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On the application of the Critical Minimum Energy Subspace method to disordered systems

Laura Hernández^{1,*} and Horacio Ceva²

¹*Laboratoire de Physique Théorique et Modélisation, UMR CNRS-Université de Cergy Pontoise.*

2 Av Adolphe Chauvin, 95302 Cergy-Pontoise Cedex, France

²*Departamento de Física, Comisión Nacional de Energía Atómica,*

Avenida del Libertador 8250, 1429 Buenos Aires, Argentina

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We discuss the recent application to strongly disordered systems of the Critical Minimum Energy Subspace (CMES) method, used to limit the energy subspace of the Wang-Landau sampling. We compare with our results on the 3D Random Field Ising Model obtained by a multi-range Wang-Landau simulation in the whole energy range. We point out at some problems that may arise when applying the CMES scheme to models having a complex free energy landscape.

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I. INTRODUCTION

In [1] Malakis, Peratzakis and Fytas introduce an interesting approximation method to allow for an easy extension of a Wang-Landau (WL) [2] study to large systems. It is based on the fact that in the thermal averages sums at a given temperature T , only some terms give a relevant contribution: those whose energies correspond to the interval around the maximum of the probability distribution of the energy at that temperature, $P_T(E)$. Hence an algorithmic procedure to determine a restricted interval $\Delta\tilde{E}$ centered in the energy \tilde{E} of the maximum of $P_T(E)$, called minimum energy subspace (MES) is proposed. In this way the WL sampling needs to be performed only in this restricted energy interval, improving the efficiency of the algorithm and diminishing the errors introduced when joining together the different parts of the density of states in a multirange simulation [3].

This algorithm is based on the equivalence of thermodynamical ensembles and on the central limit theorem: the energy probability distribution at a given temperature T approaches a Gaussian. Moreover, for a continuous transition, it is supposed that this remains the case *even at* $T_c(L)$, the critical temperature of a sample whose linear size is L . Then one expects that the width of the critical MES (CMES) will be of the same order that the standard deviation of the energy:

$$\Delta\tilde{E} \propto \sqrt{NT^2C} \quad (1)$$

where volume of the system is given by $N = L^d$, with d the space dimension, T is the temperature and C the specific heat.

The CMES is iteratively built, starting from the central value \tilde{E} and extending the interval on both sides of

it, until the difference between the specific heat calculated using the whole energy interval (or the exact one, if known) and the one calculated using the restricted iterated interval is less than a given error. Assuming that one imposes the same level of error for all the sizes, a lattice size dependence remains: the center of the CMES \tilde{E} and its boundaries are functions of L . At the critical temperature, using the scaling law for the specific heat one gets:

$$\frac{\Delta\tilde{E}}{L^{d/2}} \approx L^{\alpha/2\nu} \quad (2)$$

In this way, performing a WL simulation over the whole energy range for small lattices and determining the CMES for this small size will be enough to extrapolate the CMES where the WL simulation has to be carried out for larger lattices.

This method has been successfully applied to the study of the pure 2D and 3D Ising model.

In this work we discuss the CMES technique applied to the 3D Random Field Ising Model (3D-RFIM). This is one of the simplest disordered systems whose hamiltonian is given by:

$$\mathcal{H} = -J \sum_{ij>} s_i s_j - \sum_i h_i s_i \quad (3)$$

with a bimodal probability distribution of the random fields of intensity h_0

$$p(h_i) = \frac{1}{2} [\delta(h_i - h_0) + \delta(h_i + h_0)] \quad (4)$$

The nature of the transition of this model is a subject of controversy since long ago. In [6] we have studied it using the multi-range version of the WL simulation on the whole relevant energy range. Our results show that for high values of the random field intensity the transition is first order. The same result had also been found in [7]

*Electronic address: Laura.Hernandez@u-cergy.fr, ceva@cnea.gov.ar

using a completely different calculation method, namely the canonical Histogram Monte Carlo.

To compare with [4], we use our previously obtained density of states (DOS) to calculate different thermal averages limiting our data only to the energy subintervals corresponding to those indicated in [4].

In the following we point out several aspects that have to be carefully considered in order to apply this technique to highly disordered systems.

II. CHARACTER OF THE TRANSITION

The CMES method is based on the assumption that the transition is second order as it is required for Equation 2 and the Gaussian-like shape of the $P_{T^*}(E)$ hypothesis to be valid.

