}{1+|ny|^p}\mathrm{d}y = \frac{\mathrm{C}}{n^{3/2}}\int_{\left[-\frac{n}{2},\frac{n}{2}\right]} \frac{|z|^{3/2}}{1+|z|^p}\mathrm{d}z,$$

which goes to 0 as soon as p is chosen bigger than 3.

Proof of (IV.28) – Following [12], straightforward computations lead to

$$\mathcal{F}_n(\mathcal{D}_n v_n)(\xi) = -n\Big(1 - e^{\frac{2i\pi\xi}{n}}\Big)\mathcal{F}_n(w_n)(\xi)\mathrm{J}_n\Big(\frac{\xi}{n}\Big),$$

where J_n is given by

$$\mathrm{J}_n(y) = \int_{\left[-\frac{1}{2},\frac{1}{2}\right]} \frac{1 + e^{2i\pi(y-2x)}}{(\Lambda + 4\gamma_n - i\Omega)(y-x,x)}\mathrm{d}x. \tag{V.43}$$

Now, by using (V.41) we finally get that

$$\mathcal{F}_n(\mathcal{D}_n v_n)(\xi) = \frac{n^{3/2}}{2}\Big(1 - e^{\frac{2i\pi\xi}{n}}\Big)\mathcal{F}_n(f)(\xi)\mathrm{I}_n\Big(\frac{\xi}{n}\Big)\mathrm{J}_n\Big(\frac{\xi}{n}\Big),$$

where I_n is defined by (V.42). By Plancherel-Parseval relation we have to prove that

$$n^3 \int_{\left[-\frac{n}{2},\frac{n}{2}\right]} \sin^2\left(\pi\tfrac{\xi}{n}\right)\left|\mathcal{F}_n(f)(\xi)\right|^2\left|\mathrm{I}_n\left(\tfrac{\xi}{n}\right)\right|^2\left|\mathrm{J}_n\left(\tfrac{\xi}{n}\right)\right|^2\mathrm{d}\xi$$
$$= n^4 \int_{\left[-\frac{1}{2},\frac{1}{2}\right]} \sin^2(\pi y)|\mathrm{I}_n(y)|^2|\mathrm{J}_n(y)|^2|\mathcal{F}_n(f)(ny)|^2\mathrm{d}y$$

vanishes, as $n \longrightarrow \infty$. By Lemma V.21 and Lemma V.27, this is equivalent to show that the following term goes to 0, as $n \longrightarrow \infty$:

$$n^4 \int_{\left[-\frac{1}{2},\frac{1}{2}\right]} \frac{|y|^4}{1+|ny|^p}\mathrm{d}y = \frac{1}{n}\int_{\left[-\frac{n}{2},\frac{n}{2}\right]} \frac{|z|^4}{1+|z|^p}\mathrm{d}z.$$

For p bigger than 5, this term goes to 0 as $n \longrightarrow \infty$.

Proof of (IV.29) – Let $\theta_n : n^{-1}\mathbb{Z} \longrightarrow \mathbb{R}$ be defined by

$$\theta_n\Big(\frac{x}{n}\Big) = v_n\Big(\frac{x}{n},\frac{x+1}{n}\Big) - v_n\Big(\frac{x}{n},\frac{x}{n}\Big)$$

and observe that

$$\frac{1}{\sqrt{n}}\tilde{\mathcal{D}}_n v_n\left(\frac{x}{n},\frac{y}{n}\right) = n^{3/2}\begin{cases}\theta_n\left(\frac{x}{n}\right), & y = x+1,\\ \theta_n\left(\frac{x-1}{n}\right), & y = x-1,\\ 0, & \text{otherwise.}\end{cases}$$

We have to show that

$$\lim_{n\longrightarrow\infty} n\sum_{x\in\mathbb{Z}} \theta_n^2(x) = 0$$

which is equivalent by Plancherel-Parseval relation to show that

$$\lim_{n\longrightarrow+\infty} n^2\int_{\left[-\frac{n}{2},\frac{n}{2}\right]} \mathcal{F}_n(\theta_n)(\xi)\mathrm{d}\xi = 0.$$

By using Lemma V.24, we have that the Fourier transform of θ_n is given by

$$\mathcal{F}_n(\theta_n)(\xi) = \int_{\left[-\frac{n}{2},\frac{n}{2}\right]} \mathcal{F}_n(v_n)(\xi-\ell,\ell)\Big(e^{-\frac{2i\pi\ell}{n}} - 1\Big)\,\mathrm{d}\ell$$

Performing a change of variables and using (V.40) and (V.41), we get that

$$\mathcal{F}_n(\theta_n)(\xi) = \frac{\sqrt{n}}{2}\mathcal{F}_n(f)(\xi)\mathrm{I}_n\Big(\frac{\xi}{n}\Big)\mathrm{K}_n\Big(\frac{\xi}{n}\Big),$$

where I_n is defined by (V.42) and K_n is given by

$$\mathrm{K}_n(y) = \int_{\left[-\frac{1}{2},\frac{1}{2}\right]} \frac{\left(e^{2i\pi(y-x)} + e^{2i\pi x}\right)\left(e^{-2i\pi x} - 1\right)}{(\Lambda + 4\gamma_n - i\Omega)(y-x,x)}\,\mathrm{d}x. \tag{V.44}$$

We need to show that

$$\lim_{n\longrightarrow\infty} n^2\|\theta_n\|_{2,n}^2 = 0.$$

By Plancherel-Parseval relation, this is equivalent to prove that

$$\lim_{n\longrightarrow\infty} n^3\int_{\left[-\frac{n}{2},\frac{n}{2}\right]} \left|\mathcal{F}_n(f)(\xi)\right|^2 \left|\mathrm{I}_n\big(\tfrac{\xi}{n}\big)\right|^2 \left|\mathrm{K}_n\big(\tfrac{\xi}{n}\big)\right|^2 \mathrm{d}\xi = 0.$$

By using the change of variables $y = \xi/n$, Lemma V.21, Lemma V.27, we have

$$n^3\int_{\left[-\frac{n}{2},\frac{n}{2}\right]} \left|\mathcal{F}_n(f)(\xi)\right|^2 \left|\mathrm{I}_n\big(\tfrac{\xi}{n}\big)\right|^2 \left|\mathrm{K}_n\big(\tfrac{\xi}{n}\big)\right|^2 \mathrm{d}\xi \leqslant \mathrm{C}n^4\int_{\left[-\frac{1}{2},\frac{1}{2}\right]} \frac{|y|^4}{1+|ny|^p}\mathrm{d}y = \frac{\mathrm{C}}{n}\int_{\left[-\frac{n}{2},\frac{n}{2}\right]} \frac{|z|^4}{1+|z|^p}\mathrm{d}z$$

which goes to 0, as $n \longrightarrow \infty$, for p bigger than 5.

2.3.6 A Few Integral Estimates

The following lemma is the new technical estimate which takes into account the extra-term coming from the velocity-flip noise of intensity γ_n.

