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SEMICLASSICAL PROPAGATION OF COHERENT STATES FOR THE HARTREE EQUATION

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1. Introduction

Let us consider the Hartree equation in $\mathbb{R}^d$:

$$\begin{gathered} i\varepsilon\partial_t\Psi^\varepsilon(x,t) = -\tfrac{\varepsilon^2}{2}\Delta\Psi^\varepsilon(x,t) + \left(V(x,t)+U(x,t)\right)\Psi^\varepsilon(x,t), \\ \Psi^\varepsilon(x,0) = \Psi_0^\varepsilon(x), \end{gathered} \tag{1}$$

where

$$V(x,t) = \int \phi(|x-y|)|\Psi^\varepsilon(y,t)|^2 dy \tag{2}$$

is a self-consistent potential given by a smooth two-body interaction, $\phi : \mathbb{R} \to \mathbb{R}$, even, and $U(\cdot,t) : \mathbb{R}^d \to \mathbb{R}$ for all $t \geq 0$, is a smooth external potential (see the next section for the precise assumptions on ϕ and U).

In a recent paper [1] the authors of the present one considered the semiclassical limit of the version of the Hartree equation corresponding to mixed states, for initial data whose Wigner functions do not concentrate at the classical limit.

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The problem we deal with in the present paper is the semiclassical asymptotics for (1) when the initial state is a coherent state centered around the point q, p of the classical phase space, namely:

$$\Psi_0^\varepsilon(x) = \varepsilon^{-\frac{d}{4}} a_0\left(\frac{x-q}{\sqrt{\varepsilon}}\right) e^{i\frac{p\cdot(x-q)}{\varepsilon}} := \psi_{qp}^{a_0}(x). \tag{3}$$

This problem was studied in [9] in the kinetic (Wigner) picture, see Théorème IV.2 therein. There it is shown that, under appropriate conditions, the solution W^ε of the Wigner equation corresponding to the dynamics (1) namely

$$\begin{aligned}\partial_t W^\varepsilon + k\cdot\partial_x W^\varepsilon &= \frac{i}{\varepsilon(2\pi)^d}\int\int e^{i\xi y}\left(V(x+\frac{\varepsilon y}{2},t) - V(x-\frac{\varepsilon y}{2},t)\right) dy\, W^\varepsilon(x,k-\xi)d\xi + \\ &+ \frac{i}{\varepsilon(2\pi)^d}\int\int e^{i\xi y}\left(U(x+\frac{\varepsilon y}{2},t) - U(x-\frac{\varepsilon y}{2},t)\right) dy\, W^\varepsilon(x,k-\xi)d\xi,\end{aligned} \tag{4}$$

where $V(x,t)$ is the same as in (1) equivalently written as

$$V(x,t) = \int \phi(|x-y|)W^\varepsilon(y,k,t)dkdy, \tag{5}$$

converges, in weak$*$-sense, to the solution of the (classical) Vlasov equation

$$\begin{gathered}\partial_t f + k\cdot\partial_x f - \partial_x V_0(x,t)\cdot\partial_k f - \partial_x U(x,t)\cdot\partial_k f = 0, \\ f(x,k,t)|_{t=0} = f_0(x,k),\end{gathered} \tag{6}$$

where

$$V_0(x,t) = \int \phi(|x-y|)f(y,k,t)dkdy,$$

and $U(x,t)$ is the same as in (1) . The initial condition for (6) is given by $f_0 = w -^* \lim_{\varepsilon\to 0} W_0^\varepsilon$. It is easy to check that the conditions of Théorème IV.2 in [9] are satisfied for $W_0^\varepsilon(x,v) = W^\varepsilon[\Psi_0^\varepsilon](x,v)$, Ψ_0^ε as in equation (3). In that case (under appropriate assumptions on the pair-interaction potential ϕ and the external potential U) it can be seen that the Wigner measure of the wave function verifies

$$W^\varepsilon[\Psi^\varepsilon](x,k,t) \rightharpoonup \delta(x-X(t))\delta(k-K(t)), \quad \text{ as } \varepsilon\to 0,$$

where

$$\dot X(t) = K(t), \qquad \dot K(t) = -\nabla U(X(t),t), \qquad X(0)=q, \qquad K(0)=p.$$

In that sense, the semiclassical limit of the problem (1) is known to be the Vlasov dynamics (6), since it is easy to recognize that, due to the smoothness of the potentials, the limiting measure $\delta(x-X(t))\delta(k-K(t))$ is the unique (weak) solution of the Vlasov equation with initial datum $\delta(x-q)\delta(k-p)$.

The goal of the present work is to strengthen this approximation. First of all, we construct L^2 approximations, as opposed to the with weak$*$-limit, and this yields an explicit control of the error in ε which allows to recover the shape with which W^ε concentrates to a δ in phase-space.

2. Main result

We will consider the Hartree equation in $\mathbb{R}^d$:

$$\begin{gathered} i\varepsilon\partial_t\Psi^\varepsilon(x,t) = -\tfrac{\varepsilon^2}{2}\Delta\Psi^\varepsilon(x,t) + \left(V(x,t)+U(x,t)\right)\Psi^\varepsilon(x,t), \\ \Psi^\varepsilon(x,0) = \Psi^\varepsilon_0(x), \end{gathered} \tag{7}$$

where

$$V(x,t) = \int \phi(|x-y|)|\Psi^\varepsilon(y,t)|^2 dy \tag{8}$$

The initial condition will be of the form

$$\Psi^\varepsilon_0(x) = \varepsilon^{-\frac{d}{4}} a_0\left(\frac{x-q}{\sqrt{\varepsilon}}\right) e^{i\frac{p\cdot(x-q)}{\varepsilon}} := \psi^{a_0}_{qp}$$

and we will make the following assumptions on a_0, ϕ and U:

Assumption 1.

$$\|a_0\|_{L^2} = \|\Psi^\varepsilon_0\|_{L^2} = 1,$$

$$x^A\partial_x^B a_0(x) \in L^2 \textit{ for any pair } A,B\in\mathbb{N}^d \textit{ with } |A|+|B|\leqslant 3,$$

$$\int x_i|a_0(x)|^2dx = 0,\ \forall\, i=1\ldots d. \tag{9}$$

$$\int k_i|\widehat{a}_0(k)|^2dk = 0,\ \forall\, i=1\ldots d. \tag{10}$$

Assumption 2.

$$C^3_b(\mathbb{R}) \ni \phi \textit{ even}$$

Assumption 3.

$$U\in C^1\left(\mathbb{R}^+_t, C^3_b(\mathbb{R}^d_x)\right).$$

Here and henceforth we denote by $C^k_b(\mathbb{R}^m)$ the space of continuous and uniformly bounded functions on $\mathbb{R}^m$ whose all derivatives up the order k are also continuous and uniformly bounded.

Theorem 2.1. *Under Assumptions 1, 2 and 3 there exists a constant C such that, $\forall\ t\geq 0$,*

$$\|\Psi^\varepsilon(\cdot,t) - e^{i\frac{\mathcal{L}(t)}{\varepsilon}+i\gamma(t)}\psi^{\beta_t}_{q(t)p(t)}\|_{L^2} \leqslant Ce^{Cte^{C\,e^{C\,t}}}\cdot\sqrt{\varepsilon}. \tag{11}$$

where β_t is the solution of

$$i\partial_t\beta_t(x) = \left(-\frac{\Delta}{2}+\frac{\phi''(0)x^2}{2}+\frac{< x,\nabla^2U(q(t),t)x >}{2}\right)\beta_t(x), \tag{12}$$

$$\beta_0(x) = a_0(x), \tag{13}$$

$$\gamma(t) = -\frac{\phi''(0)}{2} \int_0^t \int \eta^2 |\beta_s(\eta)|^2 d\eta ds, \tag{14}$$

$(q(t), p(t))$ is the Hamiltonian flow associated with $\frac{p^2}{2} + U(q,t) + \phi(0)$ issued from (q,p),

$$\mathcal{L}(t) := \int_0^t \left(p(s)^2/2 - U(q(s),s) - \phi(0)\right) ds$$

(the Lagrangian action along such Hamiltonian flow).

