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

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Abstract

We discuss the recent application to strongly disordered systems of the Critical Minimum Energy Subspace (CrMES) 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 CrMES scheme to models having a complex free energy landscape.

1 Introduction

The study of phase transitions via Monte Carlo simulations has recently regained new interest due to the introduction of the so called "extended ensemble methods", like multicanonical simulations [1], broad histogram thecniques [2], entropic sampling [3], Wang-Landau method [4], among others. These new thechniques increased significantly the accuracy of the Monte Carlo studies in the cases where large free energy barriers separate different wells in the free energy landscape. This step forward in the developement of the Monte Carlo method is analog to the already largely used clustering methods [5] [6], which help to overcome the critical slowing down observed at second order transitions.

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Following the arrival of these new methods an avalanche of thechniques were developped to further improve accuracy and performance of the different algorithms. Each one of these has been validated through the application to well known systems, typically those that can be solved exactly like the 2d Ising model or those whose numerical or aproximated analytical results are out of discussion like the Potts model for $q = 5$ (to test the case of first order transitions).

Recently, Malakis, Peratzakis and Fytas [7] introduced an interesting approximation method to allow for an easy extension of a Wang-Landau (WL) [4] 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 the corresponding 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 [8].

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 (CrMES) will be of the same order that the standard deviation of the energy:

$$\Delta\tilde{E} \propto \sqrt{NT^2C} \tag{1}$$

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 CrMES 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 becomes 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 CrMES $\tilde{E}$ and its boundaries are functions of L. At the critical temperature, using the scaling law for the specific heat one gets:

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

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

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

In this work we are interested in the application of this technique to highly disorder systems, as has been proposed in [9] for the 3D Random Field Ising Model (3D-RFIM) with bimodal distribution of the random fields. The aim of this work is to show, by the study of the 3D-RFIM, why the generalization of the CrMES method to highly disordered systems is not straightforward.

The article is organised as follows in Sec. II we describe the method used in this work, in section III we present our results and in Sec.IV we discuss how these results point out to the aspects of the proposed method that have to be handled with extreme care when applying it to the study of highly disordered systems.

2 Description of model and the method

The 3D-RFIM is one of the simplest disordered systems; its hamiltonian is given by:

$$\mathcal{H} = -J \sum_{<ij>} s_i s_j - \sum_i h_i s_i \tag{3}$$

where h_i are the local fields of intensity h_0 which we assume to be distributed as follows:

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

The nature of the transition of this model is a subject of controversy since long ago. In [10] we have studied it using the multi-range version of the WL simulation on the whole relevant energy range. Our results for high values of the random field intensity show strong first order properties. The same result had also been found in [11] using a completly different calculation method, namely the canonical Histogram Monte Carlo and similar features have also been found in the case of a gaussian distribution of random fields [12]

To analyse the method proposed in [9] we start from the density of states (DOS) calculated using a multi-range WL simulation on the whole energy

space [10] and we recalculate thermal averages limiting our DOS data only to the energy subintervals corresponding to those indicated in [9].

With this procedure we are able to point out to the different aspects that should be handled with special care in order to apply this technique to highly disordered systems.

3 Discussion of results

The fact that the nature of the transition of the 3D RFIM is still a matter of controversy calls for a special attention on the validity of the hypotesis of the methods used to study this model.

Let's discuss first the relationship between the nature of the transition and the CrMES technique. The method introduced in [7] is based on the assumption that one deals with a second order transition. This 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 [9] [12], 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^*. In very rare cases it has been found that the double peak is a finite size effect [13]. Recently it has been reported that this could be the case for the 3D-RFIM [14], though further calculations involving sizes beyond $L = 32$ are needed.

In any case the energy probability distribution at the transition temperature T^* for a given finite L, cannot be approached by a single gaussian. In fact its central value $\tilde{E}$ corresponds then to the ***minimum*** of $P_{T^*}(E)$. Moreover, in the case of first order transitions Eqs. 1 and 2 are not valid, and the probability distribution may be approached by a double gaussian [15].

A modified version of the CrMES method adapted to a system undergoing a first order transition has been proposed in [16]. It is worthwhile noticing that this work deals with a system presenting geometrically frustrated interactions but no quenched disorder.