Lemma V.26. *Recall that* G_n *and* G_0 *are defined by* (V.36) *and* (V.37). *There exists a constant* $\mathrm{C} > 0$ *such that for any* $|y| \leqslant 1/2$ *and for any positive integer n,*

$$|\mathrm{G}_n(y) - \mathrm{G}_0(y)| \leqslant \mathrm{C}\left[\sin^2(\pi y) + \gamma_n^2\,|\sin(\pi y)|^{-1/2} + \gamma_n\,|\sin(\pi y)|^{1/2}\right]. \tag{V.45}$$

Proof. We compute the function G_n thanks to the residue theorem. For any $|y| \leqslant 1/2$ we denote by $w := w(y)$ the complex number $w = e^{2i\pi y}$. By denoting $z = e^{2i\pi x}$, for $|x| \leqslant 1/2$, we have that

$$\Lambda(y-x,x) = 4 - z(w^{-1}+1) - z^{-1}(w+1),$$
$$i\,\Omega(y-x,x) = z(1-w^{-1}) + z^{-1}(w-1).$$

We denote by $\mathcal{C}$ the unit circle positively oriented. Therefore,

$$\mathrm{G}_n(y) = \frac{1}{16i\pi}\oint_{\mathcal{C}} f_w(z)\mathrm{d}z$$

where the meromorphic function f_w is defined by

$$f_w(z) = \frac{[(w-1) + z^2(1-w^{-1})]^2}{z^2\big(z^2 - 2z(1+\gamma_n) + w\big)}.$$

The poles of f_w are 0 and z_-, z_+ which are the two solutions of $z^2 - 2z(1+\gamma_n) + w$. We can check that

$$z_\pm = (1+\gamma_n) \pm \sqrt{\alpha}\, e^{i\theta/2}, \tag{V.46}$$

where

$$\begin{aligned}\alpha^2 &= 4(1+\gamma_n)^2 \sin^2(\pi y) + \left[(1+\gamma_n)^2 - 1\right]^2,\\ \theta &= \arctan\left(\frac{(1+\gamma_n)^2 - \cos(2\pi y)}{\sin(2\pi y)}\right) - \frac{\pi}{2}\operatorname{sgn}(y).\end{aligned}$$

Observe that $|z_-| < 1$ and $|z_+| > 1$. Indeed, since

$$\frac{(1+\gamma_n)^2 - \cos(2\pi y)}{\sin(2\pi y)} = \frac{\gamma_n^2 + 2\gamma_n + 2\sin^2(\pi y)}{\sin(2\pi y)}$$

we have that $|\theta| < \pi/2$ (distinguish the case $y > 0$ and the case $y < 0$). Moreover $\gamma_n > 0$ so that a simple geometric argument permits to conclude that $|z_+| > 1$. Since $z_- z_+ = 1$, we have $|z_-| < 1$. By the residue theorem, we have

$$\oint_C f_w(z)\mathrm{d}z = 2\pi i\left[\operatorname{Res}(f_w, 0) + \operatorname{Res}(f_w, z_-)\right]$$

where $\operatorname{Res}(f_w, a)$ denotes the value of the residue of f_w at pole a. An elementary computation shows that

$$\begin{aligned}\operatorname{Res}(f_w, 0) &= \frac{2(w-1)^2}{w^2},\\ \operatorname{Res}(f_w, z_-) &= \lim_{z \longrightarrow z_-}(z - z_-) f_w(z) = \frac{1}{z_- - z_+}\frac{\left[(w-1) + (1-w^{-1})\, z_-^2\right]^2}{z_-^2}.\end{aligned}$$

By using the fact that $z_-^2 = 2z_-(1+\gamma_n) - w$, we obtain that

$$\begin{aligned}\mathrm{G}_n(y) &= \frac{1}{8}\left[\operatorname{Res}(f_w, 0) + \operatorname{Res}(f_w, z_-)\right] = \frac{(w-1)^2}{4w^2}\left[1 + \frac{2(1+\gamma_n)^2}{z_- - z_+}\right]\\ &= \frac{(w-1)^2}{4w^2}\left[1 - \frac{(1+\gamma_n)^2}{\sqrt{\alpha}} e^{-i\theta/2}\right]\\ &= \frac{(w-1)^2}{4w^2} - \frac{(w-1)^2}{4w^2}\frac{(1+\gamma_n)^{3/2}}{\sqrt{2|\sin(\pi y)|}}\left[1 + \frac{(2+\gamma_n)^2}{4(1+\gamma_n)^2}\frac{\gamma_n^2}{\sin^2(\pi y)}\right]^{-1/4} e^{-i\theta/2}\\ &= \frac{(w-1)^2}{4w^2} - \frac{(w-1)^2}{4w^2}\frac{(1+\gamma_n)^{3/2}}{\sqrt{2|\sin(\pi y)|}} e^{-i\theta/2} + \varepsilon_n(y)\end{aligned}$$

where

$$\varepsilon_n(y) = \frac{(w-1)^2}{4w^2}\frac{(1+\gamma_n)^{3/2}}{\sqrt{2|\sin(\pi y)|}} e^{-i\theta/2}\left\{1 - \left[1 + \frac{(2+\gamma_n)^2}{4(1+\gamma_n)^2}\frac{\gamma_n^2}{\sin^2(\pi y)}\right]^{-1/4}\right\}.$$

We deal separately with two terms: first,

$$\left|\frac{(w-1)^2}{4w^2}\right| = \sin^2(\pi y).$$

Second, after noticing that

$$\frac{1}{4} \leqslant \frac{(2+\gamma_n)^2}{4(1+\gamma_n)^2} \leqslant 1,$$

we get

$$\left|1 - \left[1 + \frac{(2+\gamma_n)^2}{4(1+\gamma_n)^2}\frac{\gamma_n^2}{\sin^2(\pi y)}\right]^{-1/4}\right| \leqslant C\left|\left[1 + C'\frac{\gamma_n^2}{\sin^2(\pi y)}\right]^{1/4} - 1\right| \leqslant C''\frac{\gamma_n^2}{\sin^2(\pi y)}.$$

Then, we get easily that

$$|\varepsilon_n(y)| \leqslant C\gamma_n^2 |\sin(\pi y)|^{-1/2}.$$

Moreover, we have that

$$|(1+\gamma_n)^{3/2} - 1| \leqslant C\gamma_n.$$

Since the derivative of arctan is bounded above by a constant, we have also that

$$\begin{aligned}
&\left|e^{-i\theta/2} - \frac{1}{\sqrt{2}}(1+i\mathrm{sgn}(y))e^{-i\pi y/2}\right| \\
&= \left|\frac{1+i\mathrm{sgn}(y)}{\sqrt{2}}\right| \left|\exp\left\{-\frac{i}{2}\left[\arctan\left(\tan(\pi y) + \frac{\gamma_n(2+\gamma_n)}{\sin(2\pi y)}\right)\right]\right\} - \exp\left\{-\frac{i}{2}\tan(\pi y)\right\}\right| \\
&\leqslant C\left|\arctan\left(\tan(\pi y) + \frac{\gamma_n(2+\gamma_n)}{\sin(2\pi y)}\right) - \tan(\pi y)\right| \leqslant C\frac{\gamma_n}{|\sin(\pi y)|}.
\end{aligned}$$

We deduce the result

$$|G_n(y) - G_0(y)| \leqslant C\left[\sin^2(\pi y) + \gamma_n^2 |\sin(\pi y)|^{-1/2} + \gamma_n |\sin(\pi y)|^{1/2}\right].$$

□

The last lemma below is widely inspired from [12].

