The CrMES scheme as an alternative to Importance Sampling: The tail regime of the order-parameter distribution

Anastasios Malakis* and Nikolaos G. Fytas
Department of Physics, Section of Solid State Physics,
University of Athens, Panepistimiopolis, GR 15784 Zografos, Athens, Greece
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We review the recently developed critical minimum energy-subspace (CrMES) technique. This scheme produces an immense optimization of popular algorithms, such as the Wang-Landau (WL) and broad histogram methods, by predicting the essential part of the energy space necessary for the estimation of the critical behavior and provides a new route of critical exponent estimation. A powerful and efficient CrMES entropic sampling scheme is proposed as an alternative to the traditional importance sampling methods. Utilizing the WL random walk process in the dominant energy subspace (CrMES-WL sampling) and using the WL approximation of the density of states and appropriate microcanonical estimators we determine the magnetic properties of the 2D Ising model. Updating \((E,M)\) histograms during the high level WL-iterations, we provide a comprehensive alternative scheme to the Metropolis algorithm and by applying this procedure we present a convincing analysis for the far tail regime of the order-parameter probability distribution.

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I. INTRODUCTION

Traditional Monte Carlo sampling methods have increased dramatically our understanding of the behavior of the standard classical statistical mechanics systems. The Metropolis method and its variants were, for many years, the main tools in condensed matter physics, particularly for the study of critical phenomena [1, 2, 3]. However, in many cases, such as for example in complex systems with effective complicated potentials, the Metropolis method and its variants are more or less inadequate methods [3, 4]. Noteworthy, the traditional importance sampling methods are not very efficient in recording of the very small probabilities in the tails of the critical order-parameter distribution [5]. This is the reason why many different simulation approaches [5, 6, 7, 8] in recent times have failed in establishing the true tail behavior of this distribution.

In Sec. II we briefly review a new simple technique, the CrMES method, which yields an immense speed up of all popular algorithms, which are used to sample the density of energy states (DOS) of a statistical system in the last decade. Provided that, the temperature range of interest is only the range around the critical temperature that determines all finite-size anomalies, our technique can be combined with any of the DOS methods [3, 4, 10, 11, 12, 13, 14, 15, 16] to speed up the simulations and establish a different methodology for the determination of the critical exponents by studying the finite-size scaling of the extensions of the dominant subspaces. In the same section we describe a CrMES-WL entropic sampling method and all magnetic properties are obtained by using the high-levels of the WL random walk process to determine appropriate microcanonical estimators. The proposed method is combined with the N-fold way [17, 18, 19] in order to improve efficiency and statistical reliability. Finally, in Sec. III we study the order-parameter distribution of the 2D Ising model and we clarify its asymptotic behavior in the far tail regime. Our conclusions are summarized in Sec. IV.

II. THE CRMES WANG-LANDAU ENTROPIC SAMPLING SCHEME

According to the CrMES method [21, 22] the total energy range \((E_{\text{min}}, E_{\text{max}})\) is restricted using the definitions:

\[
(E_{-}, E_{+}), \quad \tilde{E}_{\pm} = \tilde{E} \pm \Delta^{\pm}, \quad \Delta^{\pm} \geq 0
\]  

*Corresponding author: amalakis@cc.uoa.gr
with respect to the value \( \tilde{E} \) producing the maximum term in the partition function of the statistical model, for instance the Ising model, at some temperature of interest. Thus, the specific heat peaks are approximated by:

\[
C^*_L(\Delta \pm) = N^{-1}T^{-2} \left\{ \tilde{Z}^{-1} \sum_{E_\pm} E^2 \exp [\tilde{\Phi}(E)] - \left( \tilde{Z}^{-1} \sum_{E_\pm} E \exp [\tilde{\Phi}(E)] \right)^2 \right\}
\]  

(2)

\[
\tilde{\Phi}(E) = [S(E) - \beta E] - \left[ S(\tilde{E}) - \beta \tilde{E} \right], \quad \tilde{Z} = \sum_{E_\pm} \exp [\tilde{\Phi}(E)]
\]  

(3)