Remarks:

- As shown in the proof of the Theorem, the constant C depends only on d, $||U||_{W^{3,\infty}}$, $||\phi||_{W^{3,\infty}}$ and $\sup\limits_{|A|+|B|\leqslant 3} ||x^B \partial_x^A a_0||_{L^2}$.
- Note that in the classical flow the nonlinear potential enters only via the inessential constant $\phi(0)$. Indeed, due to the symmetry and smoothness of ϕ, we have $\phi'(0) = 0$ so that, in case of concentration as $\varepsilon \to 0$, the self-consistent field ∇V vanishes.
- A similar problem for $\phi''(0) \geq 0$ has been faced in [2] in a semirigorous way. Here we treat the case $\phi''(0) \leq 0$ as well and present an explicit control of momenta and derivatives of the solutions (see Lemma 2.3 below) which allow us to estimate the error in L^2.
- For a related result (Gross-Pitaevskii equation with a different scaling) see [3].
- Assumption 1 can be relaxed by dismissing equation (9). Indeed even if (9) does not hold one can always make a change of variables $x \mapsto x - \int x|a_0(x)|^2 dx$. However in that case one would have to adjust appropriately the external potential, which of course is not translation invariant.

3. Proofs

3.1. A Lemma.

We first prove the following

Lemma 3.1. *$b_t(x) := e^{i\gamma(t)}\beta_t(x)$ as defined by (12,13,14) is the unique solution of the equation:*

$$\begin{gathered}\left(i\partial_t + \tfrac{1}{2}\Delta\right) b_t(x) = \tfrac{\phi''(0)}{2} \int |x-\eta|^2 |b_t(\eta)|^2 d\eta \; b_t(x) + \tfrac{<x, \nabla^2 U(q(t),t) x>}{2} b_t(x), \\ b_0(x) = a_0(x).\end{gathered} \tag{15}$$

Proof.

$$i\partial_t b_t(x) = -\gamma'(t) b_t(x) + e^{i\gamma(t)} i\partial_t \beta_t(x). \tag{16}$$

By virtue of equations (12), (13) and (14) we find

$$\begin{gathered} i\partial_t b_t(x) = \tfrac{\phi''(0)}{2} \int \eta^2 |\beta_t(\eta)|^2 d\eta \; b_t(x) + e^{i\gamma(t)} \left(-\tfrac{\Delta}{2}\beta_t(x) + \tfrac{\phi''(0)}{2} x^2 \; \beta_t(x) + \tfrac{<x,\nabla^2 U(q(t),t)x>}{2} \; \beta_t(x)\right), \\ b_0(x) = a_0(x), \end{gathered} \tag{17}$$

namely

$$\begin{gathered} i\partial_t b_t(x) = -\tfrac{\Delta}{2} b_t(x) + \tfrac{\phi''(0)}{2} x^2 \ b_t(x) + \tfrac{\phi''(0)}{2} \int \eta^2 |\beta_t(\eta)|^2 d\eta \ b_t(x) + \tfrac{<x,\nabla^2 U(q(t),t)x>}{2} \ b_t(x), \\ b_0(x) = a_0(x). \end{gathered} \tag{18}$$

We first notice that the equation (12) for $\beta_t(x)$ is a linear Schrödinger equation with an harmonic potential; therefore the solution $\beta_t(x)$ of the initial value problem (12)-(13) is uniquely determined in $L^2(\mathbb{R}^d)$ and

$$\|\beta_t\|_{L^2} = \|a_0\|_{L^2} = 1, \quad \forall \ t \in \mathbb{R}. \tag{19}$$

As a consequence of that, it turns out that equation (18) can be rewritten as

$$\begin{gathered} i\partial_t b_t(x) = -\tfrac{\Delta}{2} b_t(x) + \tfrac{\phi''(0)}{2} \int x^2 |\beta_t(\eta)|^2 d\eta \ b_t(x) + \tfrac{\phi''(0)}{2} \int \eta^2 |\beta_t(\eta)|^2 d\eta \ b_t(x) + \tfrac{<x,\nabla^2 U(q(t),t)x>}{2} \ b_t(x), \\ b_0(x) = a_0(x). \end{gathered} \tag{20}$$

Furthermore, it is easy to check that if

$$x a_0(x), \ \partial_x a_0(x) \in L^2(\mathbb{R}^d), \tag{21}$$

then

$$x\beta_t(x), \ \partial_x \beta_t(x) \in L^2(\mathbb{R}^d), \text{ for all } t, \tag{22}$$

(see Observation 4.3 below).
Condition (21) is satisfied under Assumption 1, so the property (22) holds and, in particular, there exists a constant C finite for any time t such that

$$\int |\eta|^2 |\beta_t(\eta)|^2 d\eta < C, \ \forall \ \ t \in \mathbb{R}. \tag{23}$$

Thus, by virtue of (23) and of Assumptions 1, 2 and 3, it follows that the initial value problem (20) is guaranteed to have a unique solution in L^2 and, clearly, $\|b_t\|_{L^2} = \|a_0\|_{L^2} = 1, \quad \forall \ t$. In fact, the equation for $b_t(x)$ has turned to be a linear Schrödinger equation with an harmonic potential (and all constants appearing in the potential terms are finite thanks to Assumptions 2 and 3 and to (23)).

Now, it remains only to recognize that (20) is exactly the same as (15). To this end it is sufficient to observe that, since the equation (12) for $\beta_t(x)$ is a linear Schrödinger equation with an harmonic potential and conditions (9) and (10) are satisfied at time $t = 0$, we are guaranteed that

$$\int \eta |\beta_t(\eta)|^2 d\eta = 0, \ \forall \ \ t. \tag{24}$$

Thus, by virtue of (24), it follows straightforwardly that (20) can be rewritten as

$$\begin{gathered} i\partial_t b_t(x) = -\tfrac{\Delta}{2} b_t(x) + \tfrac{\phi''(0)}{2} \int |x-\eta|^2 |\beta_t(\eta)|^2 d\eta \ b_t(x) + \tfrac{<x,\nabla^2 U(q(t),t)x>}{2} \ b_t(x), \\ b_0(x) = a_0(x). \end{gathered} \tag{25}$$

Finally, it is clear, by the definition of $b_t(x)$, that $|\beta_t(x)| = |b_t(x)|$ for any x and t. Therefore (25) turns to be exactly the same as (15). $\square$

3.2. **Proof of Theorem 2.1.** We seek an approximate solution to equation (1) of the form as e.g. in [6, 7, 8, 11, 12]

$$\Psi^\varepsilon(x,t) = \varepsilon^{-\frac{d}{4}} a(\frac{x-q(t)}{\sqrt{\varepsilon}}, t) e^{i\frac{p(t)\cdot(x-q(t))}{\varepsilon}} e^{i\frac{\mathcal{L}(t)}{\varepsilon}} \tag{26}$$

where

$$\dot{q}(t) = p(t), \ \dot{p}(t) = -\nabla U(q(t),t). \tag{27}$$

By inserting the ansatz (26) in equation (1) we get

$$\begin{aligned} i\varepsilon\partial_t\Psi^\varepsilon(x,t) \ &= \ \varepsilon^{-\frac{d}{4}}\left[i\varepsilon\partial_t a(\frac{x-q(t)}{\sqrt{\varepsilon}},t) - i\sqrt{\varepsilon}\nabla a(\frac{x-q(t)}{\sqrt{\varepsilon}},t)\cdot\dot{q}(t) + \right.\\ &\left. - \mathcal{L}'(t)a(\frac{x-q(t)}{\sqrt{\varepsilon}},t) - (\dot{p}(t)(x-q(t)) - p(t)\dot{q}(t))\, a(\frac{x-q(t)}{\sqrt{\varepsilon}},t)\right]\times \\ &\times e^{i\frac{p(t)\cdot(x-q(t))}{\varepsilon}} e^{i\frac{\mathcal{L}(t)}{\varepsilon}}, \end{aligned} \tag{28}$$

and

$$\begin{aligned} -\frac{\varepsilon^2}{2}\Delta\Psi^\varepsilon(x,t) \ &= \ \varepsilon^{-\frac{d}{4}}\left[-\frac{\varepsilon}{2}\Delta a(\frac{x-q(t)}{\sqrt{\varepsilon}},t) + \frac{p^2(t)}{2}a(\frac{x-q(t)}{\sqrt{\varepsilon}},t) + \right.\\ &\left. - i\sqrt{\varepsilon}\nabla a(\frac{x-q(t)}{\sqrt{\varepsilon}},t)\cdot p(t)\right] e^{i\frac{p(t)\cdot(x-q(t))}{\varepsilon}} e^{i\frac{\mathcal{L}(t)}{\varepsilon}}, \end{aligned} \tag{29}$$

while, with regard to the potential terms in (1), we find

$$\begin{aligned} (V(x,t)+U(x,t))\,\Psi^\varepsilon(x,t) \ &= \ \varepsilon^{-d/4}\left(\int\phi(|x-y|)\varepsilon^{-d/2}|a(\frac{y-q(t)}{\sqrt{\varepsilon}},t)|^2dy + U(x,t)\right)\times \\ &\times a(\frac{x-q(t)}{\sqrt{\varepsilon}},t)e^{i\frac{p(t)\cdot(x-q(t))}{\varepsilon}} e^{i\frac{\mathcal{L}(t)}{\varepsilon}}. \end{aligned} \tag{30}$$

