Density of states determined from Monte Carlo simulations

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We describe method for calculating the density of states by combining several canonical monte carlo runs. We discuss how critical properties reveal themselves in $g(ε)$ and demonstrate this by applying the method several different phase transitions. We also demonstrate how this can used to calculate the conformal charge, where the dominating numerical method has traditionally been transfer matrix.

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I. INTRODUCTION

Since it was devised by Metropolis in 1953[1] Monte Carlo (MC) simulations based on the Metropolis algorithm have had a tremendous impact on physics; SIAM recently rated the algorithm among the ten most influential numerical algorithms of the previous century[2]. For a historical summary, and a review of modern MC methods we refer to the proceedings of the conference hosted to celebrate the 50th anniversary of the algorithm[3]. For general references to Monte Carlo simulations see e.g. Refs. 4, 5, 6.

The Metropolis algorithm is well suited to calculate quantities which can be expressed as

$$\langle O \rangle = \frac{1}{N} \sum_i \hat{O} |\psi_i\rangle,$$

(1)

i.e. as averages of values obtained by operating an operator $\hat{O}$ on a series of states $|\psi_i\rangle$. Focusing on phase space Eq. 1 can be denoted a local estimator, in the sense that only one point in phase space is involved at a time. Some quantities like entropy and free energy can not be expressed like Eq. 1; their evaluation requires simultaneous knowledge of global portions of phase space. Entropy and free energy can in principle be obtained by thermodynamic integration[4],

$$F(T) = U(T) - T \int_0^T dT' \frac{CV(T')}{T'},$$

(2)

but this technique does not seem to be much used.

Eq. 1 represents the absolutely simplest way to get MC results. A simulation produces a series of states $|\psi_i\rangle$ distributed according to the Boltzmann distribution, the mean over these states is calculated. Both the initial step of obtaining the data, and the final post-processing can be done differently. With multicanonical sampling[5] the Markov chain is altered to (ideally) yield a flat energy histogram; and the results reweighted back afterwards. The Wang-Landau histogram method[6, 7] can be seen as combined data collection and post-processing; when the simulation is complete we have built up an estimate $\hat{g}(ε)$ of the density of states (DOS). For some situations like first order transitions and disordered media these methods have very efficient.

During the simulation we can build up an estimate of the complete density $P_0(ε)$, and clearly it would be beneficial to utilize this information. This insight is the key to histogram methods. In 1989 Ferrenberg and Swendsen[8] published a method to combine results obtained at different couplings. The method was highly efficient, and Ferrenberg-Swendsen reweighting has become an essential tool for MC practitioners. The use of rawdata from several couplings allow for reweighting to a much broader range of couplings than ordinary single histogram methods.

In 1990 Alves, Berg and Villanova (ABV)[9] developed a variation of the Ferrenberg-Swendsen multihistogram technique; specifically targeted at calculating the density of states. To apply the FS method one must solve a set of nonlinear equations self consistently, this can fail if the overlap between the various histograms is insufficient. This is not the case for the ABV method which can always be applied as long as every histogram has finite overlap with at least one other histogram. We have developed a method to calculate DOS which is a minor variation of ABV’s original method.

The density of states is an elusive quantity, and not very much used in statistical mechanics. In addition to presenting a method to calculate $g(ε)$ we have here-for also briefly discussed statistical mechanics based on $g(ε)$ in section III and several applications in IV. Some of these applications are well known results from traditional canonical thermodynamics, however there are also properties which are more easily learned based on microcanonical thermodynamics.

The main focus of this paper is to determine the density of states from canonical Monte Carlo simulation. The density of states is the central quantity in microcanonical thermodynamics; hence this naturally becomes an important formalism for further analysis of the DOS...
based results. The study of microcanonical thermodynamics has seen increasing interest the latest years; see e.g. Ref. 14 for a general introduction, and Refs. 15, 16, 17 for some recent applications.