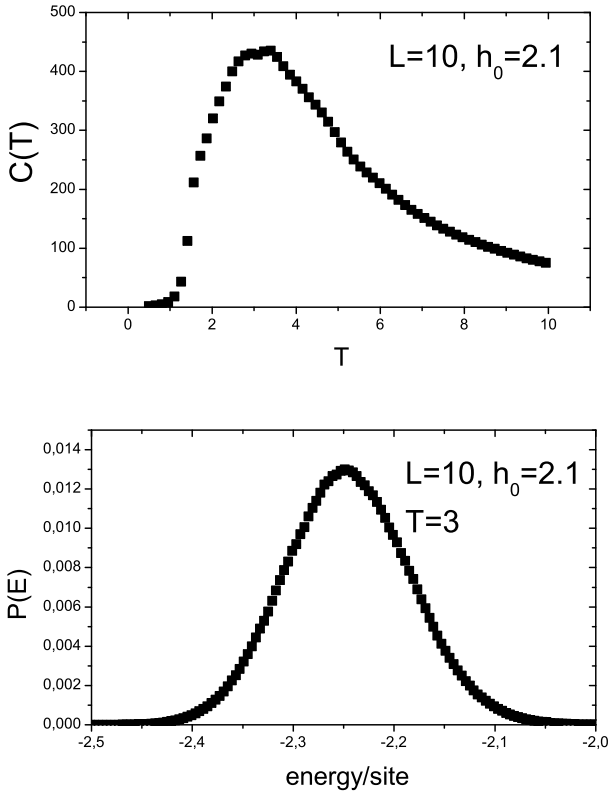

Fig. 1. $L = 10$, $h_0 = 2.1$ (a) Specific heat vs. temperature, (b) Probability density for T=3, corresponding to the maximum of (a).

It is clear that when studying systems where the free energy landscape has a complex structure due to the existence of a quenched disorder, the possibility of a crossover to a first order transition must be kept in mind.

Moreover finite size effects and sample to sample fluctuations are sensitive points studying highly disordered systems.

As it is often the case, the signatures of a first order transition are observed only for large enough sizes. For smaller sizes the transition looks continuous, as the correlation lenght may easily reach the size of the system.

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 linear size $L = 10$ 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. The appealing idea of the CrMES technique should be considered step by step in this case. In [7] it is proposed to carry WL simulations in the whole energy range on lattices

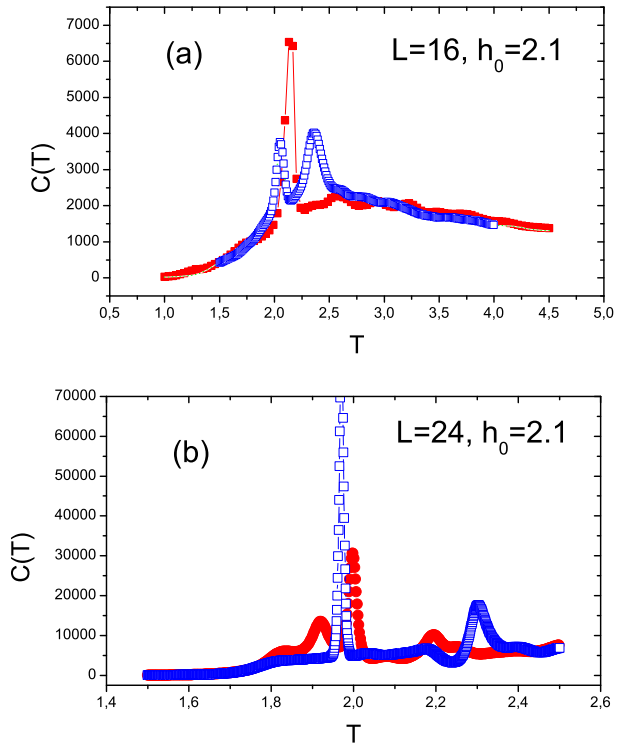

Fig. 2. $h_0 = 2.1$ Specific heat vs. temperature, comparison of two different realizations of quenched disorder for two sizes (a)$L = 16$, (b) L=24

of (preferably small) size L to determine the CrMES at this size. Then a new CrMES corresponding to a lattice of size $L' > L$ is calculated via Eq. 2 in order to perform the WL simulation at this bigger size L' only in a restricted energy interval.

Figure 2 shows that when the size increases new peaks which are absent for smaller sizes, may appear in the specific heat curve. Moreover the location of these peaks is strongly sample dependent. In figure 2 the specific heat curves of two different realisations at the same field are shown for $L = 16$ (a) and $L = 24$ (b).