LEMMA V.27. *The functions* I_n, J_n, *and* K_n, *respectively defined by* (V.42), (V.43) *and* (V.44), *satisfy for any* $y \in \mathbb{R}$ *and any positive integer n,*

$$\begin{aligned}
|I_n(y)| &\leqslant C|\sin(\pi y)|^{3/2} \\
|J_n(y)| &\leqslant C|\sin(\pi y)|^{-1/2} \\
|K_n(y)| &\leqslant C|\sin(\pi y)|^{1/2}
\end{aligned}$$

where C *is a positive constant which does not depend on* y *nor on* n.

Proof. We divide the proof into three parts, corresponding to the three inequalities.

1. As previously, we compute I_n by using the residue theorem. For any $|y| \leqslant 1/2$ we denote by $w := w(y)$ the complex number $w = e^{2i\pi y}$. Then we have

$$I_n(y) = -\frac{1}{4i\pi}\frac{w-1}{w}\oint_C f_w(z)\mathrm{d}z, \tag{V.47}$$

   where the meromorphic function f_w is defined by

$$f_w(z) = \frac{(z-1)(z^2+w)}{z^2(z-z_+)(z-z_-)} \tag{V.48}$$

with $z_\pm$ defined by (V.46). We recall that $|z_-| < 1$ and $|z_+| > 1$ so that by the residue theorem we have

$$\mathrm{I}_n(y) = -\frac{w-1}{2w}\left[\mathrm{Res}(f_w, 0) + \mathrm{Res}(f_w, z_-)\right].$$

A simple computation shows that

$$\mathrm{Res}(f_w, 0) = 1 - 2/w, \quad \mathrm{Res}(f_w, z_-) = 1/z_-.$$

It follows that

$$\mathrm{I}_n(y) = -\frac{w-1}{2w}\left[\frac{1}{z_-} + 1 - \frac{2}{w}\right].$$

Replacing w and z_- by their explicit values we get the result.

2. Then we also compute J_n by using the residue theorem:

$$\mathrm{J}_n(y) = -\frac{1}{4i\pi}\oint_{\mathcal{C}} f_w(z)\mathrm{d}z$$

where the meromorphic function f_w is defined by

$$f_w(z) = \frac{(z^2 + w)}{z^2(z - z_+)(z - z_-)}$$

with $z_\pm$ defined by (V.46). By the residue theorem, we get

$$\mathrm{J}_n(y) = -\frac{1}{2}\left(\mathrm{Res}(f_w, 0) + \mathrm{Res}(f_w, z_-)\right).$$

A simple computation shows that

$$\mathrm{Res}(f_w, 0) = -\frac{w}{2}, \quad \mathrm{Res}(f_w, z_-) = \frac{2}{z_-(z_- - z_+)}.$$

By using the explicit expressions for w, $z_\pm$, we get the result.

3. Finally, it is not difficult to see that

$$\mathrm{K}_n(y) = -\frac{w}{w-1}\mathrm{I}_n(y),$$

and by the first estimate the result follows.

□

3 CEMRACS Project: An Inverse Problem in Homogenization

During Summer 2013, I participated in the scientific event of the SMAI (the french Society of Applied and Industrial Mathematics) called CEMRACS (Centre d'Été Mathématique de Recherche Avancée en Calcul Scientifique). It consists in an intensive five weeks long research session. CEMRACS 2013 was devoted to *Modelling and simulation of complex systems: stochastic and deterministic approaches*.

I have worked on an inverse problem in stochastic homogenization with W. Minvielle (École des Ponts), A. Obliger (Université Pierre et Marie Curie) and F. Legoll (École des Ponts). Our research has lead to a submitted article [62], which is summarized in this section.

3.1 Introduction

Our work has a physical origin: for physicists, modelling porous media is a challenge, in particular because geometry of such materials can be extremely complex. One possible approach (followed in this work) consists in completely forgetting the exact geometry of the system except for a few parameters, and consider that channels form a simple network like $\mathbb{Z}^d$. This leads to the so-called *pore-network models* (PNM), initially introduced by Fatt in the 1950s [39]. Some microscopic properties are assigned to the network elements (channels conductances in this work) and rules are defined to compute the *homogenized* properties, which are then compared to the available experimental data. The aim is to construct a microscopic network with the effective properties of a real representative sample of rock.

We adopt a stochastic model: at the microscopic scale, the physical properties are described by a random field. In particular, we are interested in monophasic transport phenomena which are described by the Darcy law. Precisely, the local flux of water is assumed to be proportional to the local pressure gradient, and the microscopic properties of interest are the channels conductances. The equation to solve is therefore a discrete linear elliptic equation in divergence form, with random coefficients. The homogenized (macroscopic) property arising with this procedure is called the *permeability*.

The channels conductances depend on their size, which is randomly distributed. In practice, this size distribution can be inferred from experiments: we denote it by $\mathcal{L}_{\text{exp}}$. Very often, the macroscopic permeability computed with $\mathcal{L}_{\text{exp}}$ is different from the experimental effective properties. The main goal of this work consists in improving that random distribution, when starting from the experimental initial guess, in order to eventually achieve a better agreement between measured and computed effective properties.

From a more mathematical standpoint, the question can be phrased in the following terms. Consider a second-order divergence-form operator whose coefficients are random. If the coefficients distribution is stationary and ergodic, then (under some additional technical assumptions) this random operator can be replaced, over large scales, by an effective operator with constant homogenized coefficients. Random homogenization theory actually provides a mean to compute macroscopic quantities if we know the microscopic ones, and to solve the so-called *forward problem*. Here we consider the *inverse problem*, and try to extract some information on the properties of the materials at the microscopic scale on the basis of macroscopic quantities.

Homogenization is an averaging process, which filters out many features of the microscopic coefficients. There is no hope to recover a full information about the microstructure (in our case, the probability distribution of the conductances) from the only knowledge of macroscopic quantities. We adopt here a more restricted objective, and we assume a functional form for the distribution of the microscopic conductances (hereafter, a Weibull distribution). Our aim is to recover the parameters (denoted hereafter by θ) of that microscopic law.

Our approach is not specific to Weibull laws, and it could be used for a wide class of distribution laws with parameters θ (we give in [62] more details). Our motivation for choosing Weibull laws comes from physical reasons: based on experimental results, it appears to be a reasonable choice.

The question of recovering the unknown parameters θ of the microscopic distribution from homogenized (and more generally macroscopic) quantities belongs to the wide family of *inverse* *problems*. In this work, a major point of interest is the selection of the macroscopic quantities which we need to know in order to uniquely determine the parameters θ.

3.2 Discrete Homogenization Theory

We first recall some elements of homogenization for discrete elliptic equations with random coefficients. We refer to [53,54] for seminal contributions on this topic. For homogenization of elliptic partial differential equations (PDEs), we refer to [35] for a general, numerically oriented presentation, to the textbooks [7,28,48] and to the review article [2].