The rest of the paper is organised as follows: In section II we present the algorithm to calculate the density of states. Section III is devoted to a short discussion of statistical mechanics based on \( g(\epsilon) \). In the final section IV we use the algorithm to study several different phase transitions.

II. ESTIMATING \( g(\epsilon) \)

When doing a MC simulation with the Metropolis algorithm the probability to be in a state \( \psi \) with energy \( \epsilon_\psi \) is proportional to

\[
g(\epsilon_\psi) e^{-\beta \epsilon_\psi}.
\]

If we record a histogram of energies from a simulation at coupling \( \beta \); we get a histogram \( h_\beta(\epsilon) \) which is proportional to \( g(\epsilon) e^{-\beta \epsilon} \). Multiplying this histogram with \( e^{\beta \epsilon} \) we get something which is proportional to \( g(\epsilon) \), i.e.

\[
\hat{g}_\beta(\epsilon) = e^{\xi \beta} e^{\beta \epsilon} h_\beta(\epsilon)
\]

is an estimator for \( g(\epsilon) \). In Eq. 4 \( e^{\xi \beta} \) is a dimensionless constant of proportionality to be determined. The density of states in Eq. 3 has an index \( \beta \) to indicate that the histogram was recorded at this coupling, but it does not have any intrinsic temperature dependence. In principle Eq. 4 can be used to estimate \( g(\epsilon) \) regardless of temperature, however practically only a small energy range around \( \langle E \rangle(T) \) will be sampled with a sufficiently high frequency.

Although Eq. 4 is useless as an immediate estimator for \( g(\epsilon) \), it provides a basis for combining results from different couplings to an estimator \( \hat{g}(\epsilon) \) which can be applied over the complete energy range. Given \( N \) different histograms \( h_i(E) \) recorded at the couplings \( \beta_1 > \beta_2 > \cdots > \beta_N \), we can combine them as

\[
\hat{g}(\epsilon) = g_0 \sum_{i=1}^{N} e^{\xi_i} h_i(\epsilon) w_i(\epsilon) e^{\beta_i \epsilon},
\]

\[
w_i(\epsilon) = \frac{h_i(\epsilon)}{\sum_{j=1}^{N} h_j(\epsilon)}.
\]

to obtain an estimator which is usable over the complete \( \epsilon \) range \([\min, h_i(\epsilon), \max, h_i(\epsilon)]\). In Eq. 5 \( w_i(\epsilon) \) is a weight function, which denotes the weight ascribed to histogram \( i \) in the estimation of \( g(\epsilon) \). The constants \( e^{\xi_i} \) are determined by joining the various histograms.

The algorithm we have applied to determine \( \xi_i \) is to set \( \xi_1 \) to an arbitrary value, and then compute \( \xi_{i>1} \) by minimising

\[
\chi^2 = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \sum_{\epsilon} h_i(\epsilon) h_j(\epsilon) \left( \xi_i + \beta_i \epsilon + \ln h_i(\epsilon) - \xi_j - \beta_j \epsilon - \ln h_j(\epsilon) \right)^2.
\]

As indicated in Eq. 6 the central principle is to minimise the pairwise difference between all the \( \hat{g}(\epsilon) \) estimates, where the estimates \( \hat{g}_\beta(\epsilon) \) are given according to Eq. 4. Minimising \( \chi^2 \) with respect to \( \xi_i \) gives \( N - 1 \) linear equations which can be solved by e.g. LU decomposition. The algorithm described by ABV uses a different weight \( w_i(\epsilon) \) and the coefficients \( \xi_i \) are determined from a recursive procedure; \( \xi_{i+1} \) is given by \( \xi_i \) and a function of the overlap between histogram \( h_i(\epsilon) \) and \( h_{i+1}(\epsilon) \) (i and \( i + 1 \) are not necessarily ordered according to coupling, see Ref. 13 for details). Apart from these differences this algorithm coincides with the one by ABV.

