M.Sc. Physics of Complex Systems

Stochastic Simulation Methods

Numerical determination of the phase diagram for the ϕ^4 model

Course
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1 Introduction

One of the most used models for the study of phase transition and critical phenomena is the so called ϕ^4 model, which is nothing but a classical continuum scalar field, $\phi(\boldsymbol{r})$, fulfiling the following Hamiltonian

$$\beta H = \int \mathrm{d}\boldsymbol{r} \left[\frac{-b}{2}\phi^2 + \frac{u}{4}\phi^4 + \frac{K}{2}\left(\boldsymbol{\nabla}\varphi^2\right) \right] \tag{1.1}$$

In this work the model will be studied numerically in the so called displacive limit, which correspond to the limit $b, u \to 0$ of the above equation. Thus, the method used at the present work is appropriate for small values of the parameters u and b.

2 The model

For the numerical study we will consider a square lattice in d dimensions whose sites will be scalar fields $\{\Phi_i\}$, $i = 1, ..., N$. The spacing of the lattice is considered to be the unit so the Hamiltonian od the discretised model is given by

$$\beta H\left\{\Phi_i\right\} = \sum_i \left[-\frac{b}{2}{\Phi_i}^2 + \frac{u}{4}{\Phi_i}^4 + \frac{K}{2}\sum_{\mu=1}^{d}\left(\Phi_{i\mu} - \Phi_i\right)^2 \right] \tag{2.1}$$

so that the equilibrium properties of the system will be obtained from the partition function

$$Z(b, u, K) = \sum_{\{\Phi_i\}} e^{-\beta H\{\Phi_i\}} = \int_{-\infty}^{\infty} \left[\prod_{i=1}^{N} \mathrm{d}\Phi_i \right] e^{-\beta H\{\Phi_i\}} \tag{2.2}$$

Note that the first sum of Eq. (2.1) runs over all the sites of the d-dimensional lattice, $N = L^d$ being L the lattice length, while the second sum runs over the nearest neighbours of each site i. Note that one of the parameters in the above Hamiltonian is redundant, as it can be absorbed in the definition of the field variables, so some parametrization can be applied. Here we'll consider the following simple and for general purpose parametrization

$$\varphi = K^{1/2}\Phi \qquad \theta = b/K \qquad \chi = u/K^2 \tag{2.3}$$

so that the Hamiltonian can be written as follows considering periodic boundary conditions

$$\beta H\left\{\varphi_i\right\} = \sum_i \left[\left(d - \frac{\theta}{2}\right){\varphi_i}^2 + \frac{\chi}{4}{\varphi_i}^4 \right] - \sum_{\langle ij \rangle} \varphi_i \varphi_j$$

Note that the Hamiltonian splits naturally as the sum of a local part and an interaction part, which will be useful in our simulations.

3 Numerical methods

As said before, in order to obtain the equilibrium properties of the system we need to compute the partition function, as the average of any desired quantity to compute is given, in the canonical ensemble, by

$$\langle G(\boldsymbol{x})\rangle = \frac{1}{M}\sum_{i=1}^{M} G(x_i)P(x_i) = \frac{1}{M}\sum_{i=1}^{M}\frac{G(x_i)e^{-\beta H(x_i)}}{Z} \tag{3.1}$$

In this work we'll do so by generating field configurations using the heat-bath Monte Carlo method. A new field at site i is generated with a probability density function $P_{\theta,\chi}(\varphi_i)$ depending on the states of its neighbours as

$$P_{\theta,\chi}(\varphi_i) = \frac{\exp\left[-(d-\theta/2)\,\varphi_i^2 - \frac{\chi}{4}\varphi_i^4 + \varphi_i \sum_u \varphi_{iu}\right]}{\int_{-\infty}^{\infty} \mathrm{d}\varphi_i \exp\left[-(d-\theta/2)\,\varphi_i^2 - \frac{\chi}{4}\varphi_i^4 + \varphi_i \sum_u \varphi_{iu}\right]} \tag{3.2}$$