![FIG. 1: Behavior of CrMMS for \( r = 10^{-4} \). The solid lines correspond to power law fits (a) for \( T = T_c \) : \( \Xi \simeq 0.513(15) \cdot L^{1.758(7)} \) and (b) for \( T = T_{LX} \) : \( \Xi \simeq 0.517(45) \cdot L^{1.741(18)} \). The dotted line represents the law \( \Xi \equiv 0.5138 \cdot L^{1.75} \), which is very close to the fit \( \Xi \simeq 0.5145(90) \cdot L^{1.7497(50)} \) corresponding to the average \( (\Xi_{T_c} + \Xi_{T_{LX}})/2 \).

To implement the above restriction we request a specified accuracy by imposing the condition:

\[
\left| \frac{C^*_L(\Delta \pm)}{C^*_L} - 1 \right| \leq r
\]  

(4)

where \( r \) measures the relative error and will be set equal to a small number \( (r = 10^{-4} \) and/or \( r = 10^{-6} \)), and \( C^*_L \) is the value of the maximum of the specific heat obtained by using the total energy range. With the help of a convenient definition \[20, 22\], we can specify the minimum energy subspace satisfying the above condition. In fact, it has been numerically verified that the finite-size extensions (denoted by \( \Delta \tilde{E} \equiv \min(\tilde{E}_+ - \tilde{E}_-) \)) close to a critical point obey the scaling law \[20\]:

\[
\psi_{C^*_L} = \frac{(\Delta \tilde{E})^2_{C^*_L}}{L^d} \approx L^{2\alpha}
\]  

(5)

To locate the CrMES we may follow the method described in \[20\], or an even simpler restriction \[22\] based on the energy probability density \( (f_{T^*_C}(E) \propto \tilde{\Phi}(E)) \). Using this later approach, we may define the end-points \( (\tilde{E}_\pm) \) of the subspaces by simply comparing the corresponding probability densities with the maximum at the energy \( \tilde{E} \):

\[
\tilde{E}_\pm : \exp \{\tilde{\Phi}(\tilde{E}_\pm)\} \leq r
\]  

(6)
FIG. 2: Behavior of CrMMS for $r = 10^{-6}$. The solid lines correspond to power law fits (a) for $T = T_c$: $\Xi \simeq 0.528(17) \cdot L^{1.761(7)}$ and (b) for $T = T_{L,x}^\ast$: $\Xi \simeq 0.536(45) \cdot L^{1.745(15)}$. The dotted line represents the law $\Xi \equiv 0.54 \cdot L^{1.75}$, which is very close to the fit $\Xi \simeq 0.532(15) \cdot L^{1.753(6)}$ corresponding to the average $(\Xi_{T_c} + \Xi_{T_{L,x}^\ast})/2$.

Alternative definitions for the CrMES have been described and tested in Ref. [22] using the 2D Ising model [20, 22], the 3D Ising model [20, 22], and the Baxter-Wu model [21, 22].

Let us now discuss the idea of producing accurate estimates for finite-size magnetic anomalies by using a simple method based on a WL random walk in an appropriately restricted energy subspace $(E_1, E_2)$. Implementing this scheme we, at the same time, accumulate data for the two-parameter $(E, M)$ histogram. A multi-range algorithm [12] is implemented to obtain the DOS and the $(E, M)$ histograms in $(E_1, E_2)$. The WL modification factor $(f_j)$ is reduced at the jth iteration according to: $f_1 = e$, $f_j \rightarrow f_j^{-1/2}$, $j = 2, \ldots, J_{\text{fin}}$. The approximation of the DOS, in the last WL iteration, $G_{WL}(E)$, and the high-level $(j \gg 1)$ WL $(E, M)$ histograms, $H_{WL}(E, M)$, are used to estimate the magnetic properties in a temperature range, which is covered, by the restricted energy subspace $(E_1, E_2)$ as:

$$\langle M^n \rangle = \frac{\sum_{E} E^{(M^n)}_E G(E)e^{-\beta E}}{\sum_{E} G(E)e^{-\beta E}} \equiv \frac{\sum_{E \in (E_1, E_2)} E^{(M^n)}_E G_{WL}(E)e^{-\beta E}}{\sum_{E \in (E_1, E_2)} G_{WL}(E)e^{-\beta E}}$$

