Materials Science-Poland, Vol. 23, No. 4, 2005

Finite-size analysis via the critical energy -subspace method in the Ising models

A. C. MALAKIS*, I. A. HADJIAGAPIOU, S. S. MARTINOS, N. G. FYTAS

Faculty of Physics, University of Athens, Panepistimioupoli Zografou, GR 15784, Athens, Greece

We briefly review some applications of the critical minimum energy-subspace method (CrMES) using the Wang–Landau sampling for the estimation of the density of states (DOS). These applications concern the two- and three-dimensional Ising models and their important conserved order parameter versions (COP), known also as the Ising models with fixed magnetization (IMFM). The recently developed CrMES scheme greatly facilitates methods for sampling the DOS of classical statistical models in large systems. In effect, the CrMES technique enables the estimation of critical behaviour using only a small part of the energy space. Specific heat curves are obtained, their peaks are located and their scaling behaviour is studied and compared with the results known from literature whenever such results exist.

Key words: *Ising model; Wang–Landau sampling; finite-size scaling*

1. Introduction to the CrMES method

The CrMES method has been developed recently [1]. It is a very efficient technique for studying specific-heat anomalies of a finite lattice model and for extracting, via finite-size analysis, its asymptotic critical behaviour. In order to present the method, let us assume that the statistical model of interest will be approached using an approximation scheme for the density of states (DOS), $G(E)$. There exist a number of such methods, developed recently, such as the Wang–Landau method [2, 3] which uses a random walk in the energy space. Any such scheme will produce errors in the calculation of the specific heat. Additional errors introduced by our CrMES technique are not even observable when compared to those corresponding to the approximate scheme for the DOS, provided that one uses a sufficiently small parameter r (see Eq. (3) below).

According to the CrMES method, the specific-heat peak of the finite system may be estimated by using only a small part of the energy space. This is a very simple idea,

*Corresponding author, e-mail: amalakis@cc.uoa.gr

closely related to the notion of the thermodynamic equivalence of ensembles and to the central limit theorem. Let us follow the basic argument presented in [1]. If $\widetilde{E}$ denotes the energy that produces the maximum term in the partition function at the temperature of interest, we may define a set of approximations to the specific heat value by restricting the statistical sums to energy ranges around the value $\tilde{E}$. Accordingly, the specific heat per particle, for an N particle system of linear dimension L, at the temperature of interest (for instance, the specific heat peak at the "pseudo-critical" temperature T_L^*), is approximated by ($k_B = 1$):

$$C_L(\tilde{E}_-, \tilde{E}_+) \equiv C_L(\Delta) = N^{-1}T^{-2}\left\{\tilde{Z}^{-1}\sum_{\tilde{E}_-}^{\tilde{E}_+} E^2 \exp[\tilde{\Phi}(E)] - \left(\tilde{Z}^{-1}\sum_{\tilde{E}_-}^{\tilde{E}_+} E \exp[\tilde{\Phi}(E)]\right)^2\right\} \quad (1a)$$

$$\tilde{\Phi}(E) = [S(E) - \beta E] - \left[S(\tilde{E}) - \beta\tilde{E}\right], \qquad \tilde{Z} = \sum_{\tilde{E}_-}^{\tilde{E}_+} \exp[\tilde{\Phi}(E)] \quad (1b)$$

where the microcanonical entropy is given by:

$$S(E) = \ln G(E) \quad (1c)$$

In the above, the restricted energy sub-ranges of the total energy range ($E_{\min}$, $E_{i\max}$) are defined with respect to the energy $\tilde{E}$, which corresponds to the maximum term in the partition function at the temperature of interest:

$$(\tilde{E}_-, \tilde{E}_+), \qquad \tilde{E}_\pm = \tilde{E} \pm \Delta^\pm, \qquad \Delta^\pm \geq 0 \quad (2)$$

Depending on the extensions of the sub-ranges in Eq. (2), the above scheme may provide good approximations to the specific heat at a particular temperature. Since by definition $\tilde{\Phi}(E)$ is negative, we should expect that for large lattices "extreme" values of energy (far from $\tilde{E}$) will have an insignificant contribution to the statistical sums, because these terms decrease exponentially fast with the distance from $\tilde{E}$. It follows that, if we request a specified accuracy, then we may greatly restrict the necessary energy range in which the DOS should be sampled. According to our technique, restricting the energy space from ($E_{\min}$, $E_{\max}$) to $(\tilde{E}_-, \tilde{E}_+)$ will therefore substantially facilitate any approximate scheme for the calculation of the density of states. The proposed restriction (CrMES) will be defined below with respect to the specific heat, in such a way that the relative errors of the specific heat maxima will be bounded by a predefined small number r.