Here we can see that the denominator of the above expression is nothing but the normalisation constant of the probability density function, which in fact we already knew from statistical mechanics. Then, by doing the following change of variables

$$a = d - \theta/2 \qquad b = \chi/4 \qquad c = \sum_u \varphi_{iu} \tag{3.3}$$

we realise that the above ugly expression can be written as follows

$$P_{\theta,\chi}(\varphi_i) = \frac{f(\varphi_i)}{\int_{-\infty}^{\infty} \mathrm{d}\varphi_i f(\varphi_i)} \qquad \text{where} \quad f(\varphi_i) = f_1(\varphi_i) f_2(\varphi_2) = \frac{1}{\sqrt{2\pi/a}} e^{-a(\varphi_i - c/2a)^2} \cdot e^{-b{\varphi_i}^4}$$

so that it is the product of a Gaussian distribution of mean $\mu = c/2a$ and variance $\sigma^2 = 1/2a$ and an exponential distribution. Then, to sample the distribution $f(\varphi_i)$ we can make use of a rejection method, as the Gaussian part can be generated exactly and the exponential part is bounded between 0 and 1. In this work we use the Ziggurat algorithm [1] to generate the Gaussian part and our random number generator is a Mersenne Twister. Then, the procedure to sample the distribution runs as follows

1. Generate a Gaussian distributed number ξ with the mean and variance specified above.
2. Generate another random number uniformly distributed between 0 and 1.
3. While $\eta > f_2(\xi)$ we return to 1. and make a new proposal.
4. When $\eta < f_2(\xi)$ we accept the proposal and φ_i takes the value of ξ.

So, in essence, we are sampling the pdf with a rejection method without repetition. To evolve the system in time we run the lattice in a sequential fashion applying the heat-bath Monte Carlo method at each time step. Note that this method assumes that u is positive and then it is constrained to θ values that accomplish $\theta < 2d$ (as the Gaussian variance has to be positive), condition fulfilled in the displacive limit object of our study.

Finally, in order to obtain accurate estimates for the different quantitites computed in the simulations we have applied the Ferrenberg and Swendsen extrapolation technique. Introducing the following notation

$$M_0 = \sum_i \varphi_i \quad M_1 = \sum_i {\varphi_i}^2 \quad M_2 = \sum_i {\varphi_i}^4 \quad M_3 = \sum_i \sum_{\mu=1}^{d} \left(\varphi_{i\mu} - \varphi_i\right)^2 \tag{3.4}$$

it can be shown that the probability density function for a point (θ', χ') in the parameter space can be determined from the known probability distribution function of another point $(\theta,\, \chi)$ in the parameter space as follows [2]

$$P_{\theta',\chi'}(M_i) = \frac{P_{\theta,\chi}(M_i) \exp\left[\frac{\theta'-\theta}{2} M_1 - \frac{\chi'-\chi}{4} M_2\right]}{\int \mathrm{d}M_1 \mathrm{d}M_2 P_{\theta,\chi}(M_i) \exp\left[\frac{\theta'-\theta}{2} M_1 - \frac{\chi'-\chi}{4} M_2\right]}$$

In this work we will be simulating a point for each of the χ considered and then extrapolating to different θ values with this extrapolation technique, so that the formula is simplifies to

$$P_{\theta',\chi}(M_i) = \frac{P_{\theta,\chi}(M_i) \exp\left[\frac{\theta'-\theta}{2} M_1\right]}{\int \mathrm{d}M_1 P_{\theta,\chi}(M_i) \exp\left[\frac{\theta'-\theta}{2} M_1\right]} \tag{3.5}$$