When the coefficients \( \xi_i \) have been determined we have all the coefficients \( \xi_{i>1} \) expressed in terms of \( \xi_1 \). For discrete models with a finite ground state degeneracy \( g_0 \) we can determine \( \xi_1 \) by requiring \( g(\epsilon_0) = g_0 \), or alternatively if the total number of states is known, this can be used to normalize \( g(\epsilon) \). In section IV we will consider both discrete models were the complete normalisation can be achieved, and continuous models were \( \xi_1 \) must be left undetermined.

Use of Eq. 6 to determine \( g(\epsilon) \) is in principle quite straightforward, but in practice it is important to be careful to avoid numeric underflow or overflow in intermediate steps, in particular the implementation must ensure that only \( \ln g(\epsilon) \) is needed in actual computations.

III. STATISTICAL MECHANICS FROM \( g(\epsilon) \)

Knowledge of \( g(\epsilon) \) is in principle equivalent to knowledge of the partition function \( Z(\beta) \), hence all the properties of a system are contained in \( g(\epsilon) \), however \( g(\epsilon) \) does not have a very prominent role in modern statistical mechanics. We will therefore express some important results based on \( g(\epsilon) \) in this section, examples/applications are given in section IV. The definition of temperature in
From this we find that the fundamental requirement $C_V(T) \geq 0$ is equivalent to $\partial^2 \ln g(\epsilon) \leq 0$. The limiting value $\partial \ln g(\epsilon) = C$ is the signature of a phase transition. A finite $\epsilon$ range with $\partial \ln g(\epsilon) = C$ means that the temperature is unchanged for this $\epsilon$ range, i.e., an indication of a first order transition; actually, as we shall see in section IV B this is slightly more complicated. When the width of the of linear part of $\ln g(\epsilon)$ diminishes the first order transition is weakened; until $\partial^2 \ln g(\epsilon) = 0$ in a isolated point only, this is the manifestation of a critical point. If we differentiate Eq. 7 with respect to $T$ we find the function $C_V(\epsilon)$

$$C_V(\epsilon) = \frac{\partial \ln g(\epsilon)}{\partial T} = -\frac{(\partial \ln g(\epsilon))^2}{\partial^2 \ln g(\epsilon)}.$$  (8)

From Eq. 8 we see that the critical properties, and in particular the critical exponent $\alpha$, must be related to how $\partial^2 \ln g(\epsilon)$ approaches zero. To infer $\alpha$ directly from the behaviour of $g(\epsilon)$ close to $\epsilon_c$ is difficult, but if we make the size dependence of $g(\epsilon)$ explicit we can use finite size scaling 

$$|\partial^2 \ln g(\epsilon, L)| L^{d-\alpha/\nu}.$$  (9)

In general, $\partial \ln g(\epsilon, L)$ will also have finite size effects, however for this only the deviation from the thermodynamic value will show critical scaling.

For microcanonical systems the externally specified variable is $\epsilon$, and not $T$, and critical scaling is governed by the difference $|\epsilon - \epsilon_c|$, see e.g. Ref. 20. Using this H"unner and Pleimling have calculated the order parameter exponent $\beta$ from microcanonical data from the two and three dimensional Ising model 13.

When we have $g(\epsilon)$ we can easily calculate $F(T)$ and $P(\epsilon, T)$

$$F(T) = -T \ln \sum_{\epsilon} g(\epsilon) e^{-\beta \epsilon},$$  (10)

$$P(\epsilon, T) = \frac{g(\epsilon) e^{-\beta \epsilon}}{\sum_{\epsilon} g(\epsilon) e^{-\beta \epsilon}}.$$  (11)

From $P(\epsilon, T)$ we can easily calculate the internal energy, and all moments thereof. If we in addition to $\epsilon$ sample other operators like the magnetisation, we can use $P(\epsilon, T)$ to find thermal averages of arbitrary operators,

$$\langle O \rangle_T = \sum_{\epsilon} \langle O \rangle_\epsilon P(\epsilon, T).$$  (12)

In Eq. 12 $\langle O \rangle_\epsilon$ is the mean of $\hat{O}$ for a given value of $\epsilon$.

