

## The Fourier Monte Carlo Approach to Lattice Spin Models

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### Abstract

Recently we have developed a Monte Carlo algorithm for lattice spin systems that relies exclusively on the use of Fourier amplitudes without making any reference to the underlying real-space configurations. This article is devoted to give a comprehensive discussion of the motivation, basic ideas and limits of this algorithm. By analyzing its construction in detail, we explain why our algorithm is of considerable use for solving certain classes of problems that may be computationally too expensive otherwise. Also, we explain how finite size scaling is properly set up to work with the algorithm. © 2010 Published by Elsevier Ltd.

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### 1. Introduction

Modern statistical mechanics aims at giving a complete prediction of macroscopic behavior of real large-scale physical systems. As we all know, this is an ambitious task. On the microscopic level, the word “real” implies the description of such systems by the first principles of quantum mechanics, while “large-scale” implies that an enormous number of these microscopic degrees of freedom may collectively interact, making it hopeless to find any “exact” solutions. A major part (if not all) of statistical mechanics is devoted to the study of “models” of various degrees of abstraction. In fact, a major lesson to be learned from the history of statistical mechanics is that while today’s most sophisticated approaches are designed with the goal to microscopically model a physical system “from first principles” as precisely as possible, intuition and physical understanding can often be gained by stripping down the model’s definition to a bare minimum, in the ideal case ending up with a simplified caricature of the original problem that is nevertheless nontrivial in the sense that it still captures the essential underlying physics. Often, this process of abstraction also reveals sometimes unexpected parallels between seemingly unrelated disciplines of physics. This fact may be best illustrated by e.g. the both elegant and fruitful idea of universality underlying the unifying renormalization group (RG) approaches to problems emerging in statistical mechanics, stochastics and quantum field theory.

Unfortunately, most of these highly idealized but still nontrivial models are – more or less by definition of non-triviality – prohibitively hard to tackle by analytic means. As famous examples like Onsager’s solution of the 2d Ising model, Baxter’s and Lieb’s studies of 2d vertex models or Berlin and Kac’s spherical model demonstrate, an exact solution, while of enormous theoretical importance, can, as a rule, only be found under severe restrictions of e.g. low spatial dimension, or in rather exotic or artificial limiting cases. And even then, the mathematics can be formidable (cf. the impressive collection of calculations gathered in [1]). A closely related strategy that may provide

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additional insight, which in turn often motivates the very definition of a model itself, is that of finding clever analytical or numerical approximation schemes like mean-field theory, perturbative expansions or renormalization group calculations.

Today, computer simulations play an extremely important role on all of these levels of abstraction and approximation. In principle, most simulations of statistical mechanics problems can be divided into molecular dynamics (MD) or Monte Carlo (MC) type of approaches. While MC as well as MD, which is based on solving the underlying equations of motion numerically, is well suited to study continuum systems, in the present article the focus will be on lattice spin systems, for which the MC scheme, which does not rely on any definition of dynamics, is usually the method of choice [2, 3, 4]. MC simulations are generally implemented by defining a set of rules for generating possible “steps” in the space of configurations of the system together with an acceptance/rejection rule of such steps that is designed in such a way that the resulting random walk asymptotically visits configurations according to the predefined probability distribution imposed by the chosen ensemble underlying the simulation.

## 2. Fourier MC algorithm

To set up the basic framework for lattice spin models, we introduce the following nomenclature.  $\Gamma$  denotes a  $d$ -dimensional simple cubic Bravais lattice with a total of  $L^d$  sites, lattice constant  $a$  and periodic boundary conditions. On each site  $\mathbf{x} \in \Gamma$  we place a generalized “spin”  $s(\mathbf{x})$ , whose value will be taken to be real for simplicity. The set  $\mathbf{s} := \{s(\mathbf{x})\}$  then defines a real spin-field configuration. To each such configuration, we assign an energy by means of a Hamiltonian  $\mathcal{H}$ , which should be bound from below for stability reasons. A random walk in configuration space is implemented by choosing a generating scheme of “moves”  $\mathbf{s} \rightarrow \mathbf{s}'$  that assigns to an “old” configuration  $\mathbf{s}$  a “new” or “trial” configuration  $\mathbf{s}'$ . Finally, we choose an ensemble to work with. In our present discussion, we will work in the canonical ensemble, measuring the prescribed temperature  $T$  in units of energy (i.e. putting  $k_B \equiv 1$ ). Acceptance of a move will be most conveniently governed by the well-known *Metropolis rule*, which can be shown to generate a random walk in configuration space that reproduces the probability distribution of the canonical ensemble, provided the moves are chosen to fulfill *ergodicity* and *detailed balance* [2, 3, 4].

Apart from these requirements, it is clear that there is still great freedom to design MC algorithms, and thus questions concerning the optimal design, performance, applicability and error analysis of MC algorithms for particular problems constitute a science of its own. However, an obvious requirement for performance is that the computation of the energy changes associated with each MC move should be computationally “inexpensive” i.e. require only a modest number of operations. Roughly speaking, in real-space implementations, efficient moves are usually “local”, i.e. only change a finite number  $O(1)$ . For models with short-range interactions between lattice sites, this seems to be rather easy to fulfill. Near phase transitions, however, where collective behavior of spins becomes dominant, such local simulation schemes turn out to be quite inefficient due to low acceptance rates and the phenomenon of so-called “critical slowing-down”. To alleviate this difficulty, sophisticated “cluster moves” were invented that allow to change many spins at the same time but still require only a manageable number of operations between successive spin configurations. Without going too much into detail [2, 3, 4], we only note here that generally these schemes also rely on a certain “locality” in the computation of the underlying energy changes.