Our WL simulation on the whole energy range shows, in agreement with other works [4] [5], that for strong disorder, and big enough lattices, the $C_L(T)$ curves may present a multiplicity of peaks. In order to estimate the transition temperature T^* , we observe that one of the maxima of $C_L(T)$, located at T^* , is associated to a $P_{T^*}(E)$ curve which shows two well separated peaks of equal height. In general, this corresponds to the highest maximum of $C_L(T)$.

The double peaked $P_{T^*}(E)$ curves are an indication of the first order character of the transition, at the transition temperature T^* .

So in this case the energy probability distribution at the transition temperature T^* cannot be approached by a Gaussian. In fact its central value \bar{E} corresponds then to the **minimum** of $P_{T^*}(E)$. Therefore Equations 1 and 2 are not valid in this case. This must be kept in mind when studying a system with a complex free energy landscape.

III. FINITE SIZE EFFECTS

To observe all these features the simulated lattices must have big enough sizes. For smaller sizes the transition appears as continuous.

Figure 1 illustrates this situation for a field $h_0 = 2.1$. In (a) one can see the specific heat curve for a sample of $L = 10$ and in (b) the corresponding $P_T(E)$. There is only one peak in $C_L(T)$ at T^* and the corresponding probability distribution shows a single “gaussian-like” peak. To apply the CMES technique one has to perform WL simulations on small lattices in the whole energy range, use them to determine the extension of the CMES at this size L and then determine the new CMES for an $L' > L$ via Eq. 2. Then the WL simulation at this bigger size L' is performed only in this new restricted interval.

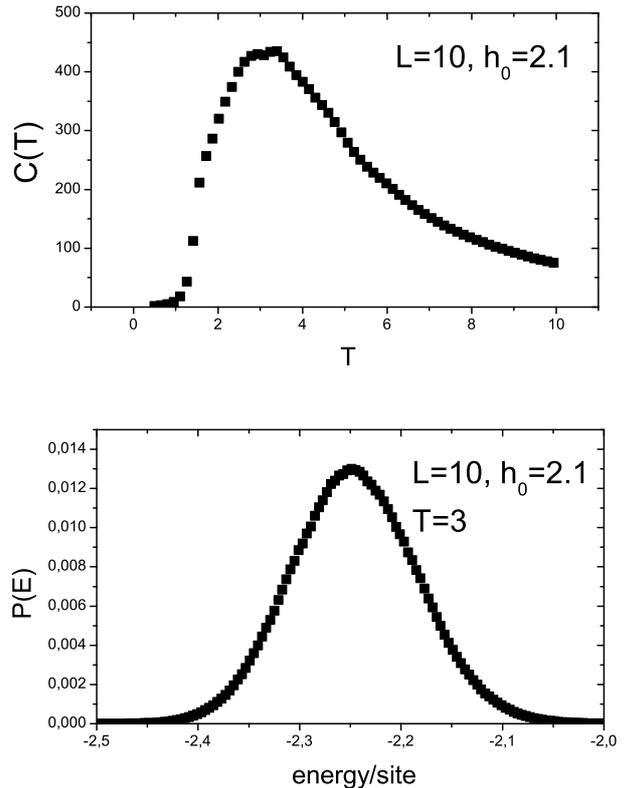


FIG. 1: $L = 10, h_0 = 2.1$ (a) Specific heat vs. temperature, (b) Probability density for $T=3$, corresponding to the maximum of (a).

For comparison, in Figure 2 we show the more complex behavior of the specific heat for $L = 16$ and $L = 24$, and the same random field.

Our results show that this finite size effect must be taken into account with some care when applying the CMES technique to highly disordered systems, because the first order nature of the transition may be hidden till quite large sizes.

In Figure 3 one can see the energy probability distribution corresponding to the maxima of $C_L(T)$ shown in Figures 1 and 2. It can be seen that for $h_0 = 2.1$, the first manifestation of the first order character of the transition appears only for $L \geq 16$. For these lattice sizes the use of multirange WL scheme is unavoidable.

IV. STRONG SAMPLE TO SAMPLE FLUCTUATIONS

We observe large sample to sample fluctuations, in agreement with other works on disordered systems [4] [5] [8] [9] [10]. In our case, the multiplicity of