3.2.1 Homogenization Result

Let us give some usual definitions for stochastic homogenization, before turning to the specific case of discrete elliptic equations. Throughout this section, $(\Omega, \mathcal{F}, \mathbb{P})$ is a probability space and we denote by $\mathbb{E}$ the corresponding expectation.

We fix an integer $d \geqslant 1$ and assume that the group $(\mathbb{Z}^d, +)$ acts on Ω. We denote by $(\tau_k)_{k\in\mathbb{Z}^d}$ this action, and assume that it preserves the measure $\mathbb{P}$, namely for all $k \in \mathbb{Z}^d$ and all $\mathrm{A} \in \mathcal{F}$, $\mathbb{P}(\tau_k \mathrm{A}) = \mathbb{P}(\mathrm{A})$. We assume that the action τ is *ergodic*: precisely, if $\mathrm{A} \in \mathcal{F}$ is such that $\tau_k \mathrm{A} = \mathrm{A}$ for any $k \in \mathbb{Z}^d$, then $\mathbb{P}(\mathrm{A}) = 0$ or 1. In addition, we introduce the following notion of stationarity:

Definition V.6. *We say that a function* $\psi : \mathbb{Z}^d \times \Omega \longrightarrow \mathbb{R}$ *is* stationary *if*

$$\forall x, z \in \mathbb{Z}^d, \quad \psi(x+z, \omega) = \psi(x, \tau_z \omega) \quad a.s. \tag{V.49}$$

We now focus on the case of discrete elliptic equations. We view $\mathbb{Z}^d$ as a lattice, whose unit vectors are denoted by e_i, $i \in \{1, ..., d\}$. Each vertex $x \in \mathbb{Z}^d$ of the lattice is connected to $2d$ other vertices: $x \pm e_i$, $i \in \{1, ..., d\}$. We write $x \sim y$ if x and y are neighbours, and $e = (x, y)$ the corresponding (non-oriented) edge. For any vertex $x \in \mathbb{Z}^d$, and any direction $1 \leqslant i \leqslant d$, we denote by $a_i(x, \omega) \in (0, \infty)$ the random conductance of the edge $(x, x + e_i)$. We next introduce the diagonal matrix A defined for any vertex $x \in \mathbb{Z}^d$ by

$$\mathrm{A}(x, \omega) := \mathrm{diag}\Big(a_1(x, \omega), \dots, a_d(x, \omega)\Big). \tag{V.50}$$

We assume that, for any direction i, the conductances $\{a_i(x, \cdot)\}_{x\in\mathbb{Z}^d}$ form an i.i.d. sequence of random variables. The matrix A is therefore stationary. We introduce discrete differential operators on the lattice $\mathbb{Z}^d$.

Definition V.7. *For a function* $g : \mathbb{Z}^d \longrightarrow \mathbb{R}$*, the gradient* $\nabla g : \mathbb{Z}^d \longrightarrow \mathbb{R}^d$ *is defined by*

$$(\nabla g)(x) = \begin{pmatrix} g(x+e_1) - g(x) \\ \vdots \\ g(x+e_d) - g(x) \end{pmatrix}.$$

For a function $\mathrm{G} = (\mathrm{G}_1, ..., \mathrm{G}_d) : \mathbb{Z}^d \longrightarrow \mathbb{R}^d$*, the function* $\nabla^\star \mathrm{G} : \mathbb{Z}^d \longrightarrow \mathbb{R}$ *is defined by*

$$-(\nabla^\star \mathrm{G})(x) = \sum_{i=1}^{d} \big(\mathrm{G}_i(x) - \mathrm{G}_i(x - e_i)\big).$$

We think of $\nabla^\star G$ as the negative divergence of G. The operator $\nabla^\star$ is the ℓ^2 transpose of ∇ in the following sense: for any compactly supported functions $g : \mathbb{Z}^d \longrightarrow \mathbb{R}$ and $G : \mathbb{Z}^d \longrightarrow \mathbb{R}^d$,

$$\sum_{x\in\mathbb{Z}^d} g(x)\nabla^\star G(x) = \sum_{x\in\mathbb{Z}^d} \nabla g(x)\cdot G(x).$$

Hereafter, the notation $a \cdot b$ stands for the usual scalar product in $\mathbb{R}^d$. We additionally define rescaled discrete differential operators as follows:

Definition V.8. *For a function $g : \varepsilon\mathbb{Z}^d \longrightarrow \mathbb{R}$, the gradient $\nabla_\varepsilon g : \varepsilon\mathbb{Z}^d \longrightarrow \mathbb{R}^d$ is defined by*

$$(\nabla_\varepsilon g)(x) = \frac{1}{\varepsilon}\begin{pmatrix} g(x+\varepsilon e_1) - g(x) \\ \vdots \\ g(x+\varepsilon e_d) - g(x)\end{pmatrix}.$$

For a function $G = (G_1, ..., G_d) : \varepsilon\mathbb{Z}^d \longrightarrow \mathbb{R}^d$, the function $\nabla_\varepsilon^\star G : \varepsilon\mathbb{Z}^d \longrightarrow \mathbb{R}$ is defined by

$$-(\nabla_\varepsilon^\star G)(x) = \sum_{i=1}^{d} \frac{G_i(x) - G_i(x-\varepsilon e_i)}{\varepsilon}.$$

Usually, the matrix field A is assumed to satisfy the following assumption:

Assumption V.28 (Ellipticity – boundedness condition). *There exist two positive deterministic constants c and C such that the matrix A defined by* (V.50) *satisfies, for all $\xi \in \mathbb{R}^d$, and for all $x \in \mathbb{Z}^d$,*

$$c|\xi|^2 \leqslant \xi \cdot A(x,\omega)\xi \leqslant C|\xi|^2 \qquad \mathbb{P} - a.s. \tag{V.51}$$

In view of (V.50), note that this simply means $0 < c \leqslant a_j(x,\omega) \leqslant C$ almost surely, for any $1 \leqslant j \leqslant d$ and any $x \in \mathbb{Z}^d$. The following homogenization result holds (we refer to [54, Theorems 3 and 4] for a proof):

Theorem V.29. *Let $\mathcal{D}$ be a bounded domain of $\mathbb{R}^d$ and $f \in \mathbf{L}^2(\mathcal{D})$. Let A be the random matrix field given by* (V.50) *satisfying Assumption V.28. Let $u_\varepsilon \in \ell^2(\varepsilon\mathbb{Z}^d;\mathbb{R})$ be the unique solution to*

$$\begin{aligned} \nabla_\varepsilon^\star\big[A(x/\varepsilon,\omega)\nabla_\varepsilon u_\varepsilon(x,\omega)\big] &= f(x) \quad \textit{in } \mathcal{D}\cap\varepsilon\mathbb{Z}^d, \\ u_\varepsilon(x,\omega) &= 0 \qquad \textit{in } (\mathbb{R}^d\backslash\mathcal{D})\cap\varepsilon\mathbb{Z}^d. \end{aligned}$$