IV. SOME APPLICATIONS

In this section we present various applications of the method presented in the preceding sections. In section IV A the results are benchmarked against the 2D Ising model, where $F(T)$ has been determined exactly even for finite systems 21. In section IV B we investigate the way phase transitions reveal themselves in $g(\epsilon)$. In section IV C we calculate the finite size corrections to the free energy in a cylindrical geometry. For conformally invariant systems 22, this is universal 23, 24, and can be used to calculate the conformal charge. We have determined the conformal charge for the 2D Ising model, and the 2D $Q = 3$ Potts model. In section IV D we discuss the problems related to models with a continuous energy distribution; and show that method is useful also for these systems, although less so. Finally in section IV E we applied the method to a large dataset obtained from a previous study of the full Ginzburg Landau (GL) model.

A. Comparisons with exact results

Due to Onsagers exact solution 25 the 2D Ising model has been one of the most used benchmarks in statistical physics. For a rectangular lattice with periodic boundary the model has been solved in closed form even for finite systems 21, this constitutes a very convenient benchmark for our approach. We have performed simulations on a $32 \times 32$ system with periodic boundary conditions, and verified that within statistical error both $F(T)$ and $C_V(T)$ agree with the exact values, see figures 1-2.

![FIG. 1: This figure shows the estimated value of $F(T)$ as symbols, and the exact value from 21 as a solid line. The small ticks on the $T$ axis indicate $T$ values were simulations have been performed. In the inset the dashed curve shows the relative error of the estimated values, and the solid lines are $\pm$ an estimated statistical error.](image)
are calculated by performing ten completely independent simulations.

B. The signature of phase transitions in \( g(\epsilon) \)

As discussed in section III all critical properties must be present in \( g(\epsilon) \). In this section we will discuss the critical properties of the \( Q = 3 \) and \( Q = 10 \) Potts model. The first model has a continuous phase transition with \( \alpha = 1/3 \) and \( \nu = 5/6 \) \cite{24}, i.e. \( \alpha/\nu = 0.4 \), the second model has a first order transition.

First we consider the \( Q = 3 \) model, for this model the goal is to determine the ratio \( \alpha/\nu \) from \( g(\epsilon, L) \). According to Eq. \( \ref{4} \) this can be done by considering how \( \partial_\epsilon^2 \ln g(\epsilon, L) \) vanishes when approaching the critical energy \( \epsilon_c \). Fig. \( \ref{3} \) shows \( L^d \partial_\epsilon^2 \ln g(\epsilon, L) \) for different system sizes, and we can see that peak approaches zero with increasing system size.

In Fig. \( \ref{2} \) we have plotted \( \min |L^d \partial_\epsilon^2 \ln g(\epsilon, L)| \), i.e. the magnitude of the peak value for the curves in Fig. \( \ref{3} \) as a function of \( L \).

The dashed line in Fig. \( \ref{2} \) has slope of \( -\alpha/\nu \approx -0.29 \); this is a significant deviation from the exact value \( \alpha/\nu = 0.40 \), however we feel that these results are sufficient to demonstrate that the critical properties, and in particular the exponents \( \alpha \) and \( \nu \) are contained in \( g(\epsilon) \). There is clearly significant finite size effects in \( \partial_\epsilon \ln g(\epsilon, L) \) also; including the factor \( \partial_\epsilon \ln g(\epsilon) \) gives the “improved” value \( \alpha/\nu \approx 0.35 \), however this can not contribute in the \( L \rightarrow \infty \) limit and we have therefore not included this factor in Fig. \( \ref{3} \). Finally Fig. \( \ref{4} \) is based on the second derivative of a sampled quantity; hence it will clearly be difficult to determine with high precision. In conclusion it is definitely possible to infer the ratio \( \alpha/\nu \) from the properties of \( g(\epsilon, L) \), but it is certainly not the most suitable way for high precision measurements. Finally we mention that the remaining critical exponents can not be obtained from \( g(\epsilon) \); their value is based on the explicit choice of fields to represent the critical state.