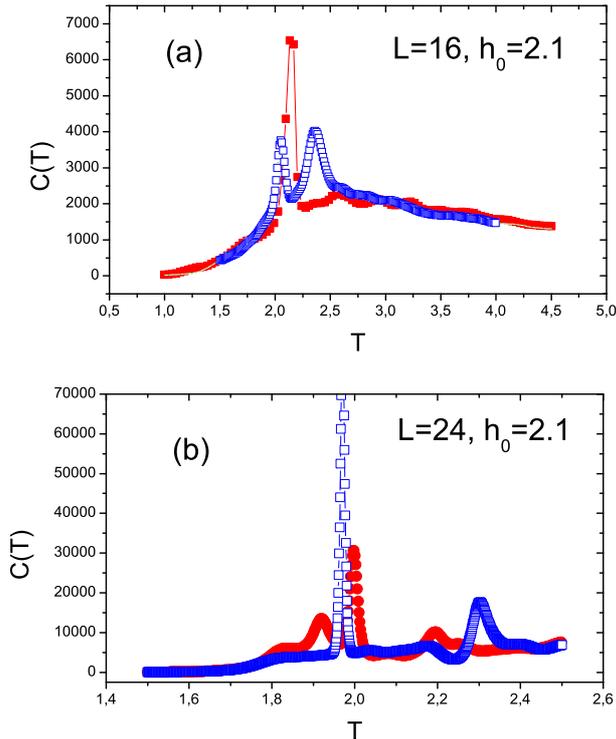


FIG. 2: $h_0 = 2.1$ Specific heat vs. temperature, comparison of two different realizations of quenched disorder for two sizes (a) $L = 16$, (b) $L=24$

peaks of the specific heat and their locations are strongly sample dependent (see Figure 2). Then the location of the maxima of $P_{T^*}(E)$, and the resulting CMES depend also strongly on the considered sample.

To take this aspect into account in [4] a “broadened CMES” for WL simulation is proposed. This broadened CMES is determined by the union of M CMES each of them calculated for a different quenched random field configuration. Then using Equation 2 the CMES is estimated for a larger size. It is assumed that for the new $L' > L$, it is enough to run the WL algorithm only in this new restricted energy interval.

Letting aside that equations 1 and 2 are not valid when the transition is first order, the fact of “somehow extending” the estimated CMES deserves some attention.

One should notice that, by definition, in the case of disordered systems the sample of size $L' > L$ is a **new, different sample** whose $P_{T^*}(E)$ may have its maxima located out of the extrapolated CMES via Eq. 2. In Figure 3(a) one can see that there is little overlap between the probability distributions, even for samples of slightly different sizes. In addition Figure 3(b) shows that this is also true for the probability distributions of two different

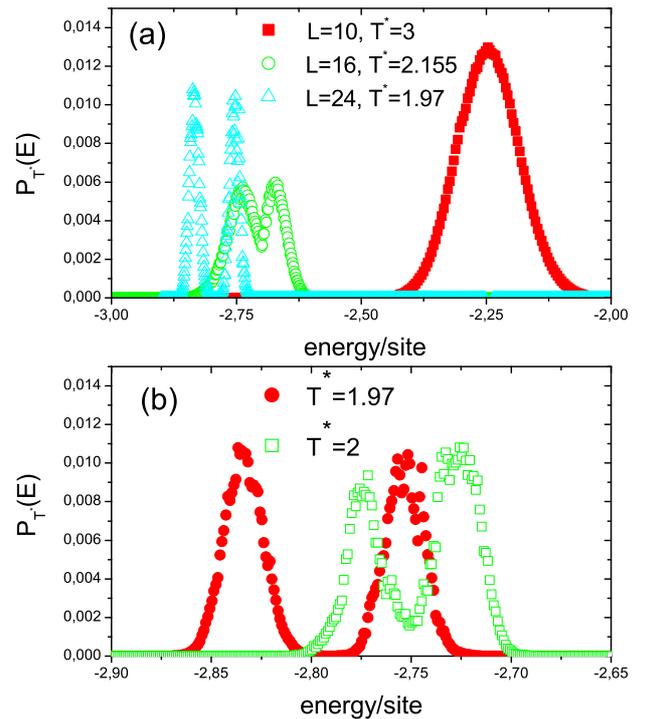


FIG. 3: (a) Probability distribution of the energy for different lattice sizes at the corresponding transition temperatures T^* . Double peaks appear in the probability distribution as $L \geq 16$ indicating a first order transition. Probability distributions of different sizes have very small overlap. It shows the size of the shift from $\Delta\tilde{E}(L)$ to $\Delta\tilde{E}(L')$. (b) Probability distribution of the energy for $L = 24$ and two different samples. One can get an estimate of the extended relevant energy interval for this size.

samples of *the same size*.

We used our data to calculate thermal properties taking into account the portions of the energy interval given in ref [4]. For $L = 24$ the broadened interval would be $\delta E = [-2.91, -1.83]$. This interval allows us to recover all the features of the model. Unfortunately, though several times smaller than the whole energy range, this interval is located in the hardest region from the convergence point of view [6]. So the multirange scheme is unavoidable and several narrow energy intervals are needed to achieve convergence.