For efficiency reasons, the Ferrenberg and Swendsen technique will be applied in a way that the average of the desired quantities will be directly extrapolated to other points in the parameter space. It is easy to see that we can compute the average of a function at a new point in the parameter space as [2]

$$\langle G(M_i)\rangle_{\theta',\chi} \approx \frac{1}{N}\sum_{k=1}^{N} G(M_i^{(k)}) P_{\theta',\chi}(x_k) = \frac{1}{N}\sum_{k=1}^{N} G(M_i^{(k)}) \frac{P_{\theta,\chi}(M_i)\exp\left[\frac{\theta'-\theta}{2}M_1\right]}{\int \mathrm{d}M_1 P_{\theta,\chi}(M_i)\exp\left[\frac{\theta'-\theta}{2}M_1\right]} \tag{3.6}$$

Then, all the quantities that we are interested in can be computed from the M_i, $i = 0, 1, 2, 3$ values defined above. In essence, magnetisation and energy are computed as follows

$$M = \langle |M_0| \rangle \qquad E = \left\langle \frac{\theta}{2}M_1 + \frac{\chi}{4}M_2 + \frac{1}{2}M_3 \right\rangle \tag{3.7}$$

while susceptibility and specific heat can be computed from their fluctuations

$$\kappa = \left(\langle M^2\rangle - \langle M\rangle^2\right)/N \qquad C = \left(\langle E^2\rangle - \langle E\rangle^2\right)/N \tag{3.8}$$

The bad news about this amazing extrapolation technique is that, in practice, it fails for points in the parameter space enough far from each other, as the statistical error is too big [2]. Then we use a rule of thumb to determine the range of θ to extrapolate without large statistical errors [3]

$$\Delta\theta < \frac{2}{\sigma(M_1)} \tag{3.9}$$

which ensures that the exponentials in the extrapolation formula do not take any large value. Moreover, note that $\sigma(M_1)$ will increase with the increase of the system size, so that $\Delta\theta$ decreases with increasing L as $\Delta\theta \sim L^{-1/\nu}$ [3].

4 Results

In this study different system sizes and different values of the χ parameter have been considered. In particular, $L = 50, 60, 70, 80, 90, 100$ and $\chi = 1.0, 0.7, 0.5, 0.25, 0.1, 0.05, 0.01$.

For a given value of the parameters (θ, χ), N_0 lattice updates have been considered to thermalise the system. Then, N_m equilibrium configurations have been measured every N_u lattice updates, considered in order to increase the statistical independence of the equilibrium configurations. The initial values of the fields on the lattice sites are set equal to the mean-field equilibrium value $\varphi_{MF} = (\theta/\chi)^{1/2}$. The particular values of N_0, N_u depend on the system size L and they are summarised along with the used N_m values in Table 1. To determine the thermalisation steps to use and the optimal lattice updates between measures a preliminary study has been done. We know that the optimal number of lattice updates, N_u between measures is given by the following relation [4]

$$N_u = \sqrt{\frac{2\tau t_1}{t_2}} \tag{4.1}$$

where t_1 correspond to the update time and t_2 to the measure time, and that the number of steps to thermalise the system should be

$$N_0 \gg \tau \tag{4.2}$$

where τ is in both equations the correlation time of, for instance, the magnetisation of the system.

Then, the dependence of τ with the system size has been computed and this allow us to choose a proper number of thermalisation steps and compute the optimal lattice updates within measures. This dependence is shown graphically and quantitatively in Fig. 1

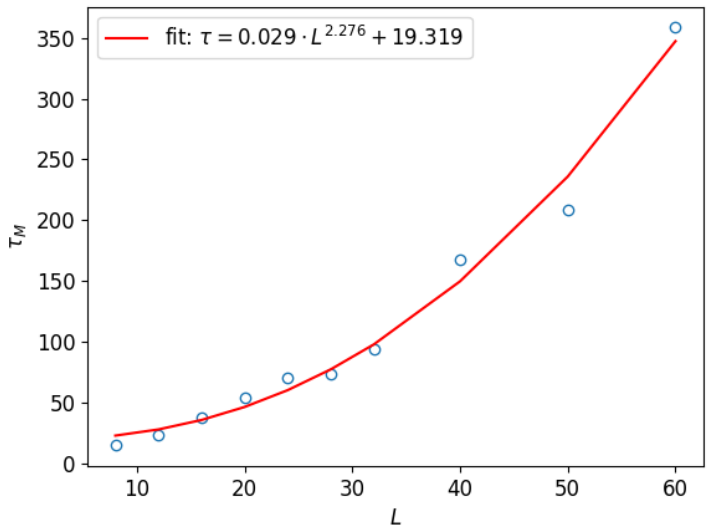


Figure 1: Dependence on τ with the system size L

We see that for our larger system size the correlation time is $\tau \sim 10^3$ so that a thermalisation of $N_0 \sim 100\tau$ should be sufficient.