When $\varepsilon \longrightarrow 0$, $u_\varepsilon(\cdot,\omega)$ converges to a homogenized solution $u^\star$ in the following sense. For any $\xi \in \mathbb{R}^d$, introduce the corrector *φ_ξ in the direction ξ as the unique solution (defined on $\mathbb{Z}^d \times \Omega$) to*

$$\begin{aligned} -\nabla^\star\left[A(\cdot,\omega)\big(\xi + \nabla\varphi_\xi(\cdot,\omega)\big)\right] &= 0 \quad \textit{in } \mathbb{Z}^d,\ \mathbb{P}-\ a.s., \\ \varphi_\xi(0,\omega) &= 0, \quad \mathbb{P}-\ a.s., \end{aligned} \tag{V.52}$$

such that $\nabla\varphi_\xi$ is stationary in the sense of (V.49) *and satisfies, for all $x \in \mathbb{Z}^d$ $\mathbb{E}[\nabla\varphi_\xi(x,\cdot)] = 0$.*

Let $A^\star$ be the constant matrix defined for $\xi \in \mathbb{R}^d$ by

$$A^\star\xi = \mathbb{E}\big[A(x,\cdot)(\xi + \nabla\varphi_\xi(x,\cdot))\big] \tag{V.53}$$

and the unique solution $u^\star \in \mathbf{H}_0^1(\mathcal{D})$ to the (continuous) PDE

$$-\text{div}\big[A^\star\widehat{\nabla}u^\star\big] = f \quad \textit{in } \mathcal{D},$$

where $\widehat{\nabla}$ *and* div *are the usual (continuous) gradient and divergence differential operators, and* $\mathbf{H}^1_0(\mathcal{D})$ *is the closure in the Sobolev space* $\mathbf{H}^1(\mathcal{D})$ *of the space* $\mathcal{C}^\infty_c(\mathcal{D})$ *of infinitely differentiable compactly supported functions.*

Then, we have the (strong) convergence $u_\varepsilon \xrightarrow[\varepsilon\longrightarrow 0]{} u^\star$, *in the sense that*

$$\varepsilon^d \sum_{x\in\mathcal{D}\cap\varepsilon\mathbb{Z}^d} |u_\varepsilon(x,\omega) - u^\star(x)|^2 \xrightarrow[\varepsilon\longrightarrow 0]{} 0 \quad \mathbb{P}-\textit{almost surely}. \tag{V.54}$$

Note that, in the right-hand side of (V.53), the vector $\mathrm{A}(\xi + \nabla\varphi_\xi)$ is stationary, and therefore the expectation may be evaluated at any $x \in \mathbb{Z}^d$. In general, φ_ξ itself is not stationary, as the one-dimensional case shows; only its gradient is.

REMARK *3.1.* From a more probabilistic point of view, the operator $\mathcal{L} := -\nabla^\star\cdot\mathrm{A}(\cdot,\omega)\nabla$ can be seen as the generator of a Markov process. More precisely, $\mathcal{L}$ describes the evolution of the environment viewed by a particle performing a continuous time random walk in a random environment (namely, the lattice $\mathbb{Z}^d$ with random edge conductances). We refer the reader to [34] for more details.

3.2.2 Approximation on Finite Boxes

The corrector problem (V.52) is untractable in practice, since it is posed in the entire lattice $\mathbb{Z}^d$. Approximations are therefore in order. The standard procedure amounts to considering finite boxes (see e.g. [23]). For a positive integer N, we denote by Λ_N the finite box $\{0,...,\mathrm{N}\}^d$ and by $\mathcal{E}_\mathrm{N}$ the set of edges in Λ_N. The *truncated corrector* φ^N_ξ defined on $\Lambda_\mathrm{N}\times\Omega$ is the unique solution to

$$-\nabla^\star\Big[\mathrm{A}(\cdot,\omega)\big(\xi + \nabla\varphi^\mathrm{N}_\xi(\cdot,\omega)\big)\Big] = 0 \quad \text{in } \Lambda_\mathrm{N},\ \mathbb{P}-a.s., \tag{V.55}$$

such that $\varphi^\mathrm{N}_\xi(\cdot,\omega)$ is Λ_N-periodic, and $\varphi^\mathrm{N}_\xi(0,\omega) = 0$, $\mathbb{P}$- a.s.

The homogenized matrix $\mathrm{A}^\star$, which is deterministic, is then approximated by the matrix $\mathrm{A}^\star_\mathrm{N}$ defined for $\xi\in\mathbb{R}^d$ by

$$\mathrm{A}^\star_\mathrm{N}(\omega)\xi = \frac{1}{|\Lambda_\mathrm{N}|}\sum_{x\in\Lambda_\mathrm{N}} \mathrm{A}(x,\omega)\big(\xi + \nabla\varphi^\mathrm{N}_\xi(x,\omega)\big). \tag{V.56}$$

Because of truncation, the practical approximation $\mathrm{A}^\star_\mathrm{N}$ is random. In the large N limit, the deterministic value is attained, thanks to ergodicity. More precisely, $\mathrm{A}^\star_\mathrm{N}(\omega)$ converges almost surely towards $\mathrm{A}^\star$ as N goes to infinity, thanks to the ergodic theorem.

REMARK *3.2.* In (V.55), we have complemented the elliptic equation in Λ_N with *periodic* boundary conditions. Other choices could be made, such as imposing homogeneous Dirichlet boundary conditions: $\varphi^\mathrm{N}_\xi(\cdot,\omega) = 0$ on $\partial\Lambda_\mathrm{N}$ (see e.g. [23] for a similar discussion in the case of continuous PDEs). In the numerical experiments of Section 3.5, we only use periodic boundary conditions, following (V.55).

In practice, we work on a finite box Λ_N, on which the apparent homogenized matrix $\mathrm{A}^\star_\mathrm{N}$ is random. It is natural to introduce M i.i.d. realizations of the random field $\mathrm{A}(x,\omega)$ and solve (V.55)–(V.56) for each of them, thereby obtaining i.i.d. realizations $\mathrm{A}^{\star,m}_\mathrm{N}(\omega)$, $1 \leqslant m \leqslant \mathrm{M}$. Let us define the empirical mean

$$\overline{\mathrm{A}}^\star_{\mathrm{N,M}}(\omega) = \frac{1}{\mathrm{M}}\sum_{m=1}^{\mathrm{M}} \mathrm{A}^{\star,m}_\mathrm{N}(\omega) \tag{V.57}$$

which is, according to the law of large numbers, a converging approximation of $\mathbb{E}\left[A_N^\star\right]$. We have that

$$\overline{A}^\star_{N,M}(\omega) \xrightarrow[M\longrightarrow\infty]{} \mathbb{E}\left[A_N^\star\right] \quad \text{a.s.}$$

The error when approximating $A^\star$ by $\overline{A}^\star_{N,M}$ can be written as the sum of two contributions,

$$A^\star - \overline{A}^\star_{N,M} = \left(A^\star - \mathbb{E}[A_N^\star]\right) + \left(\mathbb{E}[A_N^\star] - \overline{A}^\star_{N,M}\right). \tag{V.58}$$

The second term in the right-hand side of (V.58) is the *statistical* error, which measures the fact that $\nabla\varphi_\xi^N$ is only an approximation of $\nabla\varphi_\xi$. The first term is the *systematic* error, due to the fact that, for any finite N, $\mathbb{E}[A_N^\star] \neq A^\star$. The dominated convergence theorem ensures that this error vanishes as $N \longrightarrow \infty$. Many studies have been recently devoted to proving sharp estimates on the rate of this convergence, following the seminal work [23]. In [42, Lemma 2.3], the authors show that the systematic error is of order N^{-1} when the corrector problem is complemented with homogeneous Dirichlet boundary conditions on $\partial\Lambda_N$, and of order $N^{-d}\ln^d(N)$ when using periodic boundary conditions.