By (28), (29) and (30) we get that the amplitude a solves the following initial value problem:

$$\begin{gathered} \left(i\partial_t + \tfrac{1}{2}\Delta\right) a(\mu,t) = \tfrac{1}{\varepsilon}V_\varepsilon(\mu,t)a(\mu,t) + \\ + \tfrac{1}{\varepsilon}\left[U(q(t)+\sqrt{\varepsilon}\mu,t) - U(q(t),t) - \sqrt{\varepsilon}\nabla U(q(t),t)\cdot\mu\right] a(\mu,t), \\ a(\mu,0) = a_0(\mu), \end{gathered} \tag{31}$$

where

$$V_\varepsilon(\mu,t) = \int\left(\phi(\sqrt{\varepsilon}|\mu-\eta|) - \phi(0)\right)|a(\eta,t)|^2 d\eta, \tag{32}$$

$q(t), p(t)$ are as in the claim of Theorem 2.1 and we have used the rescaling $\mu = \frac{x-q(t)}{\sqrt{\varepsilon}}$. Note that we should have

$$V_\varepsilon(\mu,t) = \int \phi\left(\sqrt{\varepsilon}|\mu-\eta|\right)|a(\eta,t)|^2 d\eta - \phi(0), \tag{33}$$

instead of (32) in equation (31). However equation (31) with potential (33) is an Hartree equation which preserves the L^2 norm so that we can replace (33) by (32).

Since $\phi \in C_b^3(\mathbb{R})$ is even $\phi'(0) = 0$ and the Taylor expansion yields

$$\begin{gathered} \phi(\sqrt{\varepsilon}|\mu-\eta|) - \phi(0) = \tfrac{\varepsilon|\mu-\eta|^2}{2}\phi''(0) + \varepsilon^{\frac{3}{2}} R(|\mu-\eta|), \\ |R(|\mu-\eta|)| \leqslant C||\phi'''||_{L^\infty}|\mu-\eta|^3, \end{gathered} \tag{34}$$

while for the terms involving U we find:

$$\begin{gathered} U(q(t)+\sqrt{\varepsilon}\mu,t) - U(q(t),t) - \sqrt{\varepsilon}\nabla U(q(t),t)\cdot\mu = \varepsilon < \mu, \tfrac{\nabla^2 U(q(t),t)}{2}\mu > + \varepsilon^{\frac{3}{2}} R_U(\mu,t), \\ |R_U(\mu,t)| \leqslant C\, \sup_{\alpha\in\mathbb{N}^d:|\alpha|=3} |\nabla^\alpha U(q(t),t)||\mu|^3, \end{gathered} \tag{35}$$

where $\nabla^2 := \nabla \otimes \nabla$.

The core of the proof is to estimates the two remainders $\varepsilon^{\frac{3}{2}}R(|\mu-\eta|)$ and $\varepsilon^{\frac{3}{2}}R_U(\mu,t)$ so that we can substitute $(\phi(\sqrt{\varepsilon}|\mu-\eta|)-\phi(0))$ by $\frac{\varepsilon|\mu-\eta|^2}{2}\phi''(0)$ (as in (34)) and $U(q(t)+\sqrt{\varepsilon}\mu,t) - U(q(t),t) - \sqrt{\varepsilon}\nabla U(q(t),t)\cdot\mu$ by $\varepsilon < \mu, \frac{\nabla^2 U(q(t),t)}{2}\mu >$ (as in (35)).

In the framework of semiclassical approximation for the linear Schrödinger equation using coherent states the method is standard (see e.g. [6, 7, 8, 11, 12]), however we establish these estimates again for completeness.

Denote $a_t(\mu) := a(\mu,t)$ and

$$h_t(\mu) = b_t(\mu) - a_t(\mu). \tag{36}$$

By straightforward substitution we get that $h_0(\mu) = 0$ (see (15)) and

$$\begin{aligned} &\left(i\partial_t + \frac{1}{2}\Delta - \underbrace{\left(\frac{\phi''(0)}{2}\int |\mu-\eta|^2|b_t(\eta)|^2 d\eta + < \mu, \frac{\nabla^2 U(q(t),t)}{2}\mu >\right)}_{V_Q(\mu,t)}\right) h_t(\mu) = \\ &= \frac{\phi''(0)}{2}\underbrace{\int |\mu-\eta|^2\left(|b_t(\eta)|^2 - |a_t(\eta)|^2\right) d\eta\ a_t(\mu)}_{I_1(\mu,t)} + \\ &-\sqrt{\varepsilon}\underbrace{\int R(|\mu-\eta|)|a_t(\eta)|^2 d\eta\ a_t(\mu)}_{I_2(\mu,t)} - \sqrt{\varepsilon}R_U(\mu,t)a_t(\mu). \end{aligned} \tag{37}$$

By standard manipulations it turns out that

$$\|h_t\|_{L^2}\frac{d}{dt}\|h_t\|_{L^2} \leqslant \frac{|\phi''(0)|}{2}|\langle I_1, h_t\rangle| + \sqrt{\varepsilon}|\langle I_2, h_t\rangle| + \sqrt{\varepsilon}|\langle R_U(\cdot,t)a_t, h_t\rangle|. \tag{38}$$

Moreover, the term involving I_1 can be estimated as follows:

$$\begin{aligned} |\langle I_1, h\rangle| &\leq \left|\int_\mu\int_\eta |\mu-\eta|^2\left(|b_t(\eta)|^2 - |a_t(\eta)|^2\right) d\eta\, \overline{a}_t(\mu)h_t(\mu)d\mu\right| = \\ &= \left|\int_\mu\int_\eta |\mu-\eta|^2\left(|b_t(\eta)| - |a_t(\eta)|\right)\left(|b_t(\eta)| + |a_t(\eta)|\right) d\eta\, \overline{a}_t(\mu)h_t(\mu)d\mu\right| \leq \\ &\leq \left|\int_\mu\int_\eta |\mu-\eta|^2|h_t(\eta)|\left(|b_t(\eta)| + |a_t(\eta)|\right) d\eta\, \overline{a}_t(\mu)h_t(\mu)d\mu\right| \leq \\ &\leq 2\,\|h_t\|^2_{L^2}\int (1+|\mu|^2)^2\left[|a_t(\mu)| + |b_t(\mu)|\right]^2 d\mu, \end{aligned} \tag{39}$$

while, thanks to (34), the term involving I_2 is estimated by:

$$\begin{aligned} |\langle I_2, h\rangle| \leq C\,\|\phi'''\|_{L^\infty}\left|\int_\mu\int_\eta |\mu-\eta|^3|a_t(\eta)|^2 d\eta\, \overline{a}_t(\mu)h(\mu,t)d\mu\right| \leq \\ \leq C\,\|\phi'''\|_{L^\infty}\left(\left(\int d\eta\,|\eta|^3|a_t(\eta)|^2\right)||a_t||_{L^2}||h_t||_{L^2} + \right. \\ +3\left(\int d\eta\,|\eta|^2|a_t(\eta)|^2\right)^{3/2}||h_t||_{L^2} + 3\left(\int d\mu\,|\mu|^4|a_t(\mu)|^2\right)^{1/2}\left(\int d\eta\,|\eta|\,|a_t(\eta)|^2\right)||h_t||_{L^2} + \\ \left. + \left(\int d\mu\,|\mu|^6|a_t(\mu)|^2\right)^{1/2}||a_t||^2_{L^2}||h_t||_{L^2}\right). \end{aligned} \tag{40}$$

One should observe here that $\int d\eta\,|\eta|\,|a_t(\eta)|^2 \leq \left(\int d\eta\,(1+|\eta|^2)\,|a_t(\eta)|^2\right)$.