Although all thermodynamic information about a phase transition is contained in \( F(T) \), it is only for a first order transition, where \( \partial_T F(T) \) is discontinuous at \( T_c \), that the phase transition stands out in \( F(T) \). Fig. \( \ref{5} \) shows \( F(T) \) for the strongly transition in the two dimensional \( Q = 10 \) Potts model; a discontinuity in \( \partial_T F(T) \) at \( T \approx 0.71 \) is easily spotted.

For second order transitions we had to revert to FSS to infer critical properties from \( g(\epsilon) \); in the case of first order transitions we can make quite powerful statements from \( g(\epsilon) \) alone. Given a first order transition between the pure states \( \epsilon_1 \) and \( \epsilon_2 \) the probability \( P(\epsilon, T) \) is bimodal, with distinct peaks at the pure energy levels \( \epsilon_1 \) and \( \epsilon_2 \). The mixed states with energy \( \epsilon_1 < \epsilon < \epsilon_2 \) are exponentially suppressed, to reproduce this behaviour we
must have

$$\ln g(\epsilon_1 + \Delta \epsilon) < \ln g(\epsilon_1) + \beta \ln \left( \frac{g(\epsilon + \Delta \epsilon)}{g(\epsilon)} \right).$$  \tag{13}$$

for $0 < \Delta \epsilon < \epsilon_2 - \epsilon_1$. Hence $\ln g(\epsilon)$ must increase weaker than linearly in the immediate vicinity of $\epsilon_1$ and then subsequently stronger than linearly afterwards such that the relation $\beta_\epsilon = \partial_\epsilon \ln g(\epsilon_1) = \partial_\epsilon g(\epsilon_2)$ is satisfied. If we insist on $\partial_\epsilon^2 \ln g(\epsilon) \leq 0$ also in the interval $\epsilon_1 < \epsilon < \epsilon_2$ $\ln g(\epsilon)$ must have a cusp in this interval; however these energy levels correspond to states which are manifest not equilibrium so it might be too strict to require $\partial_\epsilon^2 \ln g(\epsilon) \leq 0$ in this particular interval. An extensive discussion of the region $\epsilon_1 < \epsilon < \epsilon_2$ can be found in discussed in Ref.\textsuperscript{27}. The various details of $g(\epsilon)$ around a first order transition are illustrated in Fig.\textsuperscript{6}.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5.png}
\caption{The free energy $F(T)$ for the $Q = 10$ Potts model which has a strong first order transition. Although there is inevitably some finite size rounding, the cusp in this figure is quite clear. Fig.\textsuperscript{6} shows a similar figure for a continuous transition, this clearly smooth in comparison.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure6.png}
\caption{Results from the $Q = 10$ Potts model. The uppermost panel shows $\ln g(\epsilon)$, the two dashed lines indicate the two energy levels $\epsilon_1$ and $\epsilon_2$. The central panel shows $\ln g(\epsilon) [\beta(\epsilon - \epsilon_1) + \ln g(\epsilon_1)]$, which clearly shows that $\ln g(\epsilon)$ has small but significant deviations from perfect linearity in the range $\epsilon_1 < \epsilon < \epsilon_2$. The bottom panel shows $P(\epsilon, T_c)$, i.e. Eq.\textsuperscript{11} at the critical point, and we can clearly see how the depression in $P(\epsilon, T_c)$ originates from the features in $\ln g(\epsilon)$. This figure very closely resembles Fig. 1 of Ref.\textsuperscript{27}.}
\end{figure}

\section{Conformal charge}

It is well known that critical systems are scale invariant; in addition the critical systems often possess further symmetries like translational and rotational invariance. Together these operations form a group $G$. Under quite mild restrictions, in particular finite length interactions, the system is actually invariant also under transformations which vary in space, this means that $G$ is the conformal group. In particular for $d = 2$ this is a very powerful result, and the application of Conformal Field Theory (CFT) has lead to many exact results for the critical state\textsuperscript{28}.