In the sequel, we want to identify the parameters of the microscopic probability distribution, knowing two macroscopic quantities:

(i) the *homogenized permeability*, which is in practice approximated by $\overline{A}^\star_{N,M}$;

(ii) the *relative variance* defined by

$$\mathbb{V}\text{arR}\left[\left(A_N^\star\right)_{ij}\right] = \frac{\mathbb{V}\text{ar}\left[\left(A_N^\star\right)_{ij}\right]}{\left(\mathbb{E}\left[\left(A_N^\star\right)_{ij}\right]\right)^2},$$

which is in practice approximated by

$$S_{N,M} = \frac{1}{(\overline{A}^\star_{N,M})^2_{ij}}\left(\frac{1}{M}\sum_{m=1}^{M}\left[\left(A_N^{\star,m}(\omega)\right)_{ij} - \left(\overline{A}^\star_{N,M}\right)_{ij}\right]^2\right). \tag{V.59}$$

3.3 The One-Dimensional Case

The purpose of this section is two-fold. On the one hand, we provide explicit formulas for the homogenized quantities in terms of the microscopic field $A(x,\omega)$. We derive these formulas assuming that (V.51) holds. On the second hand, we show that we can relax Assumption (V.51).

In the one-dimensional case, the problem (V.55)–(V.56) can be analytically solved. We have

$$A_N^\star(\omega) = \left(\frac{1}{N}\sum_{x\in\Lambda_N}\frac{1}{A(x,\omega)}\right)^{-1}, \quad \text{for almost all } \omega. \tag{V.60}$$

Likewise, the problem (V.52)–(V.53) can also be solved, yielding the formula

$$A^\star = \mathbb{E}\left[\frac{1}{A(x,\cdot)}\right]^{-1} \tag{V.61}$$

which can be evaluated at any $x \in \mathbb{Z}$ due to the stationarity of A. First, it can be checked that the homogenization convergence (V.54) holds, and second, that $A_N^\star(\omega)$ indeed converges to $A^\star$ when

$N \longrightarrow \infty$. We note that, as soon as $A(x,\omega) > 0$ a.s. for any $x \in \mathbb{Z}$ and $A^{-1}(x,\cdot) \in L^1(\Omega)$ (this latter condition being independent of x), (V.60) and (V.61) are well-defined. The following theorem states that these assumptions are enough for homogenization to hold in the one-dimensional case (and is proved in [62]).

Theorem V.30. *Let $\mathcal{D}$ be a bounded domain of $\mathbb{R}$, and $f \in \mathcal{C}_0(\overline{\mathcal{D}})$. Let A be a stationary random scalar field (defined on $\mathbb{Z} \times \Omega$), which is almost surely positive and finite, and such that $A^{-1}(x,\cdot) \in \mathbf{L}^1(\Omega)$. Let $u_\varepsilon \in \ell^2(\varepsilon\mathbb{Z};\mathbb{R})$ be the unique solution to*

$$\begin{aligned} \nabla_\varepsilon^\star\big[A(x/\varepsilon,\omega)\nabla_\varepsilon u_\varepsilon(x,\omega)\big] &= f(x) \quad \text{in } \mathcal{D} \cap \varepsilon\mathbb{Z}, \\ u_\varepsilon(x,\omega) &= 0 \qquad \text{in } (\mathbb{R}\backslash\mathcal{D}) \cap \varepsilon\mathbb{Z}, \end{aligned}$$

and let $u^\star \in \mathbf{H}_0^1(\mathcal{D})$ be the unique solution to the (continuous) boundary value problem

$$-\big[A^\star(u^\star)'\big]' = f \qquad \text{in } \mathcal{D},$$

where $A^\star$ is defined by (V.61). Then $u_\varepsilon(\cdot,\omega)$ converges to the homogenized solution $u^\star$ when $\varepsilon \longrightarrow 0$, in the sense that

$$\varepsilon \sum_{x \in \mathcal{D}\cap\varepsilon\mathbb{Z}} |u_\varepsilon(x,\omega) - u^\star(x)|^2 \xrightarrow[\varepsilon\longrightarrow 0]{} 0 \quad \textit{almost surely}. \tag{V.62}$$

From now on we assume that the conductances $\{a_i(x,\omega)\}$ are independently identically distributed according to the Weibull law of parameter $(\lambda^4, k/4)$. For any $k > 0$, Assumption (V.51) is not satisfied. However, when $k > 4$, the conditions for having Theorem V.30 are satisfied, and we know that

$$A^\star = \frac{\lambda^4}{\Gamma(1-4/k)} \tag{V.63}$$

where Γ is the Euler Gamma function. The variance of $A_N^\star$ is finite if and only if $k > 8$.

3.4 A Parameter Fitting Problem

We now describe the problem we consider, first in the general case (Section 3.4.1), next in the one-dimensional case (Section 3.4.2). In that latter section, we also motivate our choice of macroscopic quantities from which we fit the parameters of the Weibull law.

3.4.1 General Case

We assume that we are given two observed quantities, the first one being the macroscopic permeability matrix

$$K_N^{\star,\text{obs}}(\omega) = e_1 \cdot A_N^{\star,\text{obs}}(\omega) e_1$$

and the second one is its relative variance S_N^{obs} for some parameters $\theta_{\text{obs}} = (\lambda_{\text{obs}}, k_{\text{obs}})$ of the Weibull law. Note that the relative variance crucially depends on the size N^d of the finite box on which it is measured (in contrast to the apparent permeability, which converges to a finite value when $N \longrightarrow \infty$). We assume here that we know this size. In practice, these three quantities, N,

$K_N^{\star,\text{obs}}$ and S_N^{obs}, can be obtained by physical experiments. Given N, $K_N^{\star,\text{obs}}$ and S_N^{obs}, our aim is to recover (an approximation of) θ_{obs}. To that aim, we consider the function

$$F_{N,M} : \quad \begin{cases} (\mathbb{R}_+^\star)^2 & \longrightarrow \quad \mathbb{R}_+ \\ \theta & \mapsto \left(\dfrac{\overline{K}_{N,M}^\star(\theta)}{K_N^{\star,\text{obs}}} - 1\right)^2 + \left(\dfrac{S_{N,M}(\theta)}{S_N^{\text{obs}}} - 1\right)^2 \end{cases} \tag{V.64}$$

which penalizes the sum of the (relative) errors between

- first, $\overline{K}_{N,M}^\star(\theta)$ (an empirical estimator of $\mathbb{E}[K_N^\star(\cdot,\theta)]$ when M is large), and $K_N^{\star,\text{obs}}$;
- second, $S_{N,M}(\theta)$ (an empirical estimator of the relative variance when M is large) and S_N^{obs}.