Finally, due to (35), the term involving $R_U(\mu,t)$ is controlled as follows:

$$\begin{aligned} |\langle R_U(\cdot,t)a_t, h_t\rangle| &\leq C \sup_{\alpha:|\alpha|=3}|\nabla^\alpha U(q(t),t)|\left(\int d\mu\,|\mu|^3|a_t(\mu)|\,|h_t(\mu)|\right) \leq \\ &\leq C\sup_t\sup_{\alpha:|\alpha|=3}|\nabla^\alpha U(q(t),t)|\left(\int d\mu\,|\mu|^6|a_t(\mu)|^2\right)^{1/2}||h_t||_{L^2}. \end{aligned} \tag{41}$$

Making use of Lemma 4.2 and equation (70) below to estimate terms of the form $||\,|\cdot|^m a_t||_{L^2} = \left(\int d\eta|\eta|^{2m}|a_t(\eta)|^2\right)^{1/2}$, for $m \leq 3$, and $||\,|\cdot|^m b_t||_{L^2} = \left(\int d\eta|\eta|^{2m}|b_t(\eta)|^2\right)^{1/2}$, for

$m \leq 2$, in terms of the same quantities evaluated at time $t = 0$, we easily show, by summing up the previous estimates, that there exist three ε-independent functions $C_1(t), C_2(t)$ such that:

$$\frac{d}{dt}||h_t||_{L^2} \leq \sqrt{\varepsilon} C_1(t) + C_2(t)||h_t||_{L^2}. \tag{42}$$

In particular $C_1(t), C_2(t)$ depend on the potentials ϕ and U and on the L^2-norm of moments and derivatives of a_0 (up to the order 3). With regard to the time dependence, $C_1(t), C_2(t)$ are double exponentials $Ce^{Ce^{Ct}}$, following Lemma 4.2 and observations 4.3, 4.4.

The conclusion follows with application of the Gronwall lemma.

□

4. Auxiliary results

Observation 4.1. *Observe that under our assumptions the nonlinear equation (31) can be shown to have, for any $T > 0$, a unique solution in $C^1\left([0,T], L^2(\mathbb{R}^d)\right)$ (see e.g. [4]). Therefore it follows (see e.g. [13]) that the corresponding* time-dependent linear *problem*

$$\left(i\partial_t + \tfrac{1}{2}\Delta\right) u(\mu, t) = \tfrac{1}{\varepsilon} \int \left(\phi(\sqrt{\varepsilon}|\mu - \eta|) - \phi(0)\right) |a(\eta, t)|^2 d\eta \; u(\mu, t) +$$

$$+ \tfrac{1}{\varepsilon} \left(U(q(t) + \sqrt{\varepsilon}\mu, t) - U(q(t), t) - \sqrt{\varepsilon} \nabla U(q(t), t) \cdot \mu\right) u(\mu, t), \tag{43}$$

$$u(x, 0) = u_0(x), \quad u_0 \in L^2(\mathbb{R}^d) \quad \|u_0\|_{L^2} = 1,$$

has a unique and well-defined L^2 propagator.

Lemma 4.2 (Propagation of Moments and derivatives for $a(x,t)$)**.** *Let $a(x,t)$ be the solution of the initial value problem (31). Suppose that for some $m \in \mathbb{N}$ there exists an ε-independent constant $M_m > 0$ such that*

$$||x^A \partial_x^B a_0||_{L^2} \leqslant M_m \tag{44}$$

for all $A, B \in \mathbb{N}^d$ such that $|A| + |B| \leqslant m$.

For $m \geq 2$, assume $\phi \in C_b^m(\mathbb{R}^d)$ and $U \in C^1(\mathbb{R}_t^+, C_b^m(\mathbb{R}_x^d))$. Then, there exists a (finite) ε-independent constant C_m such that

$$||x^A \partial_x^B a(t)||_{L^2} \leqslant C_m e^{C_m e^{C_m t}} M_m, \tag{45}$$

for all $A, B \in \mathbb{N}^d$ such that $|A| + |B| \leqslant m$.

For $m = 1$ inequality (45) holds by assuming $\phi \in C_b^2(\mathbb{R}^d)$ and $U \in C^1(\mathbb{R}_t^+, C_b^2(\mathbb{R}_x^d))$, while in the case $m = 0$ formula (45) becomes an equality and holds with unitary constant (for all t) by simply assuming $\phi \in C_b^0(\mathbb{R}^d)$ and $U \in C^1(\mathbb{R}_t^+, C_b^1(\mathbb{R}_x^d))$.

Remark: The proof makes no use of an energy conservation argument, and this is the reason why the Lemma can be established for both signs of $\phi''(0)$.

Proof. Denote

$$\psi^{A,B}(x, t) = x^B \partial_x^A a(x, t), \tag{46}$$

e.g. $\psi^{0,0}(x,t) := a(x,t)$.
It is straightforward to check that

$$\Big(i\partial_t + \tfrac{1}{2}\Delta - \tfrac{1}{\varepsilon}V_\varepsilon(x,t) - \tfrac{1}{\varepsilon}U(q(t)+\sqrt{\varepsilon}x,t) + \tfrac{1}{\varepsilon}U(q(t),t) + \tfrac{1}{\sqrt{\varepsilon}}\nabla U(q(t),t)\cdot x\Big)\,\psi^{A,B}(x,t) =$$

$$= -\sum_{k=1}^{d}\Big[\tfrac{B_k(B_k-1)}{2}\psi^{A,B-2e_k}(x,t) + B_k\psi^{A+e_k,B-e_k}(x,t)\Big] + \tfrac{1}{\varepsilon}\sum_{0\leqslant l<A}\prod_{k=1}^{d}\tbinom{A_k}{l_k}\partial_x^{A-l}V_\varepsilon(x,t)\psi^{l,B}(x,t)+$$

$$+\tfrac{1}{\varepsilon}\sum_{0\leqslant l<A}\prod_{k=1}^{d}\tbinom{A_k}{l_k}\partial_x^{A-l}U(q(t)+\sqrt{\varepsilon}x,t)\psi^{l,B}(x,t) - \tfrac{1}{\sqrt{\varepsilon}}\sum_{\substack{0<l\leqslant A,\\ |l|=1}}\prod_{k=1}^{d}\tbinom{A_k}{l_k}\partial_x^{l}\left(\nabla U(q(t),t)\cdot x\right)\psi^{A-l,B}(x,t) \tag{47}$$

where $B=(B_1,\dots,B_k,\dots,B_d)$, $l=(l_1,\dots,l_k,\dots,l_d)$, $A=(A_1,\dots,A_k,\dots,A_d)$ and $0\le l<A$ means that $0\le l_k<A_k$ for any $k=1,2,\dots,d$. The consistent initial data for (47) are defined by

$$\psi^{A,B}(x,0) = x^B\partial_x^A a_0(x),$$

and in particular $\psi^{0,0}(x,0) := a_0(x)$.

Some remarks with regard to our notation are in order; it is clear for example that if $B_k=0$ or $B_k=1$, then the first term on the right-hand side yields no contribution. Similarly for $B_k=0$ in the second term and $|A|=0$ for the remaining terms respectively.
The derivation of (47) is straightforward by induction.

Denote by $P(t,\tau)$ the propagator associated with the left-hand side of equation (47), which is known to be uniquely well defined in L^2 (see Observation 4.1). As a consequence, for $m=0$, the result claimed by Lemma 4.2 follows from the existence of the propagator. We will proceed for $m\in\mathbb{N}$ by induction.

We will work with vectors including all the moments and derivatives, namely, $\overrightarrow{\Psi} = \{\psi^{A,B}\}_{A,B:|A|+|B|\le m}\in X_m$ and

$$||\overrightarrow{\Psi}||_{X_m} = \sum_{0\leqslant|A|+|B|\leqslant m}||\psi^{A,B}||_{L^2},$$

where $X_0 := L^2(\mathbb{R}^d)$.