Table 1: Simulation details

L	50	60	70	80	90	100
N_0	10^5	10^5	10^5	10^5	10^5	10^5
N_u	15	15	20	25	30	30
N_m	10^6	10^6	10^6	10^6	10^6	10^6

Before starting the long runs we have to make sure that the extrapolation technique works. To do so, two different but close points were simulated and then an extrapolation was performed from both points. The fact that the extrapolated values of θ agree within the statistical errors, as can be seen in Fig. 3, give support to the validity of the extrapolation scheme.

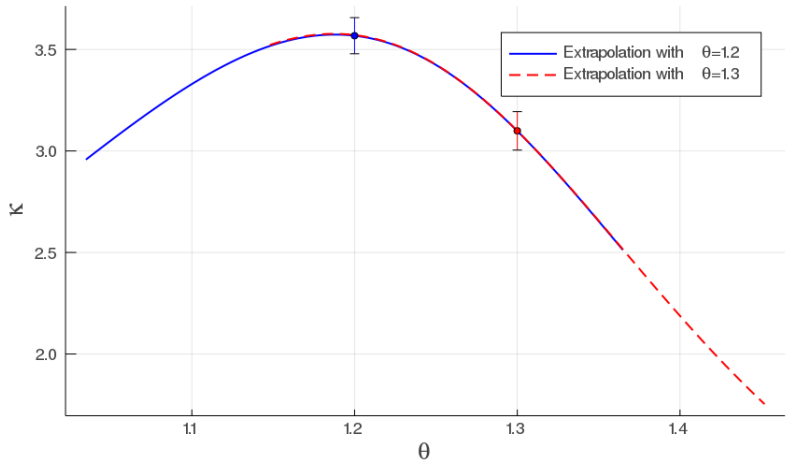
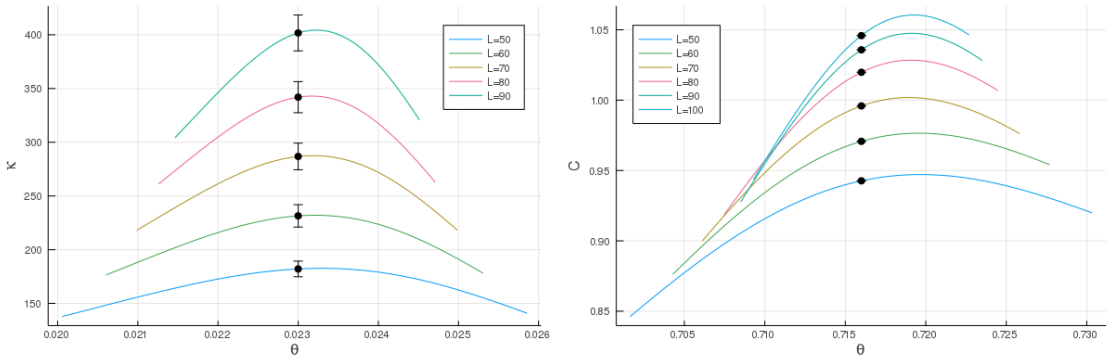


Figure 2: Extrapolation of the susceptibility from two close θ points at $\chi = 1.0$ in a system of size $L = 8$.

Now we directly show a sample of the results obtained for the susceptibility and specific heat each for a different value of χ.