Different weights could be assigned to the error on the permeability and the error on its relative variance. We eventually cast our parameter fitting problem in the form of the optimization problem

$$\inf_{\theta \in (0,\infty)\times\mathcal{K}} F_{N,M}(\theta),$$

where $\mathcal{K} \subset (0,\infty)$ is the admissible set of parameters k such that homogenization holds (even if Assumption (V.51) is not satisfied for any $k > 0$) and the variance of $K_N^\star$ is also well-defined. In the one-dimensional case, $\mathcal{K} = (8,\infty)$.

3.4.2 The One-Dimensional Case

In the one-dimensional case, explicit computations are available, in particular when $M \longrightarrow \infty$ and $N \longrightarrow \infty$. In [62] we prove the following lemma:

Lemma V.31. *The function* $F_\infty^{1D} := \lim_{M\longrightarrow\infty} \lim_{N\longrightarrow\infty} F_N^{1D}(\theta)$ *has a unique minimizer, which is* θ_{obs}.

Homogenization is an averaging process, which filters out many features of the microscopic coefficient A. These features cannot be recovered from the knowledge of macroscopic quantities. The above lemma shows that, if one assumes a given form for the probability distribution of A (here, a Weibull distribution), then one is able to recover the two parameters, knowing two macroscopic quantities, the permeability and its relative variance.

It is also obvious from (V.63) that the knowledge of the macroscopic permeability is not enough to uniquely determine the two parameters λ and k of the Weibull law. Additional information is needed. Our choice of considering the relative variance of the permeability is motivated by the following observation. This quantity, in the one-dimensional case, only depends (at first order in N) on k and does not depend on λ, so that it permits to estimate the parameter k. Once k has been identified, the macroscopic permeability yields an estimation of λ, by using (V.63).

In [62], we have ploted the function $\theta \mapsto F_\infty^{1D}(\theta)$ for $\lambda_{\text{obs}} = 1$ and $k_{\text{obs}} = 15$. We observe that the function is not degenerated at its minimum, in the sense that its hessian matrix at θ_{obs} is positive definite, with eigenvalues equal to 16 and 0.04. We thus expect that a standard algorithm (such as the Newton algorithm) will be able to converge to the minimizer of F_∞^{1D}. This is indeed the case, as shown in Section 3.5.

Finally, we show in [62] that we can approximate the function to minimize by an explicit function F_N^{1D}, that does not depend on M. This function is consistent in the sense that it almost surely converges, when $N \longrightarrow \infty$, to the exact function $F_\infty^{1D}(\theta)$. On the other hand, $F_N^{1D}(\theta,\omega)$ is random, and thus somewhat mimics the difficulties that one would encounter in the multi-dimensional case when working with $F_{N,M}(\theta)$.

3.5 Numerical Simulations

We briefly explain how in practice we minimize the function F_N^{1D}, before turning to our numerical results. As pointed out in the introduction, we only consider here the one-dimensional case, and postpone the study of two-dimensional examples to a future work.

Optimization algorithm – We show in [62] how to compute the first and second derivatives of the function $F_N^{1D}(\theta, \omega)$ with respect to $\theta = (\lambda, k)$. Then, we use the Newton algorithm, and compute a sequence θ_j according to

$$\theta_{j+1} = \theta_j - \mu_j \left[\mathcal{H}\left(F_N^{1D}\right)(\theta_j)\right]^{-1} \nabla F_N^{1D}(\theta_j), \tag{V.65}$$

where $\mathcal{H}\left(F_N^{1D}\right) \in \mathbb{R}^{2\times 2}$ is the Hessian matrix of F_N^{1D} and $\nabla F_N^{1D} \in \mathbb{R}^2$ is the gradient of F_N^{1D} (for the sake of simplicity, we keep implicit the dependence with respect to ω). In turn, $\mu_j > 0$ is the step-size, which is chosen by using a line-search algorithm (along the descent direction prescribed by the Newton algorithm), with Goldstein's (respectively Armijo's) rule to increase (respectively decrease) the step-size.

We note that the function $\theta \mapsto F_\infty^{1D}(\theta)$ is not convex. It is possible to find some θ such that the Hessian matrix $\mathcal{H}\left(F_\infty^{1D}\right)(\theta)$ is not positive definite, but rather has (at least) one negative eigenvalue. We thus cannot expect the function $\theta \mapsto F_N^{1D}(\theta)$ to be convex (even for large values of N), and the Newton algorithm to be globally convergent. We are therefore careful to start the Newton iterations from an initial guess θ_0 (given by physical experiments) that we hope to be close enough to the minimizer of F_N^{1D}.

Numerical results – In all what follows, we set $N = 10^5$. Our first numerical test is to check whether the Newton algorithm (V.65) is indeed able to minimize the function $\theta \mapsto F_N^{1D}(\theta, \omega)$. We pick once for all one realization of the i.i.d. random variables and we run the Newton algorithm (V.65) starting from several initial guesses θ_0. We observe that it indeed always converges to θ_{obs} in a limited number of iterations. We also remark that, for some initial guesses, using an adaptive step-size μ_j as in (V.65) is critical: if, in contrast, one uses the step-size $\mu_j = 1$, then the algorithm may not converge, or converges within a much larger number of iterations.

For our second test, we proceed as follows. We first set $\theta_{ref} = (\lambda_{ref}, k_{ref}) = (1, 15)$, pick one realization of the i.i.d. random variables $\overline{\omega}$ and define all the macroscopic observed quantities computed with this realization. We now fix the initial guess $\theta_0 = (1.1, 16.5)$ (10% off the reference value θ_{ref}) and set $M = 500$. For any $1 \leqslant m \leqslant M$, we apply the following procedure:

- we draw a realization of N i.i.d. random variables ω_m.
- we run the Newton algorithm (V.65) to minimize the function $\theta \mapsto F_N^{1D}(\theta, \omega_m)$. The optimal parameter found by the algorithm depends on ω_m and is denoted by $\theta_{opt}(\omega_m)$. Since ω_m is different from the reference realization $\overline{\omega}$, we have in general $\theta_{opt}(\omega_m) \neq \theta_{ref}$.

We show on Figure V.3 the histogram of the optimal parameters $\theta_{opt}(\omega_m)$ for $1 \leqslant m \leqslant M$. We see that these histograms are centered close to the reference value (k_{ref}, resp. λ_{ref}). There is however a small bias, i.e. $\mathbb{E}[\theta_{opt}] \neq \theta_{ref}$. We also observe that the width of these histograms (related to the variance of k_{opt} and λ_{opt}) is quite small.

REMARK *3.3.* Of course, the variance of k_{opt} and λ_{opt} is related to N. In the limit $N \longrightarrow \infty$, the function $F_N^{1D}(\theta, \omega)$ almost surely converges to a deterministic limit, and we thus expect k_{opt} and λ_{opt} to almost surely converge to a deterministic limit. But this is not the regime we are interested in, since in practice (in the two-dimensional case), we have to work with the *random* function $F_{N,M}$.