The CrMES part of the energy spectrum is well defined if we know the exact DOS for a finite system. Given any small number r and the exact DOS, one can easily calculate the minimum energy subspace (MES), compatible with the above requirements. An algorithmic approach has been described in [1]. The resulting sub-space (its end-

points and its extension) depends, of course, on the temperature, on the value of the small parameter *r*, and on lattice size. We write for its extension:

$$\Delta\tilde{E} \equiv \Delta\tilde{E}(T,r,L) \equiv \min(\tilde{E}_{+} - \tilde{E}_{-}) : \left| \frac{C_L(\Delta^{\pm})}{C_L} - 1 \right| \leq r \tag{3}$$

The extension of this dominant energy subspace, determining the behaviour of the system, is much smaller than the total energy range, $\Delta\tilde{E}(T,r,L) \ll (E_{\max} - E_{\min})$, and we should expect that its value will be of the same order, with the standard deviation of the energy distribution. Therefore, we propose that, given a small parameter *r*, the extensions of the CrMES part of the spectrum satisfy:

$$\Delta\tilde{E} \propto \sigma_E = \sqrt{NT^2C} \tag{4}$$

From the central limit theorem we know that the energy distribution should approach a Gaussian far from the critical point and that the energy subspace determining all thermodynamic properties is at most of the order of $\sqrt{N}$. Close to a critical point, the extensions $\Delta\tilde{E}^* \equiv \Delta\tilde{E}(T_L^*,r,L)$ of the CrMES at the "pseudo-critical" temperature, (as well as the extensions $\Delta\tilde{E}_c \equiv \Delta\tilde{E}(T_c,r,L)$ at the exact critical temperature), should scale as:

$$\frac{\Delta\tilde{E}^*}{L^{d/2}} \approx L^{\alpha/2\nu} \tag{5}$$

where α and ν are the specific heat and correlation length critical exponents, respectively. Note that for the square Ising lattice a logarithmic scaling law should be expected. The proposed scaling equation (Eq. (5)) follows from the well-known finite-size scaling behaviour of the specific heat $(C_L \approx L^{\alpha/\nu})$ and hypothesis (Eq. (4)).

In order to obtain the minimum energy subspace satisfying Equation (3) from the density of states *G*(*E*) we may define successive "minimal" approximations (*j* = 1, 2, 3, …) to the specific heat $C_L(j)$, as in [1]. With the help of these approximations we obtain the following relative errors:

$$r_j = \left| \frac{C_L(j)}{C_L} - 1 \right| \tag{6}$$

Then we fix our requirements by specifying a particular level of accuracy for all finite lattices. In effect, we define the (critical) MES as the subspace "centered" at $\tilde{E}(\tilde{E}^*)$, corresponding to the minimum subspace for which the relative error of the specific heat satisfies the relation $r_j \leq r$. Demanding the same level of accuracy for all lattice sizes, we produce a size dependence on all parameters of the above energy

ranges. That is, we should expect that the "centre" $\tilde{E}(T,r,L)$ and the end-points $\tilde{E}_{-}(T,r,L),\tilde{E}_{+}(T,r,L)$ of the (critical) MES are all functions of L. In particular, the extensions $\Delta\tilde{E}^{*}=\Delta\tilde{E}(T_L^{*},r,L)$ of the CrMES should obey the scaling law (Eq. (5)). It is therefore possible to find approximations to these functions using the total energy range for small lattices and then to extrapolate in order to estimate the CrMES for larger lattices.