(a) Susceptibility for $\chi = 0.01$

(b) Specific heat for $\chi = 0.5$

Figure 3: Two examples of the extrapolated values for susceptibility and specific heat

As we can see the maximums ob both susceptibility and heat capacity tend to a particular value θ_c. We know that at the critical value this quantities should diverge but strictly speaking this only happens in an infinite system. For a finite system we observe maxima that sharpen and their location shifts with increasing L towards the asymptotic value $\theta_c = \theta_c(L = \infty)$. Finite size scaling theory provides a way in which the infinite limit can be recovered. In particular we know that $\theta_c(L)$ should tend to θ_c as

$$\theta_c^i(L) = \theta_c + a_i L^{1/\nu} + b_i L^{-\omega} + \cdots \tag{4.3}$$

where the index i stands for susceptibility and heat capacity, as both should tend to the same critical value of θ; ν is the critical behaviour of the correlation length ($\nu = 1$ in $d = 2$) and the rest are higher order corrections to the leading scaling term. Then, it is clear that we have to fit Eq. (4.3) but this is not free of problems. Typically $\omega = 3/4$ when $\nu = 1$ but as we move to the displacive limit the exponent ν is expected to jump to its mean-field value $\nu = 1/2$. Thus, we have considered two methods to determine the critical parameter θ_c:

A) We have plotted $\theta_c(L)$ vs $1/L$ and allowed a linear extrapolation towards the origin ($L = \infty$) by fitting the last few points. This is not very precise but provides some graphical support. An example for some values of χ can be seen in Fig. 4.

B) We have considered Eq. (4.3) with $\nu = 1/2$ and ω as a variable parameter between 1 and 2. This method is much more precise and the dispersity of the fitted values θ_c as ω varies allows us to give errors to θ_c. The obtained values are summarised in Table 2 and will be used later to plot the phase diagram of the system.

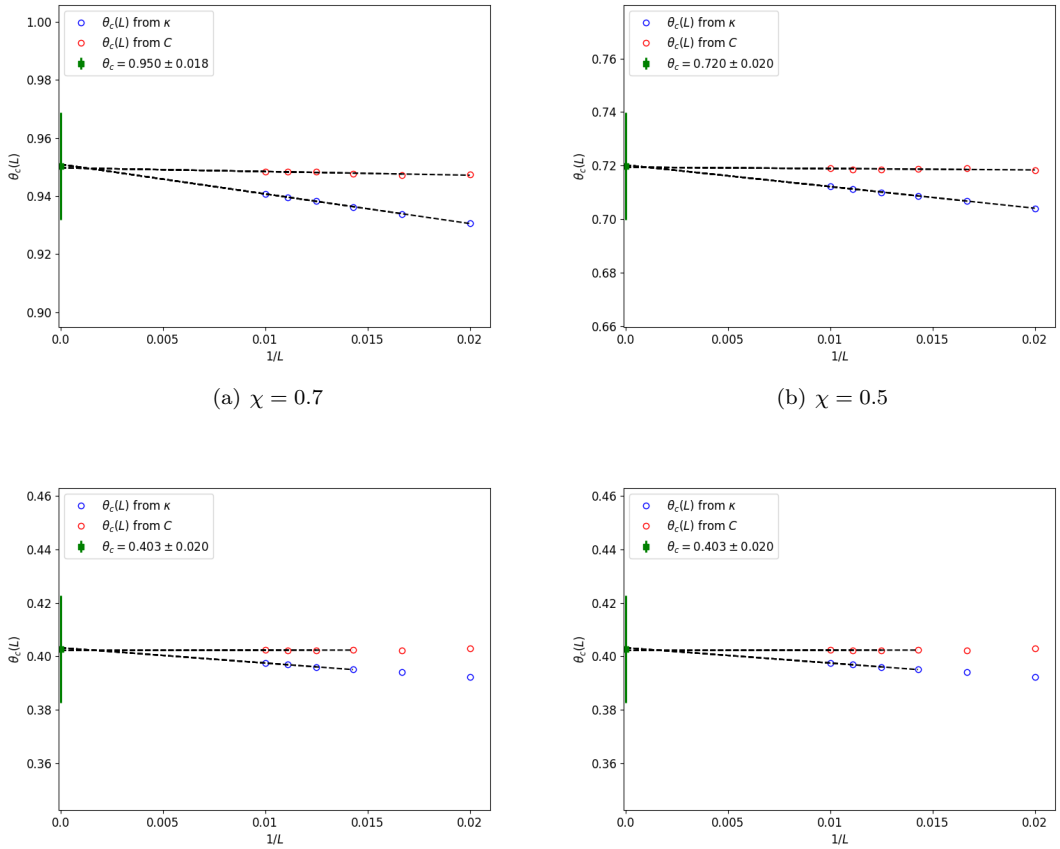
C) Finally, to five further support to the assigned values of θ_c a finite size scaling test has been performed. We know that several quantities, for instance magnetisation, should have a scaling behaviour of the form