Consider an infinitely long strip of width $W$, due to the finite width there will be finite size corrections to the free energy density. One of the most fundamental results from conformal invariance is that the leading finite size correction for this system is universal\textsuperscript{23, 24}

$$f_W = f_B - \frac{\pi c}{6W^2} + O\left( \frac{1}{W^4} \right).$$  \tag{14}$$

In Eq.\textsuperscript{14} $f_W$ is the free energy density of the strip, $f_B$ is the bulk free energy density of an infinite system and $c$ is the conformal charge or anomaly. The conformal charge is a dimensionless number which uniquely characterises a given universality class. In two dimensions the Ising model has $c = 0.5$ and the $Q = 3$ Potts model has $c = 0.8$\textsuperscript{22}.

Eq.\textsuperscript{14} is a finite size scaling expression which should be very useful for numeric evaluation of $c$. However, since the use of Eq.\textsuperscript{14} requires knowledge of the free energy MC has not been extensively used; see however for instance\textsuperscript{29} for a numerical test of another Conformal Field Theory conjecture by MC methods. The numerical evaluation of $c$ has been dominated by transfer matrix methods\textsuperscript{22, 30}, see however Ref.\textsuperscript{31} for a study of the $Q = 3$ Potts model very similar to the present one.

Using the method presented in this paper we have calculated $c$ for the Ising model and the $Q = 3$ Potts model. We have considered cylindrical systems of length...
$L$ and circumference $W$, we have considered $W = \{4, 5, 6, 8, 10, 12, 16\}$, and for each $W$ we have used $L = \{W, 2W, 4W, 8W, (16W)\}$, $L = 16W$ was only considered for the Ising model. From this we have extrapolated to find

$$f_W = \lim_{L \to \infty} \frac{1}{LW} F(L, W).$$  \tag{15}$$

Plots of $f_W$ are shown in Fig. 7 and $c$ has been determined from a least squares fit to these curves. The curves in Fig. 7 show that there are quite significant corrections to the $W^{-2}$ term for small $W$, and the numerical results $c = 0.49 \pm 0.07$ for the Ising model was obtained by excluding all $W < 8$. Including an additional fourth order term $\alpha W^{-4}$, and including all the results we get $c = 0.55 \pm 0.06$. Most of the computational resources were spent on the Ising model, and the $Q = 3$ Potts model has low quality, the solid line corresponds to $c = 0.86 \pm 0.19$, this was obtained by retaining only the four largest $W$ values.

**D. Continuous systems**

The method we have presented can to some extent also be applied to systems with a continuous energy distribution, however for these systems the full normalisation of $g(\epsilon)$ is difficult. The method used to normalise $g(\epsilon)$ for discrete systems so far require that (i) the ground-state is sampled, and (ii) that the histograms have sufficient overlap. For a system with a truly continuous energy distribution sampling of the ground-state requires $T \equiv 0$, and this will generate histograms without overlap. Even for models with a very small energy gap, like e.g. the $Z_q$ model for large $q$ a large fraction of the computational resources must be spent close to the ground state to ensure that both the conditions are met. Attempts to generalise the Wang Landau histogram sampling to continuous systems are faced with essentially the same problems.

Due to the problems with normalisation we must generally content with a function $\ln g(\epsilon) = \ln g(\epsilon) + C$ where $C$ is an unknown, dimensionless constant. This will induce a linear error $\Delta F(T) = -T \ln C$ in the free energy, but since Eq. \ref{eq:15} is independent of $C$ all remaining thermodynamics will be unaffected by the incomplete normalisation.

The $Z_q$ clock model is a planar spin model where the real angle $\phi \in [0, 2\pi]$ is approximated with the discrete variable $\theta_i = i2\pi/q$, in the limit $q \to \infty$ the converges to the XY model. Numerical simulations of the XY model are customarily done using the $Z_q$ model with $q$ “large enough”, values of $q = 32$ or 64 are often used. Furthermore it has been shown that already at $q = 5$ the critical properties are governed by the XY critical point. To learn about the behaviour $g(\epsilon)$ for continuous systems we have done a short simulation of a $32 \times 32$ system for the $Z_q$ model with $q = 2048$, according to the discussion above this should with a good capture the properties of the continuous $q \to \infty$ system. Fig. 8 shows $\ln g(\epsilon)$ for the $Z_q$ model with $q = 2048$ along with the Ising model.