(7)

The microcanonical averages $\langle M^n \rangle_E$ are obtained from the $H_{WL}(E, M)$ histograms as:

$$\langle M^n \rangle_E \cong \langle M^n \rangle_{E, WL} \equiv \sum_{M} M^n \frac{H_{WL}(E, M)}{H_{WL}(E)} \quad \text{and} \quad H_{WL}(E) = \sum_{M} H_{WL}(E, M)$$

(8)

and the summation in the magnetization $M$ runs over all values generated in the restricted energy subspace $(E_1, E_2)$.

The accuracy of the magnetic properties obtained from the above averaging process depends on many factors. However, since the detailed balance condition depends on the control parameter $(f_j)$, we classify our recipes utilizing the $j$-range used for updating the $(E, M)$ histogram during the WL process. The high-level recipes WL($J_{\text{init}}, J_{\text{fin}}$) and their N-fold versions WL(N-fold:$J_{\text{N-fold}}, J_{\text{fin}}$) give excellent estimates, as shown in detail in Ref. [22]. The extensions of the CrMES defined with the help of the thermal finite-size anomalies (specific heat maximum and energy cumulant minimum), and also with the help of magnetic finite-size anomaly (susceptibility maximum) obey a clear logarithmic dependence on the lattice size [22], as should be expected for the 2D Ising model.

Consider now the probability density of the order-parameter at some temperature of interest $T$:

$$P_T(M) \cong \frac{\sum_{E \in (E_1, E_2)} H_{WL}(E, M) G_{WL}(E)e^{-\beta E}}{\sum_{E \in (E_1, E_2)} G_{WL}(E)e^{-\beta E}}$$

(9)
If $\tilde{M}$ is the value that maximizes (9), we locate the critical minimum magnetic subspaces (CrMMS) by:

$$\tilde{M}_{\pm} : \frac{P_{T,\chi}(\tilde{M}_{\pm})}{P_{T,\chi}(M)} \leq r \quad (10)$$

and we should expect the following scaling law to hold:

$$\Xi_{T,\chi} \equiv \Xi_{P_{T,\chi}(M)} \equiv \frac{(\Delta \tilde{M})^2}{L^d} \approx L^{\gamma/\nu} \quad (11)$$

![FIG. 3: Illustration of the universal scaling function $p^*(x)$ for $L = 60$ and $L = 120.$](image)

In Figs. 1, 2 we present the behavior of the extensions of the CrMMS, obtained using the magnetic space restriction (10) for two values of $r$, namely $r = 10^{-4}$ and $r = 10^{-6}$. These extensions were determined at the exact critical temperature $T_c$ and at the pseudocritical temperatures $T_{L,\chi}$ of the susceptibility, as indicated in the figures. The power laws and the resulting exponents are given in the corresponding figure captions. It is clear that the law (11) is very well satisfied and the estimation of $\gamma/\nu$ via this route is quite good, giving $\gamma/\nu = 1.7497(50)$ for $r = 10^{-4}$ and $\gamma/\nu = 1.753(6)$ for $r = 10^{-6}$, respectively. It is of interest to point out that, an attempt to estimate $\gamma/\nu$ using this route and the Metropolis algorithm will most likely yield a marked underestimation, which will be more pronounced for the case $r = 10^{-6}$. This effect, has been discussed in Ref. [22] and is a result of the very slow equilibration process of this algorithm in the far tail regime of the order-parameter distribution. Next, we consider the tail regime of the universal order-parameter distribution, we analyze its asymptotic behavior and finally examine the possibility of extracting estimates of the exponent $\delta$ from this behavior.