$$m(\theta, L) = L^{\beta/\nu} f(tL^{-1/\nu}) \tag{4.4}$$

As the ϕ^4 model belongs to the same universality class of the Ising model the critical exponents will be that of the Ising model and clearly here $t = 1 - \theta/\theta_c$. We have also considered the scaling behaviour of the fourth order cumulant, $\rho = 1 - \dfrac{\langle M^4 \rangle}{3 \langle M^2 \rangle^2}$, given by

$$\rho(\theta, L) = f(tL^{-1/\nu}) \tag{4.5}$$

First of all we should note that the values obtained for the critical coupling by both A) and B) methods agree within errors. Then, the finite size scaling behaviour of the commented quantities seems to hold for the different values of the system size considered here, but, as we can see in Fig. 5, as χ decreases so it does the quality of the scaling. This is so because as χ tends to the displacive limit the exponents should jump to their mean field values. Moreover, the obtained values for the critical coupling match within errors with the ones obtained previously in [3].



(a) $\chi = 0.7$

(b) $\chi = 0.5$

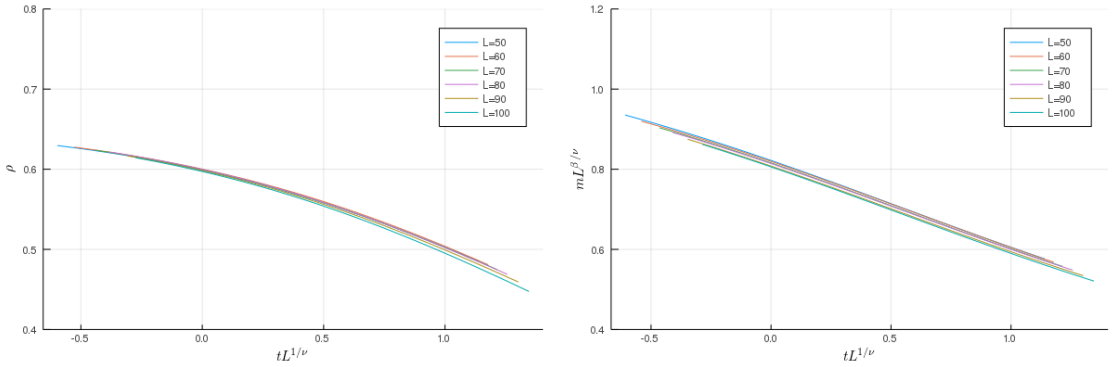
(c) $\chi = 0.25$

(d) $\chi = 0.01$

Figure 4: Determination of the critical coupling value by fitting the last points with a straight line. The green point correspond to the extrapolated θ value at the origin ($L = \infty$) as the average of the extrapolation values obtained considering the maximums in the specific heat and susceptibility.