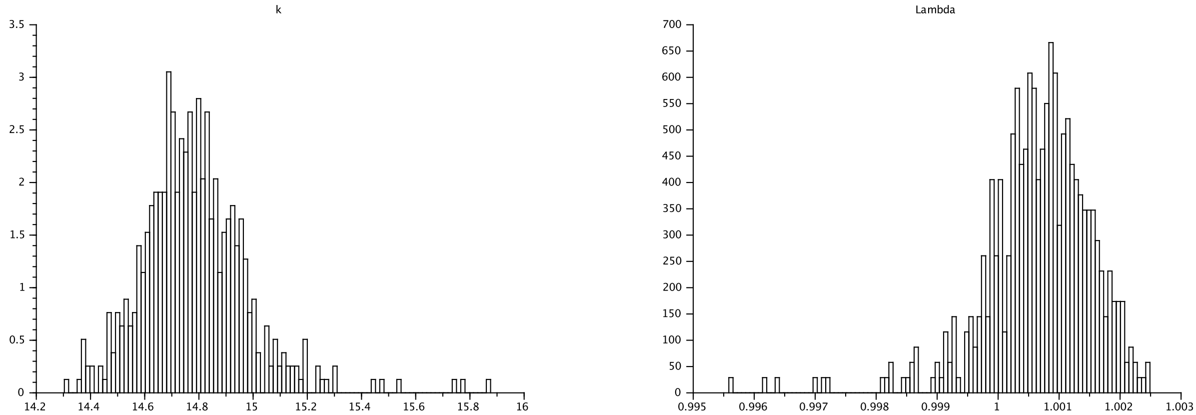

Figure V.3: **Left**: distribution of $k_{\text{opt}}(\omega)$. **Right**: distribution of $\lambda_{\text{opt}}(\omega)$.

We next compare the variance of θ_{opt} with the amount of randomness introduced in the function $F_N^{1D}(\cdot, \omega)$. We show on Figure V.4 the histograms, for $1 \leqslant m \leqslant M$, of the two macroscopic quantities $K_N^\star(\theta_0, \omega_m)$ and of $S_N(k_0, \omega_m)$, for the initial guess parameter $\theta_0 = (1.1, 16.5)$. We observe that the relative variance of the optimal parameters is roughly of the same order of magnitude as the relative variance introduced in the function to minimize.

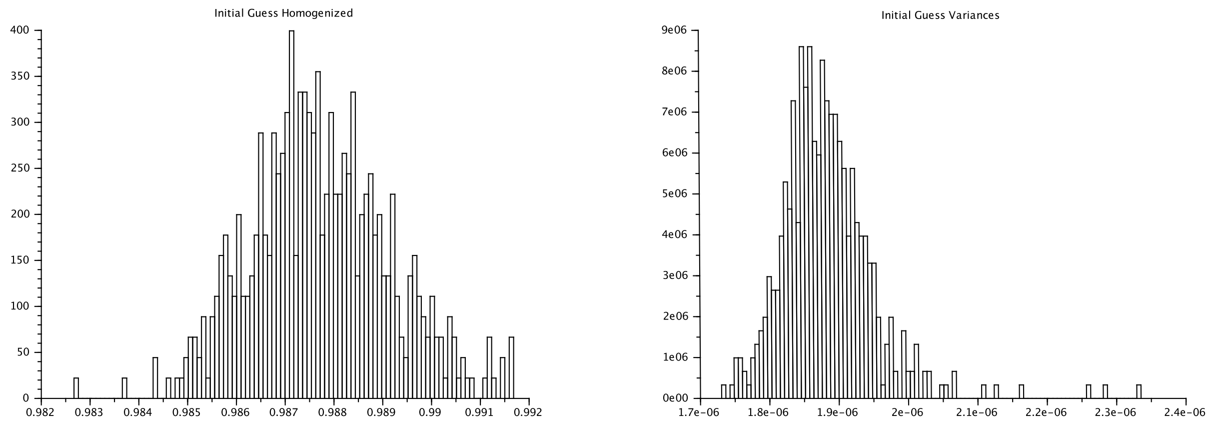

Figure V.4: **Left**: distribution of $K_N^\star(\theta_0, \omega)$. **Right**: distribution of $S_N(k_0, \omega)$.

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Résumé

L'équation de la chaleur est un phénomène macroscopique, émergeant après une limite d'échelle diffusive (en espace et en temps) d'un système d'oscillateurs couplés. Lorsque les interactions entre oscillateurs sont linéaires, l'énergie évolue de manière balistique, et la conductivité thermique est infinie. Certaines non-linéarités doivent donc apparaître au niveau microscopique, si l'on espère observer une diffusion normale. Pour apporter de l'ergodicité, on ajoute à la dynamique déterministe une perturbation stochastique qui conserve l'énergie.

En premier lieu nous étudions la dynamique Hamiltonienne d'un système d'oscillateurs linéaires, perturbé par un bruit stochastique dégénéré conservatif. Ce dernier transforme à des temps aléatoires les vitesses en leurs opposées. On montre que l'évolution macroscopique du système est caractérisée par un système parabolique non-linéaire couplé pour les deux lois de conservation du modèle.

Ensuite, nous supposons que les oscillateurs évoluent en environnement aléatoire. La perturbation stochastique est très dégénérée, et on prouve que le champ de fluctuations de l'énergie à l'équilibre converge vers un processus d'Ornstein-Uhlenbeck généralisé dirigé par l'équation de la chaleur.

Il est désormais connu que les systèmes unidimensionnels présentent une diffusion anormale lorsque le moment total est conservé en plus de l'énergie. Dans une troisième partie, on considère deux perturbations, l'une préservant le moment, l'autre détruisant cette conservation. En faisant décroître l'intensité de la seconde perturbation, on observe une transition de phase entre un régime de diffusion normale et un régime de superdiffusion.

Abstract

The heat equation is known to be a macroscopic phenomenon, emerging after a diffusive rescaling of space and time. In linear systems of interacting oscillators, the energy ballistically disperses and the thermal conductivity is infinite. Since the Fourier law is not valid for linear interactions, non-linearities in the microscopic dynamics are needed. In order to bring ergodicity to the system, we superpose a stochastic energy conserving perturbation to the underlying deterministic dynamics.

In the first part we study the Hamiltonian dynamics of linear coupled oscillators, which are perturbed by a degenerate conservative stochastic noise. The latter flips the sign of the velocities at random times. The evolution yields two conservation laws (the energy and the length of the chain), and the macroscopic behavior is given by a non-linear parabolic system.

Then, we suppose the harmonic oscillators to evolve in a random environment, in addition to be stochastically perturbed. The noise is very degenerate, and we prove a macroscopic behavior that holds at equilibrium: precisely, energy fluctuations at equilibrium evolve according to an infinite dimensional Ornstein-Uhlenbeck process driven by the linearized heat equation.

Finally, anomalous behaviors have been observed for one-dimensional systems which preserve momentum in addition to the energy. In the third part, we consider two different perturbations, the first one preserving the momentum, and the second one destroying that new conservation law. When the intensity of the second noise is decreasing, we observe (in a suitable time scale) a phase transition between a regime of normal diffusion and a regime of super-diffusion.