For the $Z_q$ model the lowest lying of the sampled states has energy $\epsilon_-$, hence the $Z_q$ curve in Fig. 8 terminates at this $\epsilon$ value. This means that $g(\epsilon)$ is undetermined in the interval $[\epsilon_0, \epsilon_-]$, where $\epsilon_0 = -2L^d$ is the ground-state energy. Furthermore overall normalisation is impossible to determine, and we have just arbitrarily fixed $\ln g(\epsilon_-) = 0$. According to Eq. \ref{eq:15} internal energy and specific heat depend only on the shape of $\ln g(\epsilon)$, and not possible vertical offset. Combined with the knowledge from pre-
vious simulations: that the $Z_g$ model for large $q$ correctly captures the thermodynamics of the XY model, we can conclude that apart from the vertical offset Fig. 8 is a faithful representation of $g(\epsilon)$ for the continuous XY model. Looking at Fig. 8 the most striking features are (i) $g(\epsilon)$ is orders of magnitude larger for the $Z_g$ model than the Ising model, and (ii) the steep sloop of $\ln g(\epsilon)$ for the $Z_g$ model; actually any gap-less model must have $\lim_{\epsilon\to 0} \partial_\epsilon g(\epsilon) \to \infty$ to produce a finite value for $C_V(T)$ in the limit $T \to 0$.

In section IV E we will reanalyse a real dataset from a large scale simulations of the Ginzburg Landau model, this constitutes a real example of a continuous system.

E. Reanalysing Ginzburg Landau results

The Ginzburg Landau (GL) model is one of the most studied models physics, and it is applied as 'meta-model' in a wide range of fields, see Ref. [35] for an extensive list of applications. In dimensionless form, the continuum version of the model is given by the functional integral

$$Z = \int \mathcal{D}A \mathcal{D}\phi \exp\left[ -\int d^dx \left( \frac{1}{4} F^\mu_\nu \phi_{\mu\nu} + |(\partial_\nu + iA_\nu)\phi|^2 + y|\phi|^2 + x|\phi|^4 \right) \right].$$ (16)

Due to the difficulties mentioned in section IV D, we are not able to calculate the overall normalisation $g_0$ of $g(\epsilon)$, nevertheless $g(\epsilon)$ shows the critical behaviour discussed in section IV E, and the behaviour of $F(y)$ clearly separates between first and second order transitions. F

In conclusion we feel that in the application to the GL model the method has proved itself, and furthermore that it provides interesting information even tough $g_0$ cannot be determined.

Software to go through the steps described in sections III and IV can be down-loaded as a c library from the authors web-site http://www.ii.uib.no/~hove/libdos/

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FIG. 9: The upper part shows the free energy $F(\beta)$, although it is rounded we can clearly see the remnants of a cusp in $F(\beta)$. The thin ticks on the $x$ axis indicate the couplings which where used. The central figure shows $\ln g(\epsilon)$, the dashed lines indicate the two meta-stable energy levels $\epsilon_1$ and $\epsilon_2$. In the lowest figure we have plotted $\ln g(\epsilon) - \hat{g}(\epsilon)$, where $\hat{g}(\epsilon)$ is a fit to a straight line on the interval $\epsilon_1 < \epsilon_2$. Although not very prominent, the structure in this plot is significant, see the discussion at the end of section IV B. The results come from a simulation of a system of $40 \times 40 \times 40$ lattice units.

FIG. 10: The two upper panels show the same as Fig. 9 for a second order transition. The lower panel shows $\partial^2 \ln g(\epsilon)$, and we can see that this approaches zero at the critical energy $\epsilon_c \approx 4600$, this can be compared to Fig. 3.