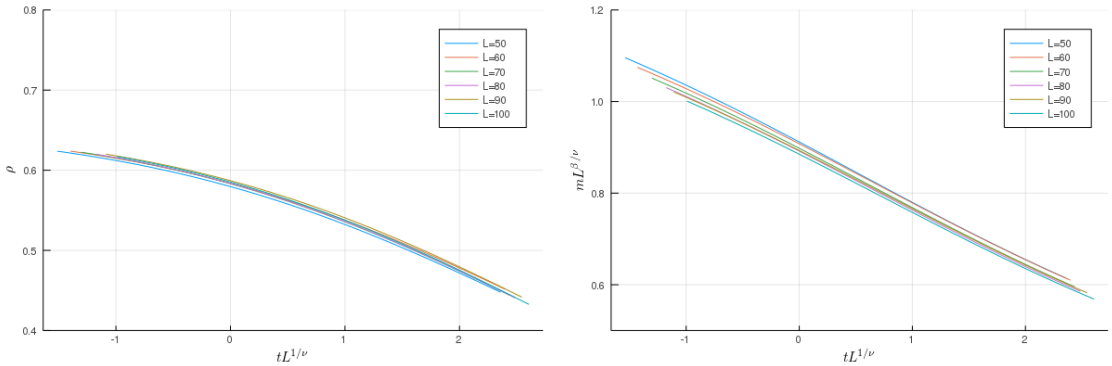
Table 2: Fitted values for θ_c

χ	θ_c
1.0	1.26880(6)
0.7	0.95098(8)
0.5	0.71874(5)
0.25	0.40294(4)
0.1	0.18346(2)
0.05	0.090379(6)
0.01	0.023608(9)



(a) Finite size scaling of ρ for $\xi = 0.7$

(b) Finite size scaling of m for $\xi = 0.7$



(c) Finite size scaling of ρ for $\xi = 0.1$

(d) Finite size scaling of m for $\xi = 0.1$

Figure 5: Caption

To finish with, we present the plot of the phase diagram obtained with the critical coupling values determined in our simulations and summarised in Table 2.

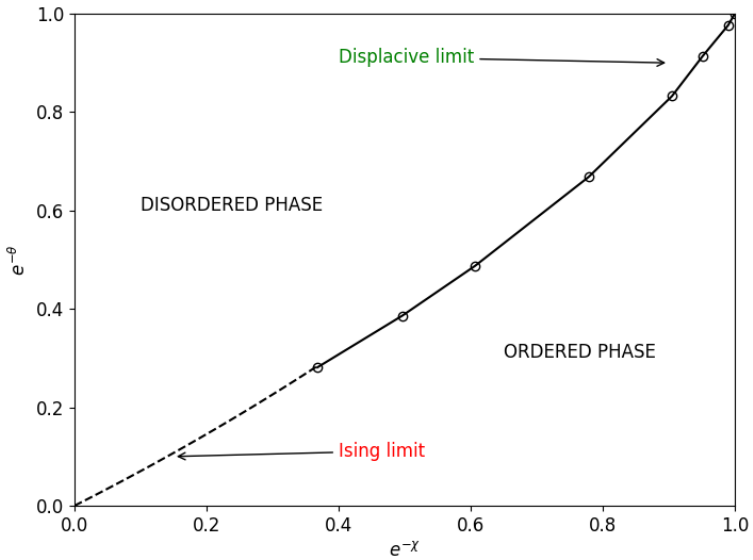


Figure 6: Phase diagram for the model studied in the present work. The dashed line corresponds to a extrapolation through the Ising limit from our data by considering the (0,0) point.

5 Conclusions

We have performed a numerical study of the ϕ^4 model defined in a square lattice in the displacive limit. The algorithm used has been the heat-bath Monte Carlo method implemented with a rejection technique, which has made use of the Ziggurat algorithm to generate Gaussian random numbers with a Mersenne Twister random number generator. Ensemble averages over the generated equilibrium configurations have been combined with the Ferrenberg and Swendsen extrapolation technique to obtain accurate estimates for the magnitudes of interest, such as magnetisation or energy. By studding the finite size behaviour of the susceptibility and specific heat a set of critical points in the parameter space have been determined, which allow us to find the phase diagram of the model.

References

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