### III. FAR TAIL REGIME OF THE ORDER-PARAMETER DISTRIBUTION

Following Smith and Bruce [5] we define the universal scaling form of the order-parameter density by:

$$p^*(x)dx \simeq p(m)dm, \quad x = m / \sqrt{\langle m^2 \rangle}, \quad m = M/N \quad (12)$$

Fig. 3 shows $p^*(x)$ for $L = 60$ and $L = 120$ obtained via the WL(N-fold:12-24) scheme. The tail regime of this universal distribution has been a matter of increasing interest in the last decade [5, 6, 23, 24, 25]. The main theme is the verification of the following conjecture for the large-$x$ behavior of $p^*(x)$ [5, 6]:

$$p^*(x) \simeq p_\infty x^\psi \exp(-a_\infty x^{\delta+1}) \quad (13)$$
with:

$$\psi = \delta - \frac{1}{2}$$  \hspace{1cm} (14)

and $p_\infty, a_\infty$ universal constants. The above hypothesis, its origin and its significance are discussed in some detail in Refs. 5, 6.

The studies of 5, 6 have provided some evidence for this conjecture and in particular for the prefactor and the relation of the exponent $\psi$ to the critical exponent $\delta$. For the 2D Ising model the exponent should have the value $\psi = 7$, if, of course, the prefactor hypothesis is valid. Smith and Bruce 5 provided numerical support for this value, but their study was not completely conclusive since it was carried out only for relatively small lattices ($L = 32$ and $L = 64$) and the $x$-window in which the value $\psi = 7$ was observed was actually quite narrow. We now present results for several lattice sizes ($L = 80, 100, 120$, and $L = 140$) reinforcing this conjecture in a very wide $x$-window. Following Smith and Bruce we fix the exponent $\delta$ in the exponential factor of Eq. (13) and fit our results ($x > 1$) in $x$-windows, each one corresponding to 50 different magnetization values, sampled during the WL(N-fold:12-24) process. Fig. 4 shows a very clear signature of the prefactor law (14) which upholds in a large $x$-window only for the large lattices ($L = 120$ and $L = 140$). On the other hand, for smaller lattice sizes ($L = 60 – 100$) the picture is similar to that presented in Ref. 5 and the expected value is obtained only in a small $x$-window. Finally, let us treat both exponents in the exponential and in the prefactor as free parameters, assuming however the validity of Eq. (14). In this case we examine whether the far tail regime could be a possible route for an independent estimation of the exponent $\delta$. Fig. 5 presents such an attempt for the case $L = 120$. The value obtained for $\psi$ (and therefore for $\delta(= 2\psi + 1)$) is accurate to the third decimal place ($\psi = 6.995(1.750)$), despite the fact of the existing large error of the fit. In fact the shown $x$-window ($x = 1.4 – 1.45$) produces good estimates for all lattice sizes $L = 60 – 140$ as should be expected by thoroughly inspecting Fig. 4.

**IV. CONCLUDING REMARKS**

In the present work we described the basic ideas and formalism behind the recently developed by the authors 21, 21, 22 critical minimum energy(magnetization) subspace CrME(M)S technique, appearing as an alternative computational method for the estimation of critical behavior of statistical systems. We presume that this new promising route will increase our comprehension of the development of the critical behavior as the lattice size increases and will further facilitate the estimation of critical exponents via finite-size scaling. It is hoped that the presented CrMES
FIG. 5: Independent estimation of the exponent \( \delta \) via fitting the universal scaling function \( p^*(x) \) in a specific \( x \)-window. The fitted line reads as \( p^*(x) = p_\infty x^\psi \exp(-a_\infty x^{2\psi}) \), yielding \( p_\infty = 2.189(2.223) \), \( \psi = 6.995(1.750) \) and \( a_\infty = 0.058(64) \), respectively.

Wang-Landau entropic sampling will provide an efficient and reliable scheme for the study of complex systems, such as the random-field Ising model and systems with competing interactions, where the critical behavior is still controversial. Furthermore, the efficiency of our approach enabled us to present here reliable data for large lattices and to clarify the asymptotic tail behavior of the universal critical distribution of the order-parameter of the 2D Ising model. This should be contrasted to the fact that all previous studies of the far tail regime of this distribution \( \cite{5, 25} \) have considered rather small lattices.

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