Figure 3 shows the energy probability distribution corresponding to the maxima of $C_L(T)$ depicted in Figures 1 and 2. It can be seen that for $h_0 = 2.1$, for $L \geq 16$, the probability distribution of the energy is double peaked. This is a signature of a first order transition, which is absent for smaller sizes. So the procedure proposed in [7] would be misleading if the starting sizes are smaller than $L = 16$. For the 3D RFIM $L = 16$ is big enough so as to render the use of multirange WL scheme necessary. Very recently a variation on the

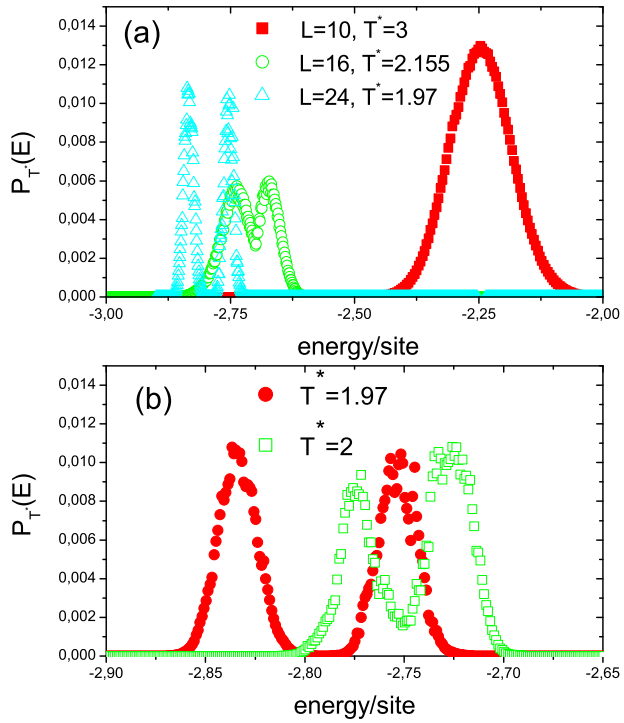

Fig. 3. (a) Probability distribution of the energy for different lattice sizes at the corresponding transition temperatures T^*. Double peaks appear in the probability distribution as $L \geq 16$ suggesting a first order transition. Probability distributions of different sizes have very small overlap. 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.

WL method has been proposed that migth improve this point [17].

Finite size effects are well known and should be generally taken into account in order to obtain results for infinite systems. The additional point when considering finite size effects in disordered systems is that changing the size implies a change of quenched disorder, which is obviously not the case in systems without disorder. This becomes particularily troublesome when large sample to sample fluctuations are observed.

The observed large sample to sample fluctuations are in agreement with other works on disordered systems [9] [12] [18] - [20]. As the multiplicity of peaks of the specific heat and their locations are strongly sample dependent (see Figure 2), the location of the maxima of $P_{T^*}(E)$, and the resulting CrMES depend also on the considered sample.

To take this aspect into account in [9] a "broadened CrMES" for WL simulation is proposed. This broadened CrMES is determined by the union of M CrMES each of them calculated for a different quenched random field configuration. Then, using Equation 2, the CrMES is estimated for a larger size. It is assumed that for the new $L' > L$, it will be enough to run the WL algorithm only in this new restricted energy interval.

Letting aside the fact that equations 1 and 2 are not valid if the transition is first order, and that in general the critical exponents are not always known in the case of a second order transition, we will now discuss in detail the idea of extending to a larger size L' the CrMES calculated for L [16].

As pointed out above, in the case of disordered systems the sample of size $L' > L$ is a ***new, different sample***, the corresponding $P_{T^*}(E)$ may have its maxima located out of the CrMES that has been extrapolated 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 samples of *the same size*.

We used the DOS obtained in [10] for the whole energy range, to recalculate thermal properties restricting the DOS to the intervals given in ref [9]. Let's consider first the case where a broadened interval is used. For $L = 24$ the broadened interval of [9] corresponds to the energy interval $\delta E = [-2.91, -1.83]$. We find that, using this broaden restricted interval, it is possible to reproduce our results issued from the complete DOS. Unfortunately, though several times smaller than the whole energy range, this interval is located in the hardest region from the convergence point of view [10]. 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, working with a very large CrMES 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 [9] are aware of this and they have proposed, as an alternative, to work on the CrMES of *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 [9] $\Delta\tilde{E}_i$.