For $m=1$ we have

$$\left(i\partial_t + \frac{1}{2}\Delta - \frac{1}{\varepsilon}V_\varepsilon(x,t) - \frac{1}{\varepsilon}U(q(t)+\sqrt{\varepsilon}x,t) + \frac{1}{\varepsilon}U(q(t),t) + \frac{1}{\sqrt{\varepsilon}}\nabla U(q(t),t)\cdot x\right)\psi^{e_j,0}(x,t) =$$

$$= \frac{1}{\varepsilon}\,\partial_{x_j}V_\varepsilon(x,t)\psi^{0,0}(x,t) + \frac{1}{\varepsilon}\,\partial_{x_j}U(q(t)+\sqrt{\varepsilon}x,t)\psi^{0,0}(x,t) - \frac{1}{\sqrt{\varepsilon}}\,\partial_{z_j}U(z,t)|_{z=q(t)}\,\psi^{0,0}(x,t), \tag{48}$$

and

$$\left(i\partial_t + \frac{1}{2}\Delta - \frac{1}{\varepsilon}V_\varepsilon(x,t) - \frac{1}{\varepsilon}U(q(t)+\sqrt{\varepsilon}x,t) + \frac{1}{\varepsilon}U(q(t),t) + \frac{1}{\sqrt{\varepsilon}}\nabla U(q(t),t)\cdot x\right)\psi^{0,e_j}(x,t) = \\ = \psi^{e_j,0}(x,t) \tag{49}$$

By virtue of the Duhamel formula we get:

$$\begin{aligned}\psi^{e_j,0}(x,t) &= P(t,0)\psi^{e_j,0}(x,0) + \int_0^t d\tau\, P(t,\tau)\,\left[\frac{1}{\varepsilon}\,\partial_{x_j}V_\varepsilon(x,\tau)\psi^{0,0}(x,\tau)\right] + \\ &+ \int_0^t d\tau\, P(t,\tau)\,\left[\frac{1}{\varepsilon}\,\partial_{x_j}U(q(\tau)+\sqrt{\varepsilon}x,\tau)\psi^{0,0}(x,\tau) - \frac{1}{\sqrt{\varepsilon}}\,\partial_{z_j}U(q(\tau),\tau)\,\psi^{0,0}(x,\tau)\right]\end{aligned} \tag{50}$$

and

$$\psi^{0,e_j}(x,t) = P(t,0)\psi^{0,e_j}(x,0) + \int_0^t d\tau\, P(t,\tau)\,\left[\psi^{e_j,0}(x,\tau)\right]. \tag{51}$$

Then, by recalling that $P(t,\tau)$ is L^2-norm preserving, we find

$$\begin{aligned}\left\|\psi^{e_j,0}(t)\right\|_{L^2} &\leq \left\|\psi^{e_j,0}(0)\right\|_{L^2} + \int_0^t d\tau\,\left\|\frac{1}{\varepsilon}\,\partial_{x_j}V_\varepsilon(x,\tau)\psi^{0,0}(\tau)\right\|_{L^2} + \\ &+ \int_0^t d\tau\,\left\|\left(\frac{1}{\varepsilon}\,\partial_{x_j}U(q(\tau)+\sqrt{\varepsilon}x,\tau) - \frac{1}{\sqrt{\varepsilon}}\,\partial_{z_j}U(q(\tau),\tau)\right)\,\psi^{0,0}(\tau)\right\|_{L^2}\end{aligned} \tag{52}$$

and

$$\left\|\psi^{0,e_j}(t)\right\|_{L^2} \leq \left\|\psi^{0,e_j}(0)\right\|_{L^2} + \int_0^t d\tau\,\left\|\psi^{e_j,0}(\tau)\right\|_{L^2}. \tag{53}$$

Now, taking into account the terms involving U in (52), we get

$$\begin{aligned}&\frac{1}{\varepsilon}\,\partial_{x_j}U(q(\tau)+\sqrt{\varepsilon}x,\tau) - \frac{1}{\sqrt{\varepsilon}}\,\partial_{z_j}U(q(\tau),\tau) = \\ &= \frac{1}{\sqrt{\varepsilon}}\partial_{z_j}U(z,\tau)|_{z=q(\tau)+\sqrt{\varepsilon}x} - \frac{1}{\sqrt{\varepsilon}}\,\partial_{z_j}U(z,\tau)|_{z=q(\tau)} = \\ &= \left[\partial^2_{z_j}U(z,\tau)|_{z=q(t)+\sqrt{\delta}\,x}\right]x_j, \quad \text{for some } \delta\in(0,\varepsilon),\end{aligned} \tag{54}$$

therefore

$$\left\| \left(\frac{1}{\varepsilon}\,\partial_{x_j} U(q(\tau)+\sqrt{\varepsilon}x,\tau) - \frac{1}{\sqrt{\varepsilon}}\,\partial_{z_j} U(q(\tau),\tau) \right) \psi^{0,0}(\tau) \right\|_{L^2} =$$

$$= \left\| \left[\partial^2_{z_j} U(z,\tau)|_{z=q(\tau)+\sqrt{\delta}\,x} \right] x_j\, \psi^{0,0}(\tau) \right\|_{L^2} = \left\| \left[\partial^2_{z_j} U(z,\tau)|_{z=q(\tau)+\sqrt{\delta}\,x} \right] \psi^{0,e_j}(\tau) \right\|_{L^2} \leq$$

$$\leq \sup_{\tau\in[0,t]} \left\| \partial^2 U(\cdot,\tau) \right\|_{L^\infty} \left\| \psi^{0,e_j}(\tau) \right\|_{L^2}. \tag{55}$$

On the other side, with regard to the term involving V_ε in (52), we have

$$\begin{aligned} \left| \frac{1}{\varepsilon}\,\partial_{x_j} V_\varepsilon(x,\tau) \right| &= \left| \int d\eta\, \partial_{x_j} \frac{1}{\varepsilon} \phi(\sqrt{\varepsilon}|x-\eta|) |\psi^{0,0}(\eta,\tau)|^2 \right| \leq \\ &\leq \int d\eta \left| \frac{\phi'(\sqrt{\varepsilon}|x-\eta|)}{\sqrt{\varepsilon}} \right| |\psi^{0,0}(\eta,\tau)|^2 \leq L \int d\eta\, |x-\eta| |\psi^{0,0}(\eta,\tau)|^2, \end{aligned} \tag{56}$$

where L is the global Lipschitz constant of ϕ' (i.e., the L^∞-norm of ϕ'') that is known to be finite since $\phi \in C^2_b(\mathbb{R}^d)$. Then, by (56) we get that

$$\begin{aligned} \left\| \frac{1}{\varepsilon} \partial_{x_j} V_\varepsilon(x,\tau) \psi^{0,0}(\tau) \right\|^2_{L^2} &\leq L^2 \int dx \int d\eta |x-\eta| |\psi^{0,0}(\eta,\tau)|^2 \int d\eta' |x-\eta'| |\psi^{0,0}(\eta',\tau)|^2 |\psi^{0,0}(x,\tau)|^2 \\ &\leq L^2 \int |x|^2 |\psi^{0,0}(x,\tau)|^2 dx + 3L^2 \left(\int |\eta| |\psi^{0,0}(\eta,\tau)|^2 d\eta \right)^2 \leqslant \\ &\leq L^2 ||\, |x| \psi^{0,0}(\tau)||^2_{L^2} + 3L^2 ||\, |x| \psi^{0,0}(\tau)||^2_{L^2}, \end{aligned} \tag{57}$$

where we made use of the fact that $||\psi^{0,0}(\tau)||_{L^2} = ||\psi^{0,0}(0)||_{L^2} = ||a_0||_{L^2} = 1$, for any time τ. At this point we observe that $||\, |x| \psi^{0,0}(\tau)||^2_{L^2} = ||\, |x| a(\tau)||^2_{L^2} = \sum_j ||\psi^{0,e_j}(\tau)||^2_{L^2}$. So that, we have just proven that there exists a constant $C > 0$ depending only on the L^∞-norm of the second derivative of ϕ, such that

$$\left\| \frac{1}{\varepsilon} \partial_{x_j} V_\varepsilon(x,\tau) \psi^{0,0}(\tau) \right\|_{L^2} \leqslant C \sqrt{\sum_j ||\psi^{0,e_j}(\tau)||^2_{L^2}} = ||\psi^{0,1}(\tau)||_{L^2}. \tag{58}$$

Now, by using (55) and (58) in (52), we obtain that

$$\|\psi^{e_j,0}(t)\|_{L^2} \leq \|\psi^{e_j,0}(0)\|_{L^2} + C \int_0^t d\tau ||\psi^{0,1}(\tau)||_{L^2} + C \int_0^t d\tau\, \|\psi^{0,e_j}(\tau)\|_{L^2}, \tag{59}$$

where C is not the same constant of formula (58) - we denoted it by the same symbol just for the sake of simplicity - since here it is depending on ϕ, as previously, but even on U (through the L^∞-norm of its second derivative, according to (55)).
Now after (55), summing over $j = 1, \ldots, d$ in equations (59) and (53) and then adding them,

we get

$$||\overrightarrow{\Psi}(t)||_{X_1} \leq ||\overrightarrow{\Psi}(0)||_{X_1} + C\int_0^t d\tau\, ||\overrightarrow{\Psi}(\tau)||_{X_1}. \tag{60}$$

The conclusion follows by applying the Gronwall lemma, i.e.

$$||\overrightarrow{\Psi}(t)||_{X_1} \leq ||\overrightarrow{\Psi}(0)||_{X_1} e^{Ct} \leq M_1 e^{Ct}, \tag{61}$$

where M_1 has been defined in (44).