2. Ising models and their COP versions

Let us review here some recent applications of the CrMES method to some well -known models of statistical mechanics, such as the Ising model. The normal Ising model is described by the Hamiltonian:

$$H=-J\sum_{<i,j>}S_iS_j,\quad S_i=\pm 1,\quad i=1,2...,N \tag{7}$$

and is primarily a model for ferromagnets. Furthermore, according to universality, it describes the properties of several systems of physical significance, including magnetic nuclear systems, and the liquid–vapour critical point [4, 5]. An important variation of the Ising model is the Ising model with fixed magnetization (IMFM), also known as the conserved-order-parameter (COP) Ising model. This variation has the same Hamiltonian, but now the sum of the partition function is restricted by the condition $\sum_i S_i=M_0$, where M_0 is the value of the fixed magnetization. The COP version is used to describe different systems and phenomena, including lattice gases and binary mixtures. Related phenomena are the formation of equilibrium crystal shapes, the roughening transition, and the non-equilibrium processes of diffusing surface clusters, phase separation and demixing [6, 7].

Consider first the three-dimensional case. For the Ising model on a cubic $L\times L\times L$ lattice, we may express the specific heat in the critical region using a renormalization group expansion of the form:

$$C_L \simeq q_0 L^{2y_t-d}+p_0+rL^{2y_t-d+y_i} \tag{8}$$

where y_i is irrelevant exponent which, according to Deng and Blote [8], is approximately $y_i = -0.821$. The above expansion is, of course, valid in the critical region, which is assumed to include both the "pseudo-critical" and exact critical temperatures for large lattices.

Using the CrMES method combined with Wang–Landau sampling, we have accurately estimated, in the corresponding energy-subspaces, the DOS for cubic lattices with linear sizes $L = 4, ..., 32$ [1]. The analysis of our specific heat data gives a thermal critical exponent of $y_t = 1.5878(31)$. This is comparable to the best estimate

known in literature [8]. Furthermore, we can use an alternative route for determining the thermal exponent, since the extensions of the CrMES at "pseudo-critical" temperatures are assumed to satisfy a similar scaling law, that is:

$$\left(\frac{\Delta \tilde{E}_r^*}{L^{d/2}} \right)^2 \simeq q(r) L^{2y_t - d} + p(r) L^{2y_t - d + y_i} \tag{9}$$

Using this new scheme, the critical exponent is found to be $y_t = 1.5860(30)$, which is also in excellent agreement with literature [8], verifying our proposal and proving its effectiveness. We point out that this is the first accurate estimation of the thermal critical exponent from specific heat data. In the past, other routes used for estimating this important critical exponent have been used [8], mainly because of the inaccuracy of previous specific heat data, but also due to the corrections due to scaling in the specific heat behaviour. The CrMES technique has improved the situation by allowing us to produce quite accurate finite-size data.

For the COP version of the three-dimensional Ising model, we have developed a non-local spin-exchange Wang–Landau algorithm. The combination of this algorithm with our CrMES scheme appears to be the most efficient route for studying the specific heat anomalies of this important variation of the Ising model. Our study of the three-dimensional COP version of the cubic Ising model has not yet been completed. We observe a striking similarity in the critical behaviour, however, suggesting that the COP version may share the same thermal exponent with the simple model, something that we have already numerically tested for the two-dimensional case, presented below.

Figures 1a, b show the specific heat peaks for several lattice sizes of the 3D Ising model and its COP version. The specific heat curves shown in these figures have been obtained from the CrMES part of the energy spectrum, and it should be pointed out that although these curves are accurate in the region of the peaks they are not reliable far away from them. However, for the COP version (Fig. 1b) and for $L = 8$, 10, and 12 the full low energy part of the energy spectrum is used in order to show an interesting secondary peak to the left of the main peak.

Consider now the two-dimensional case. For the normal square Ising model, a spin-flip Wang–Landau algorithm is used, whereas a non-local spin-exchange Wang–Landau algorithm is used for its COP version. Specific heat values are obtained in the appropriate critical region, implementing the CrMES method. The application is carried out for both the exact critical temperature T_c and the "pseudo-critical" temperature T_L^*, by restricting the Wang–Landau random walk in an appropriate energy range, wide enough to cover both minimum energy subspaces for the two temperatures and to accurately estimate the extensions of the corresponding MES.