Conceptually $\Delta\tilde{E}_i$ corresponds to the region where the energy probability distribution at the transition temperature is significative for the sample i and, in the case of a double peaked distribution, it contains the two peaks. Hence, we identify $\Delta\tilde{E}_i$ as the energy interval where $P_{T^*}(E)$ is different from zero. We

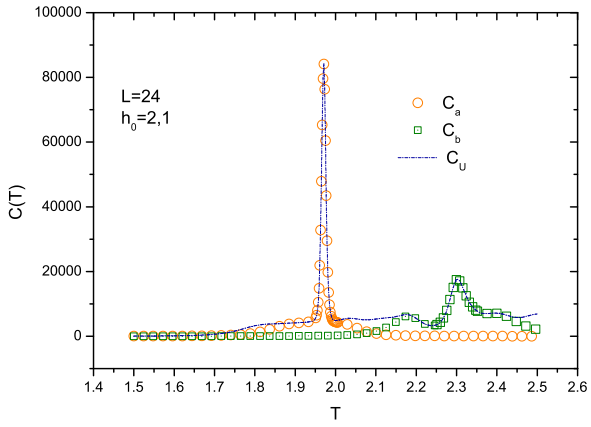

Fig. 4. (a) Specific heat as a function of temperature T, for $L = 24$, $h_0 = 2.1$ obtained from thermal averages using the DOS restricted to three different energy intervals. Interval $\Delta\tilde{E}_U(L)$ corresponds to the levels given in [9] for L=24, this union interval reproduces a multi-peaked $C_u(T)$ 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

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 separated peaks. Each of them determines a T^* and hence a restricted energy interval.

We show that the whole structure of $C_L(T)$ cannot be reproduced using the DOS restricted to the interval associated with only one of the peaks. When $C_L(T)$ is re-calculated 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 let's imagine that we determine the CrMES for a lattice size L. *As a larger size implies a new different quenched disorder*, 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' of size L'. In that case the results calculated for L' will not correspond to the transition region of this new sample.

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4 Conclusions

We show, using the example of the 3D-RFIM, that the CrMES method has to be applied with extreme care to the study of highly disordered systems, because the existence of strong quenched disorder may lead to first order transition properties and strong sample to sample fluctuations.

To begin with, it is worthwhile noticing that when dealing with disordered systems, increasing L automatically changes the distribution of the quenched disorder. Hence, if the interval $\Delta\tilde{E}(L)$ calculated for a sample of size 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 CrMES 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, and there is a risk using this method, to seize only one of them. This migth explain the anomalous behaviour observed in Fig.5 of [9] for the largest sizes studied in that work.

The actual nature of the transition of the 3D-RFIM, still under discussion, does not change the source of the problem. Would the transition be found second order in the thermodynamic limit, the use of Eqs. 1 and 2 would be justified. Nevertheless this would neither change the problem of sample to sample fluctuations, nor the fact that when working with finite sizes $P_{T^*}(E)$ would still be double peaked.

References

[1] B. A. Berg, T. Neuhaus, Phys. Rev. Lett. **68** 9 (1992)

[2] P. M. C. de Oliveira, T. J. P. Penna, H. J. Herrmann, Braz, J. Phys **26** 677 (1997)

[3] J.Lee, Phys. Rev. Lett. **71** 211 (1993)

[4] Fugao Wang and D. P. Landau, Phys. Rev. Lett. **86** 2050 (2001)

[5] R. H. Swendsen and J. S. Wang, Phys. Rev. Lett. **58** 86 (1987)

[6] U. Wolff, Phys. Rev. Lett. **62** 361 (1989a)

[7] A.Malakis, A. Peratzakis and N. G. Fytas, Phys.Rev.E **70** 066128 (2004)

[8] Fugao Wang and D. P. Landau, Phys. Rev. E **64** 056101 (2001)

[9] Anastasios Malakis and Nikolaos Fytas, Phys.Rev.E **73** 016109 (2006)

[10] Laura Hernández and Horacio Ceva, Physica A387,2793 (2008)

[11] Laura Hernández and H. T. Diep Phys.Rev.B **55** 14080 (1997)

[12] Yong Wu and Jonathan Machta Phys. Rev. B **74** 064418 (2006)

[13] H. Behringer and M.Pleimling, Phys. Rev. E74, 011108 (2006)

[14] N.G. Fytas, A. Malakis and K. Eftaxias, J.Stat.Mech. P03015 (2008)

[15] K. Binder, D.P. Landau, Phys.Rev.B **30** 1477 (1984); M.S.S. Challa, D.P. Landau, K. Binder, Phys.Rev.B **34** 1841 (1986)

[16] A. Malakis, N.G. Fytas and P. Kalozoumis, Physica A383, 351 (2007).

[17] A. G. Cunha-Netto, A. A. Caparica1, Shan-Ho Tsai3, Ronald Dickman and D. P. Landau arXiv 0808-1210v1

[18] Giorgio Parisi and Nicolas Sourlas, Phys. Rev. Lett. **89** 257204, (2002)

[19] Nicolas Sourlas, Computer Physics Communications 121-122, 183 (1999)

[20] Shai Wiseman and Eytan Domany, Phys. Rev. Lett. 81, 22 (1998)