For $m \geq 2$, the previous inductive step from $m = 1$ applies almost verbatim: first, by virtue of the Duhamel formula, we write the solution of equation (47) by using the propagator $P(t,\tau)$ associated with the time evolution on the left-hand side. Then, by using the L^2-control on $P(t,\tau)$, it only remains to show that the "source terms" appearing on the right-hand side of (47) are suitably uniformly bounded in terms of $||\psi^{A,B}||_{L^2}$ or $||\overrightarrow{\Psi}||_{X_m}$. The way to do that is by using $||\psi^{A,B}||_{L^2}, |A|+|B| < m$ as constants now.

For example, let us look at the term involving the potential V_ε on the right-hand side of (47), i.e.

$$\begin{aligned}\frac{1}{\varepsilon}\sum_{0\leqslant l<A}\prod_{k=1}^{d}\binom{A_k}{l_k}\partial_x^{A-l}V_\varepsilon(x,t)\psi^{l,B}(x,t) &= \frac{1}{\varepsilon}\sum_{\substack{0\leqslant l<A\\ |A-l|=1}}\prod_{k=1}^{d}\binom{A_k}{l_k}\partial_x^{A-l}V_\varepsilon(x,t)\psi^{l,B}(x,t) + \\ &\quad + \frac{1}{\varepsilon}\sum_{\substack{0\leqslant l<A\\ |A-l|>1}}\prod_{k=1}^{d}\binom{A_k}{l_k}\partial_x^{A-l}V_\varepsilon(x,t)\psi^{l,B}(x,t).\end{aligned} \tag{62}$$

The estimation for any of the terms in the last sum reads as:

$$\begin{aligned}&||\partial_x^{A-l}\int \tfrac{1}{\varepsilon}\phi(\sqrt{\varepsilon}|x-\eta|)|\psi^{0,0}(\eta,t)|^2 d\eta\ \psi^{l,B}(x,t)||_{L^2}^2 \leqslant \\ &\leqslant \left(\varepsilon^{\frac{|A-l|-2}{2}}||\phi^{(A-l)}(x)||_{L^\infty}\right)^2 ||\int |x-\eta||\psi^{0,0}(\eta,t)|^2 d\eta\ \psi^{l,B}(x,t)||_{L^2}^2 \leqslant \\ &\leqslant 2D||\,|\eta|\psi^{0,0}(t)||_{L^2}||\psi^{l,B}(t)||_{L^2}||\,|x|\psi^{l,B}(t)||_{L^2} + D||\,|\eta|\psi^{0,0}(t)||_{L^2}||\psi^{l,B}(t)||_{L^2}^2 + D||\,|x|\psi^{l,B}(t)||_{L^2}^2 = \\ &= 2D||\psi^{0,1}(t)||_{L^2}||\psi^{l,B}(t)||_{L^2}||\psi^{l,B+1}(t)||_{L^2} + D||\psi^{0,1}(t)||_{L^2}^2||\psi^{l,B}(t)||_{L^2}^2 + D||\psi^{l,B+1}(t)||_{L^2}^2,\end{aligned} \tag{63}$$

where D is a constant only depending on $||\phi^{(A-l)}(x)||_{L^\infty}$ (that is finite under our assumptions since $A-l \leq m$). Furthermore, it is clear that, by construction, we are guaranteed that the exponent $\frac{|A-l|-2}{2}$ for ε is non negative.
On the other side, the estimate for any of the terms in the first sum on the right-hand side of

(62) is given by

$$
\begin{gathered}
||\partial_x^{A-l}\int\tfrac{1}{\varepsilon}\phi(\sqrt{\varepsilon}|x-\eta|)|\psi^{0,0}(\eta,t)|^2d\eta\ \psi^{l,B}(x,t)||^2_{L^2}\le\\
\leqslant L||\int|x-\eta||\psi^{0,0}(\eta,t)|^2d\eta\ \psi^{l,B}(x,t)||^2_{L^2}\leqslant\\
\leqslant 2L||\ |\eta|\psi^{0,0}(t)||_{L^2}||\psi^{l,B}(t)||_{L^2}||\ |x|\psi^{l,B}(t)||_{L^2}+L||\ |\eta|\psi^{0,0}(t)||_{L^2}||\psi^{l,B}(t)||^2_{L^2}+L||\ |x|\psi^{l,B}(t)||^2_{L^2}=\\
=2L||\psi^{0,1}(t)||_{L^2}||\psi^{l,B}(t)||_{L^2}||\psi^{l,B+1}(t)||_{L^2}+L||\psi^{0,1}(t)||^2_{L^2}||\psi^{l,B}(t)||^2_{L^2}+L||\psi^{l,B+1}(t)||^2_{L^2},
\end{gathered}
\tag{64}
$$

where L is the global Lipshitz constant of ϕ' (see (56)), which is guaranteed to be finite since $\phi\in C_b^m(\mathbb{R}^d)$, with $m\ge 2$.

Now, by virtue of the estimate we proved for $m=1$ (see (60)), from (63) and (64) we find that

$$
\begin{gathered}
||\partial_x^{A-l}\int\tfrac{1}{\varepsilon}\phi(\sqrt{\varepsilon}|x-\eta|)|\psi^{0,0}(\eta,t)|^2d\eta\ \psi^{l,B}(x,t)||^2_{L^2}\leqslant\\
\le KM_1e^{Ct}||\psi^{l,B}(t)||_{L^2}||\psi^{l,B+1}(t)||_{L^2}+KM_1e^{Ct}||\psi^{l,B}(t)||^2_{L^2}+K||\psi^{l,B+1}(t)||^2_{L^2},
\end{gathered}
\tag{65}
$$

where $K=max\{D,L\}$ and and we recall that $|l|+|B|\le|A|-1+|B|\le m-1$ and $|l|+|B|+1\le|A|-1+|B|+1\le m$. Thus:

$$
||\partial_x^{A-l}\int\tfrac{1}{\varepsilon}\phi(\sqrt{\varepsilon}|x-\eta|)|\psi^{0,0}(\eta,t)|^2d\eta\ \psi^{l,B}(x,t)||^2_{L^2}\le K(M_1e^{Ct}+1)||\overrightarrow{\Psi}(t)||^2_{X_m}. \tag{66}
$$

Concerning the terms involving the potential U on the right-hand side of (47), the idea is quite similar. In fact, we observe that

$$
\begin{gathered}
\tfrac{1}{\varepsilon}\sum_{0\leqslant l<A}\prod_{k=1}^{d}\tbinom{A_k}{l_k}\partial_x^{A-l}U(q(t)+\sqrt{\varepsilon}x,t)\psi^{l,B}(x,t)-\\
-\tfrac{1}{\sqrt{\varepsilon}}\sum_{\substack{0<l\leqslant A,\\|l|=1}}\prod_{k=1}^{d}\tbinom{A_k}{l_k}\partial_x^{l}\left(\nabla U(q(t),t)\cdot x\right)\psi^{A-l,B}(x,t)=\\
=\sum_{\substack{0<l\leqslant A,\\|l|=1}}C_{A,l,B}\Big(\tfrac{1}{\varepsilon}\partial_xU(q(t)+\sqrt{\varepsilon}x,t)\psi^{A-l,B}(x,t)-\tfrac{1}{\sqrt{\varepsilon}}\partial_x\left(\nabla U(q(t),t)\cdot x\right)\psi^{A-l,B}(x,t)\Big)+\\
+\tfrac{1}{\varepsilon}\sum_{\substack{0\leqslant l<A,\\|A-l|>1}}\prod_{k=1}^{d}\tbinom{A_k}{l_k}\partial_x^{A-l}U(q(t)+\sqrt{\varepsilon}x,t)\psi^{l,B}(x,t),
\end{gathered}
\tag{67}
$$

where we made a discrete change of variable $l\mapsto A-l$ in the first term of the left-hand side.

Now, with regard to first term of the right-hand side, the estimation that has to be used is exactly the one we did in (55), thus one finds, $\forall\, l:\ |l|=1$

$$\begin{aligned}&\left\|\frac{1}{\varepsilon}\partial_x U(q(t)+\sqrt{\varepsilon}x,t)\psi^{A-l,B}(t)-\frac{1}{\sqrt{\varepsilon}}\partial_x\left(\nabla U(q(t),t)\cdot x\right)\psi^{A-l,B}(t)\right\|_{L^2}\leq\\&\leq\sup_t\left\|\partial^2 U(\cdot,t)\right\|_{L^\infty}\left\|\psi^{A,B}(t)\right\|_{L^2}\leq\sup_t\left\|\partial^2 U(\cdot,t)\right\|_{L^\infty}||\overrightarrow{\Psi}(t)||_{X_m}\end{aligned}\tag{68}$$

(the adjustment for $l=0$ is obvious).
Now, for the last term in (67) we have

$$\begin{aligned}&\left\|\frac{1}{\varepsilon}\partial_x^{A-l}U(q(t)+\sqrt{\varepsilon}x,t)\psi^{l,B}(x,t)\right\|_{L^2}\leq\varepsilon^{\frac{|A-l|-2}{2}}\sup_t||\partial^{(A-l)}U(\cdot,t)||_{L^\infty}\left\|\psi^{l,B}(t)\right\|_{L^2}\leq\\&\leq\sup_t||\partial^{(m)}U(\cdot,t)||_{L^\infty}||\overrightarrow{\Psi}(t)||_{X_m},\end{aligned}\tag{69}$$

where we used that $A-l\leq A\leq m$, $|A-l|-2\geq 0$ and $l+B<A+B\leq m$.