Let us now discuss the finite-size behaviour of the specific heat for the normal Ising model (with freely fluctuating magnetization) on a square $L \times L$ lattice. It is known from the work of Ferdinand and Fisher [9] that close to the critical temperature $T_c = 2(J/k_B)/\ln(1+\sqrt{2})$, the finite-size behaviour is described by the following expansion:

$$C_L(T) = A_0 \ln L + B(T) + B_1(T)\frac{\ln L}{L} + B_2(T)\frac{1}{L} + ... \tag{10}$$

where the critical amplitude A_0 and the first B coefficients are given in [9] for both the exact critical and "pseudo-critical" temperature of the normal Ising model. In particular, the coefficient B_1 is zero for the exact critical temperature but non-zero for the "pseudo-critical" temperature. The amplitude A_0 (main singularity) does not vary in the range of the validity of the expansion and is therefore the same for the specific heat sequence at the exact critical and for the sequence of specific heat peaks at the "pseudo-critical" temperatures.

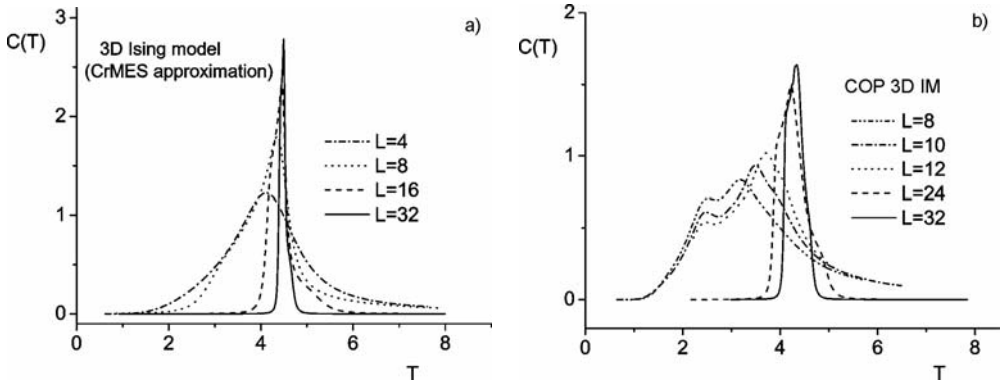

Fig. 1. Specific heat for: a) small lattices in the 3D Ising model. For large sizes, only the neighbourhoods of the peaks are reliable, since the curves have been derived from the corresponding CrMES; b) the COP versions of small lattices in the 3D Ising model. For L = 8, 10, and 12, the CrMES has been intentionally extended to the low-energy part of the spectrum down to the ground state in order to illustrate the existence of a secondary peak

Using our CrMES method and the algorithms mentioned above, we have verified the scaling law (Eq. (10)) for the square Ising model by accurately estimating the amplitude A_0 and the first B-coefficients from our specific heat data [1]. Furthermore, we have confirmed that the finite-size extensions of the CrMES satisfy an analogous scaling law, namely:

$$\left(\frac{\Delta\tilde{E}(r)}{L^{d/2}}\right)^2 \simeq A(r)\ln L + B_1(r)\frac{\ln L}{L} \tag{11}$$

Figure 2 presents the behaviour of the CrMES extensions in function of lattice size. As proposed based on physical grounds, this figure shows a clear logarithmic dependence, pointing out that our technique is a new route for estimating the critical behaviour. Our scaling proposal (Eq. (5)) also gives an interesting interpretation of the ratio α/ν, as discussed in the concluding remarks.

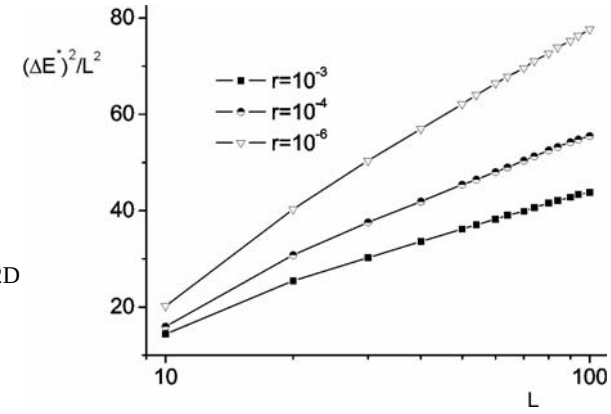

Fig. 2. Demonstration of the proposed logarithmic scaling law (Eq. (11)) for the 2D Ising model. Three levels of accuracy (r) have been used in order to define the corresponding CrMES parts of the energy spectrum