In conclusion, from the efficiency and precision point of view, broadening the CMES too much guarantees that all the thermodynamical properties will be correctly reproduced, but the computational effort required is at least comparable to performing WL in the whole energy range.

The authors of [4] are aware of this and they have proposed, as an alternative, to work on the CMES of

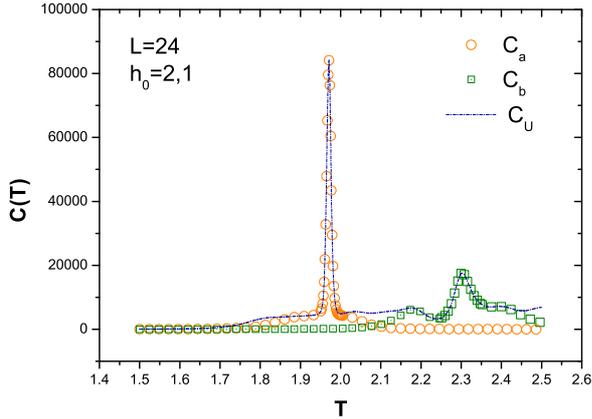


FIG. 4: (a) Specific heat as a function of temperature T , for $L = 24$, $h_0 = 2.1$ obtained from thermal averages using the DOS restricted to three different energy intervals. Interval $\Delta\tilde{E}_U(L)$ corresponds to the levels given in [4] for $L=24$, this union interval reproduces a multi-peaked $C_u(T)$ curve coincident to the one obtained with the whole DOS for the sample i . On the other hand the restricted intervals $\Delta\tilde{E}_a(L)$ and $\Delta\tilde{E}_b(L)$ give the curves $C_a(T)$ and $C_b(T)$ respectively centered around the temperatures $T_a \approx 1.97$ and $T_b \approx 2.3$. These temperatures correspond to the peaks of the complete DOS, that gave rise to the restricted intervals, as could be expected

each sample. To study this proposal we use our data calculated in the full energy range for each sample i and we identify the relevant part of the energy axis for the transition of the considered sample. This is noted by analogy with [4] $\Delta\tilde{E}_i$.

Conceptually $\Delta\tilde{E}_i$ corresponds to the region where the energy probability distribution at the transition temperature is more significative for the sample i . Hence, we identify $\Delta\tilde{E}_i$ as the energy interval where $P_{T^*}(E)$ is different from zero. We then recalculate the thermal averages using only the DOS restricted to $\Delta\tilde{E}_i$. For the

sample shown here the $C_L(T)$ curve we obtained using the whole DOS has two peaks. The whole structure of $C_L(T)$ cannot be reproduced using a restricted interval associated with only one of the peaks. When $C_L(T)$ is recalculated using the DOS restricted to the interval $\Delta\tilde{E}_i^a$ ($\Delta\tilde{E}_i^b$) corresponding to the temperature T_a (T_b) of one of the peaks, the other is not reproduced (see Figure 4).

Now lets imagine that we determine the CMES for a lattice size L . As a larger size implies a new sample, it is possible that the extrapolation to $L' > L$ gives a $\Delta\tilde{E}'$ which doesn't include the highest peak of the new sample i' . In that case the results calculated for L' will not correspond to the transition region of this new sample.

V. CONCLUSIONS

The application of the CMES method to the 3D-RFIM has to be done with extreme care, for several reasons that were considered in this work.

To begin with, it is worthwhile noticing that increasing L implies changing the sample. Hence, if the interval $\Delta\tilde{E}_U(L)$ calculated for L contains the information to reproduce the highest peak of $C_L(T)$, due to the large sample to sample fluctuations there is no warranty that the new, extrapolated interval for L' will reproduce the corresponding peak of $C'_L(T)$. Then one is forced to broaden the interval at L to calculate it at L' . It should be noticed, however, that there is no rule to control this; additionally, if the interval is substantially enlarged, the computational effort is similar to that required when one uses the WL method on the whole energy range.

Moreover, performing a WL simulation on the whole energy range for small lattices, in order to determine the nature of the transition before using the CMES method should be considered with some care, because it is a methodology prone to reach incorrect conclusions, as we have shown in Figure 3.

As the lattice size increases the two peaks of $P_{T^*}(E)$ become well separated, so one risk is to seize only one of them; this may explain the anomalous behaviour observed in Fig.5 of [4] for the largest sizes studied in that work.

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