Similar (simpler, in fact) estimates can be shown for the other terms on the right-hand side of (47).

□

Observation 4.3. [Propagation of moments and derivatives for $\beta_t(x)$] *$\beta_t(x)$ was defined in equations (12), (13). Under the assumptions of Lemma 4.2, regularity estimates for $\beta_t(x)$ analogous to Lemma 4.2 for $a(x,t)$ hold, i.e., for any $t>0$*

$$||x^B\partial_x^A\beta_t||_{L^2}\leqslant C_m(t)\sum_{|A'|+|B'|\leqslant m}||x^{B'}\partial_x^{A'}a_0||_{L^2},\quad\forall\ A,B\in\ \mathbb{N}^d:\ |A|+|B|\leq m.$$

Remarks:

- The proof is in fact simpler with respect to the one of Lemma 4.2: it can be checked easily that, due to the fact that we have to deal with harmonic potentials, the terms that arise from the differentiation of the potentials turn to be exactly of the form $x\beta_t(x)$ ($\sim||\overrightarrow{\Psi}_\beta(t)||_{X_1}$ if we denote by $\psi_\beta^{A,B}(x,t)$ the quantities $x^B\partial_x^A\beta_t(x)$ and we define $\overrightarrow{\Psi}_\beta(t)$ consistently), i.e., precisely the kind of objects we want to recover to apply the Gronwall Lemma (see the proof of Lemma 4.2).

- As a consequence of Observation 4.3, by Assumptions 1, 2, 3 we are guaranteed that, in particular, there exists a ε-independent constant $C>0$ depending on the L^∞-norm of the second x-derivative of $U(x,t)$ and on $|\phi''(0)|$, such that

$$\int dx\,|x|^2|\beta_t(x)|^2 < \left(\int dx\,|x|^2|a_0(x)|^2\right) e^{Ct} < \infty, \quad \forall\ t.$$

We remind that this is exactly what we need to make the proof of Theorem 2.1 work succesfully (see (23)).

Observation 4.4. [Propagation of Moments and derivatives for $b_t(x)$] *Although apparently $b_t(x)$ solves a nonlinear equation, it can be obtained as the solution of a linear Schrödinger equation with an harmonic potential whose coefficients are determined by the L^2-norm of the first moment of $\beta_t(x)$, by $\phi''(0)$ and $\nabla^2 U$ (see (25) and Lemma 3.1).*
Therefore, as a consequence of Observation 4.3, it follows that, as long as $U \in C^1\left(\mathbb{R}_t^+, C_b^m(\mathbb{R}_x^d)\right)$ and $\phi''(0)$ is finite, we can get a result for $b_t(x)$ e.g. analogous to Lemma 4.2 for $a(x,t)$, i.e.

$$x^B\partial_x^A b_t \in L^2, \quad \forall\ A,B \in\ \mathbb{N}^d:\ |A|+|B| \leq m\ \ \forall\ t,$$

under the same assumption (44) on the (common) initial datum $a_0(x)$.

Note that, in particular, by Assumptions 1, 2, 3 we are guaranteed that there exists a ε-independent constant $C_t > 0$ depending on the L^∞-norm of the second x-derivative of $U(x,t)$, on $|\phi''(0)|$ and on time t (but finite for any t), such that

$$\int dx\,|x|^{2m}|b_t(x)|^2 < C_t, \quad \forall\ t, \quad m \leq 3. \tag{70}$$

We observe that (70), for $m = 2$, is exactly what we need to make the proof of Theorem 2.1 work succesfully (see (39), (40) and (41)).

5. Higher order approximations

On the basis of the above results, it seems natural to ask whether it is possible to go beyond the $\sqrt{\varepsilon}$-approximation discussed previously (see (11)) and to find higher order corrections $a_t^{(k)}(\mu)$ to the amplitude $a_t^{(0)}(\mu) := b_t(\mu)$ so that the right-hand side of (11) gets of size of any power of ϵ, as this is the case for the linear Schrödinger equation [11, 12]. Although we will not present all the (tedious) details of the construction, we claim that one can determine a semiclassical expansion

$$a_t^\varepsilon(\mu) = a_t^{(0)}(\mu) + \sqrt{\varepsilon}\,a_t^{(1)}(\mu) + \varepsilon\,a_t^{(2)}(\mu) + \cdots + \varepsilon^{k/2}a_t^{(k)}(\mu) + \ldots, \tag{71}$$

with

$$a_0^{(k)}(\mu) = \delta_{k,0}a_0(\mu), \tag{72}$$

such that

$$\Psi^\varepsilon(x,t) = e^{i\frac{\mathcal{L}(t)}{\varepsilon}+i\gamma(t)}\psi^{\beta_t}_{q(t)p(t)} + O(\epsilon^\infty).$$

In order to determine the equations governing the evolution for each coefficient $a_t^{(k)}(\mu)$ we need to look at the expansion for the potential terms appearing in (31). With regard to the nonlinear part involving the pair interaction ϕ, we get:

$$\begin{aligned}\frac{1}{\varepsilon}\left(\phi(\sqrt{\varepsilon}|\mu-\eta|)-\phi(0)\right) &= \frac{|\mu-\eta|}{\sqrt{\varepsilon}}\phi'(0)+\frac{|\mu-\eta|^2}{2}\phi''(0)+\frac{\sqrt{\varepsilon}|\mu-\eta|^3}{3!}\phi'''(0)+\\ &+ \cdots+\frac{(\sqrt{\varepsilon})^k|\mu-\eta|^k}{k!}\phi^{(k)}(0)+\ldots \end{aligned}\tag{73}$$

In Theorem 2.1 we were assuming $\phi\in C_b^3(\mathbb{R})$. Clearly, if we want to go to higher orders in the approximation we need more smoothness on ϕ and on the external potential U. Therefore, here and henceforth we assume:

$$\phi\in C_b^\infty(\mathbb{R}),\quad \text{and} \quad \phi \ \ \text{even}\tag{74}$$

so that we have

$$\frac{1}{\varepsilon}\left(\phi(\sqrt{\varepsilon}|\mu-\eta|)-\phi(0)\right)=\frac{|\mu-\eta|^2}{2}\phi''(0)+\cdots+(\sqrt{\varepsilon})^{2n-1}\frac{|\mu-\eta|^{2n}}{(2n)!}\phi^{(2n)}(0)+\ldots \quad n\geq 2\tag{75}$$

Observation 5.1. *Assumption (74) is actually too strong if one wants to deal with an approximation up to a certain order k.*

With regard to the linear terms in (31) involving the external potential U, we get:

$$\tfrac{1}{\varepsilon}\left(U(q(t)+\sqrt{\varepsilon}\mu,t)-U(q(t),t)-\sqrt{\varepsilon}\nabla U(q(t),t)\cdot\mu\right)=$$

$$=<\mu,\tfrac{\nabla^2U(q(t),t)}{2}\mu>+\cdots+(\sqrt{\varepsilon})^{n-1}\tfrac{\nabla^nU(q(t),t)}{n!}\cdot\mu^n+\ldots$$

where of course $n\geqslant 3$. Here we are using the notation

$$\nabla^nU\cdot\mu^n=\sum_{\substack{\alpha_1\ldots\alpha_d:\\ \sum\alpha_i=n}}\frac{\partial^nU}{\partial x_1^{\alpha_1}\ldots\partial x_d^{\alpha_d}}\ \mu^{\alpha_1}\ldots\mu^{\alpha_d}.\tag{76}$$