Finally, we present some new results for the COP version of the square Ising model, which we have extensively studied for several values of the fixed magnetization. For the IMFM, a critical temperature for any constant value of magnetization M_0 has been proposed by Kastner [7]:

$$M_0 = \left[1 - \left(\sinh\frac{2J}{k_B T_0}\right)^{-4}\right]^{1/8}, \qquad T_0 = T_c(M_0) \tag{12}$$

Note that for $M_0 = 0$, the above formula (Eq. (12)) produces a critical temperature that has the same value as the normal Ising model ($T_c = T_c(M_0 = 0)$). We have verified that for the main component $M_0 = 0$ the Ferdinand–Fisher expansion is well obeyed, and we have estimated the first B-coefficients and the main amplitude A. We found that the amplitude A of the main logarithmic term is also the same for the IMFM at both the "pseudo-critical" and exact critical temperatures and obeys the value of the normal Ising model case, namely:

$$A(M_0 = 0) = A_0 = \frac{8}{\pi}K_c^{\,2} = \frac{2}{\pi}\left[\ln(1+\sqrt{2})\right]^2 = 0.494538 \tag{13}$$

Furthermore, the coefficient B_1 of the expansion appears to be very close to zero at the exact critical temperature, and in fact our optimum fitting attempts are based on this conjecture. In conclusion, for the $M_0 = 0$ IMFM shares an exceptionally similar scaling behaviour with the normal Ising model.

We have also studied the scaling behaviour of the specific heat for several other values of fixed magnetization. For lattice sizes L in the range of 10–150, the logarithmic behaviour of the specific heat seems to prevail and the amplitude A of the optimum fitting tends to zero as $M_0 \to 1$. Note that, according to our data, if this behaviour is correct, then the amplitude A is much smaller at the critical temperature proposed in Equation (12) than the value obtained for the sequence of "pseudo-critical" temperatures. It will be interesting to see whether this behaviour will also be observed for much larger lattice sizes.

3. Conclusions

The CrMES technique is an efficient approximation scheme which greatly facilitates the sampling of the density of states in large systems. The relevant energy range used is in general a very small portion of the whole energy space. Therefore, the method is very efficient compared to the original Wang–Landau random walk, which covers the entire energy space. In effect, our proposal combines the idea of entopic sampling with that of importance sampling in a systematic way, without producing additional errors. The applications presented here have shown that the general approach is very reliable, and that not only the critical temperatures, but also the critical exponents can be estimated with high accuracy. This new method might be applicable to complex systems. The route proposed for calculating the ratio of the critical exponents α/ν from the scaling law (Eq. (5)) also provides an interesting interpretation for this ratio. Thus, α/ν may be comprehended as an index that determines the expansion of the dominant energy-subspace as we increase the lattice size. This provides new insight into the critical behaviour of a statistical system, and we think that similar interpretations may be found for other critical exponents.

References

[1] MALAKIS A., PERATZAKIS A., FYTAS N. G., Phys. Rev. E, 70 (2004), 066128.
[2] WANG F., LANDAU D. P., Phys. Rev. Lett., 86, 2050, (2001).
[3] WANG F., LANDAU D. P., Phys. Rev. E, 64(2001), 056101.
[4] DOMB C., Adv. Phys., 9 (1960), 149.
[5] FISHER M. E., Rep. Prog. Phys., 30 (1967), 615.
[6] PLEIMLING M., SELKE W., J. Phys. A: Math. Gen., 33 (2000), L199–L202.
[7] KASTNER M., J. Stat. Phys., 109 (2002), 133.
[8] DENG Y., BLOTE H. W. J., Phys. Rev. E, 68 (2003), 036125.
[9] FERDINAND A. E., FISHER M. E., Phys. Rev., 185 (1969), 832.

Received 23 September 2004
Revised 5 May 2005