Analogously to what we observed for the pair-interaction ϕ, we need more smoothness for U, so that here and henceforth we require:

$$U\in C^1(\mathbb{R}_t^+,C_b^\infty(\mathbb{R}_x^d)).\tag{77}$$

Now, inserting (71), (75) and (76) in (31) we readily arrive to a sequence of problems for the coefficients $a_t^{(k)}(\mu)$ of the expansion (71). For $k=0$ we obviously find:

$$\begin{cases}\left(i\partial_t+\dfrac{\Delta_\mu}{2}+\dfrac{\phi''(0)}{2}\displaystyle\int d\eta\,|\mu-\eta|^2|a_t^{(0)}(\eta)|^2+<\mu,\dfrac{\nabla^2U(q(t),t)}{2}\mu>\right)a_t^{(0)}(\mu)=0,\\ a_0^{(0)}(\mu)=a_0^\varepsilon(\mu),\end{cases}\tag{78}$$

namely, the initial value problem that we had for $b_t(\mu)$ in the previous sections (see (15)). Then, for $k=1$, we find:

$$\begin{cases} \left(i\partial_t + \frac{\Delta_\mu}{2} + \frac{\phi''(0)}{2}\int d\eta\,|\mu-\eta|^2|a_t^{(0)}(\eta)|^2 + <\mu, \frac{\nabla^2 U(q(t),t)}{2}\mu>\right) a_t^{(1)}(\mu) = \\ = \frac{\phi''(0)}{2}\left(\int d\eta\,|\mu-\eta|^2 2\Re[\overline{a}_t^{(0)}(\eta)a_t^{(1)}(\eta)]\right) a_t^{(0)}(\mu) + \frac{\nabla^3 U(q(t),t)}{3!}\cdot\mu^3\, a_t^{(0)}(\mu), \\ a_0^{(1)}(\mu) = 0. \end{cases} \tag{79}$$

This is a linear initial value problem where the left-hand side is known to have a unique well-defined L^2-propagator $P^{(0)}(t)$ due to the existence and uniqueness in L^2 of the solution $a_t^{(0)}(\mu)$ of the zero-order initial value problem (78) and to the L^2-control on its first moment (see Observation 4.4 and (70)). Then, it is easy to see that, writing the solution $a_t^{(1)}(\mu)$ through the Duhamel formula (with "leading" propagator $P^{(0)}(t)$), the well-posedness in L^2 for (79) is guaranteed by the L^2-control on the source term $\frac{\nabla^3 U(q(t),t)}{3!}\cdot\mu^3\, a_t^{(0)}(\mu)$ (which is achieved thanks to the smoothness of U and to the L^2-control on the third moment of $a_t^{(0)}(\mu)$ - see (70)) and by the following estimate:

$$\begin{aligned} &\left\|\frac{\phi''(0)}{2}\left(\int d\eta\,|\mu-\eta|^2 2\Re[\overline{a}_t^{(0)}(\eta)a_t^{(1)}(\eta)]\right) a_t^{(0)}(\mu)\right\|_{L^2}^2 = \\ &= \left(\frac{\phi''(0)}{2}\right)^2 \int d\mu \int d\eta|\mu-\eta|^2\overline{a}_t^{(0)}(\eta)a_t^{(1)}(\eta)\int d\eta'|\mu-\eta'|^2\overline{a}_t^{(0)}(\eta')a_t^{(1)}(\eta')\,|a_t^{(0)}(\mu)|^2 + \\ &+ \left(\frac{\phi''(0)}{2}\right)^2 \int d\mu \int d\eta|\mu-\eta|^2 a_t^{(0)}(\eta)\overline{a}_t^{(1)}(\eta)\int d\eta'|\mu-\eta'|^2 a_t^{(0)}(\eta')\overline{a}_t^{(1)}(\eta')\,|a_t^{(0)}(\mu)|^2 \leq \\ &\leq C_{a_t^{(0)}}\left\|a_t^{(1)}\right\|_{L^2}^2. \end{aligned} \tag{80}$$

Here $C_{a_t^{(0)}} > 0$ is a constant that only depends on the moments of $a_t^{(0)}(\mu)$ up to order 3, depending on the potentials U (trought the L^∞-norm of its second derivative) and ϕ (through the quantity $|\phi''(0)|$) and on the initial derivatives and moments of $a_t^{(0)}(\mu)$ up to the order 3 (see Observation 4.4), that, as in the previous sections, we assume to be finite. By virtue of (80) and the L^2-control on the term involving U in (79), the Duhamel formula and the Gronwall lemma allow to conclude that

$$a_t^{(1)} \in L^2(\mathbb{R}^d), \quad \forall\, t. \tag{81}$$

Moreover, following the same lines of the proofs presented and discussed in the previous sections (see Lemma 4.2, Observation 4.4 and subsequent remarks), it can be easily checked that by assuming enough regularity for the (zero-order) "full" initial datum $a_0^{(0)}(\mu) = a_0(\mu)$, in such a way that we control in L^2 a sufficiently high number of moments and derivatives, we can control the derivatives and moments of $a_t^{(1)}(\mu)$ up to any fixed order m, i.e:

$$x^B\partial_x^A a_t^{(1)} \in L^2(\mathbb{R}^d), \quad \forall\, t, \qquad \forall\;\; A,B\in\mathbb{N}^d : |A|+|B| \leq m. \tag{82}$$

This will be crucial to go on with the higher orders dynamics because, for example, the equation for the second coefficient $a_t^{(2)}(\mu)$ is

$$\begin{cases} \left(i\partial_t + \frac{\Delta_\mu}{2} + \frac{\phi''(0)}{2}\int d\eta\,|\mu-\eta|^2|a_t^{(0)}(\eta)|^2 + <\mu, \frac{\nabla^2 U(q(t),t)}{2}\mu>\right) a_t^{(2)}(\mu) = \\ = \frac{\phi''(0)}{2}\left(\int d\eta\,|\mu-\eta|^2 2\Re[\overline{a}_t^{(0)}(\eta)a_t^{(2)}(\eta)]\right) a_t^{(0)}(\mu) + \frac{\nabla^4 U(q(t),t)}{4!}\cdot\mu^4\, a_t^{(0)}(\mu) + \\ + \frac{\phi^{(4)}(0)}{4!}\left(\int d\eta\,|\mu-\eta|^4|a_t^{(0)}(\eta)|^2\right) a_t^{(0)}(\mu) + \frac{\phi''(0)}{2}\left(\int d\eta\,|\mu-\eta|^2|a_t^{(1)}(\eta)|^2\right) a_t^{(0)}(\mu) + \\ + \frac{\phi''(0)}{2}\left(\int d\eta\,|\mu-\eta|^2 2\Re[\overline{a}_t^{(0)}(\eta)a_t^{(1)}(\eta)]\right) a_t^{(1)}(\mu) + \frac{\nabla^3 U(q(t),t)}{3!}\cdot\mu^3\, a_t^{(1)}(\mu). \\ a_0^{(2)}(\mu) = 0, \end{cases} \tag{83}$$

So, again, as for the case $k = 1$, we obtained a linear initial value problem where the propagator associated with the left-hand side is $P^{(0)}(t)$, that is known to be uniquely well-defined in L^2. Then, as before, the solution $a_t^{(2)}(\mu)$ can be written through the Duhamel formula, applying the propagator $P^{(0)}(t)$ to the term $\frac{\phi''(0)}{2}\left(\int d\eta\,|\mu-\eta|^2 2\Re[\overline{a}_t^{(0)}(\eta)a_t^{(2)}(\eta)]\right) a_t^{(0)}(\mu)$ and to the various source terms in (83). The term which is linear in $a_t^{(2)}(\mu)$ is estimated as in (80) while the source terms are controlled in L^2 by virtue of the control on moments and derivatives of $a_t^{(0)}(\mu)$ and $a_t^{(1)}(\mu)$. In the end, by using the Gronwall lemma, we get

$$a_t^{(2)} \in L^2(\mathbb{R}^d), \quad \forall\, t. \tag{84}$$

and, moreover, by assuming a sufficiently high number of moments and derivatives of the (zero-order) "full" initial datum $a_0^{(0)}(\mu) = a_0(\mu)$ to be controlled in L^2, we can control as well the derivatives and moments of $a_t^{(2)}(\mu)$ up to any fixed order m, i.e:

$$x^B\partial_x^A a_t^{(2)} \in L^2(\mathbb{R}^d), \quad \forall\, t, \qquad \forall\ A, B \in \mathbb{N}^d : |A| + |B| \le m. \tag{85}$$

At this point it is clear how to proceed in general. The equation for $a_t^{(k)}(\mu)$ is a linear Schrödinger equation with a source term involving the coefficients $a_t^{(n)}(\mu)$ with $n < k$, which have been estimated by the previous steps. The L^2-control of $a_t^{(k)}(\mu)$ follows by the L^2-control on a sufficiently high number of moments and derivatives of $a_t^{(n)}(\mu)$ with $n < k$.

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