On the other hand, for models with long-range interactions, we may be in trouble. Suppose that interactions between any two of the  $N = L^d$  sites of the lattice cannot be neglected. Then, changing one spin at site  $\mathbf{x}$  requires  $N - 1 = O(N)$  operations, which is bad news since usually one needs to extrapolate simulation results to the thermodynamic limit. Below, we will encounter this situation in the example of compressible spin models, where the accompanying strain induces long-range interactions. Another source of problems is the possible presence of certain constraints imposed on the system which may restrict the choice of admissible MC moves. The coarse graining (CG) problem, also to be discussed below, is a prominent member of this class. Both situations may be visualized under the following common viewpoint. Suppose that the dependence of Hamiltonian  $\mathcal{H}[\mathbf{s}]$  on  $\mathbf{s}$  is formulated not directly in terms of the individual on-site spins  $s(\mathbf{x})$ , but rather in terms of some collective coordinates built from these spins in the sense that the Hamiltonian has a manageable (“local” i.e. diagonal or almost diagonal) structure only when expressed through these coordinates. Then obviously the favorable candidates for MC moves are those that are formulated directly in terms of this collective coordinates rather than in terms of the original real-space spins.

For translation-invariant systems, the collective coordinates that immediately come to mind are defined by Fourier transformation (FT), as they have the pleasant effect of diagonalizing the harmonic parts of a given Hamiltonian. In

its discrete form on a lattice, the Fourier transform and its inverse are given by

$$\tilde{s}(\mathbf{k}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{x} \in \Gamma} s(\mathbf{x}) e^{-i\mathbf{k}\mathbf{x}}, \quad s(\mathbf{x}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in \Gamma^*} \tilde{s}(\mathbf{k}) e^{i\mathbf{k}\mathbf{x}}. \quad (1)$$

Here,  $\tilde{\Gamma} = \{\frac{2\pi}{aL}\mathbf{z}, \mathbf{z} \in \mathbb{Z}^d\}$  denotes the space of all  $\mathbf{k}$ -vectors that are consistent with periodic boundary conditions,  $\Gamma_* = \{\frac{2\pi}{a}\mathbf{z}, \mathbf{z} \in \mathbb{Z}^d\}$  denotes the set of reciprocal vectors of our original (direct) lattice, and its (first) Brillouin zone is the quotient space  $\Gamma^* := \tilde{\Gamma}/\Gamma_*$  of all  $\mathbf{k}$ -vectors modulo addition of reciprocal vectors. The collection of complex amplitudes  $\tilde{s}(\mathbf{k})$ ,  $\mathbf{k} \in \Gamma^*$  gives an alternative representation of any real-space spin configuration  $s$ . However, in general these amplitudes are *not* independent degrees of freedom! Suppose – just for the sake of the argument – that they were. Then, since the FT diagonalizes any Ising-like Hamiltonian

$$\mathcal{H}[s] = - \sum_{\mathbf{x}, \mathbf{y} \in \Gamma} \frac{J(\mathbf{x} - \mathbf{y})}{2} s(\mathbf{x}) s(\mathbf{y}) = - \sum_{\mathbf{k} \in \Gamma^*} \frac{\tilde{J}(\mathbf{k})}{2} |\tilde{s}(\mathbf{k})|^2 \quad (2)$$

$$\tilde{J}(\mathbf{k}) = \sum_{\mathbf{x}} J(\mathbf{x}) e^{-i\mathbf{k}\mathbf{x}} \quad (3)$$

it seems at first glance that we would have paved the way to immediately solving the Ising model immediately for any dimension! Of course, this is ridiculous. In reality, the restriction  $s^2(\mathbf{x}) = 1$  of the range of spin variables  $s(\mathbf{x} \in \Gamma)$  to be of Ising type yield a set of  $N$  complicated constraints on the collection of possible Fourier amplitudes, which are therefore by no means independent. From this we conclude that Fourier amplitudes are rather useless for encoding MC moves in strict Ising systems.

But what if we relax the Ising condition  $s^2(\mathbf{x}) = 1$  and only require that  $s(\mathbf{x})$  is a real number? In direct space, we then have to deal with  $N$  independent real-valued degrees of freedom. To understand how precisely these are encoded in terms of Fourier amplitudes, let us first introduce the map  $\mathbf{k} \rightarrow \mathbf{k}^*$  on  $\Gamma^*$  which is induced by the reflection  $\mathbf{k} \rightarrow -\mathbf{k}$  about the origin of  $\tilde{\Gamma}$ . For real-valued spins, it is then easy to see that the Fourier amplitudes must satisfy the set of constraints  $\tilde{s}(\mathbf{k}^*) = \tilde{s}^*(\mathbf{k})$ ,  $\mathbf{k} \in \Gamma^*$ . However, for a simple cubic  $d$ -dimensional system, there are exactly  $2^d$  distinct “high-symmetry vectors”  $\mathbf{h} \in \Gamma^*$  for which  $\mathbf{h}^* = \mathbf{h}$ , and consequently the corresponding amplitudes  $\tilde{s}(\mathbf{h})$  must be real-valued, which makes for  $2^d$  real degrees of freedom. In particular, the zero mode  $\tilde{s}(\mathbf{0}) = \sqrt{Nm}$ , which corresponds to the high-symmetry vector  $\mathbf{h} = \mathbf{0}$ , is proportional to the average “magnetization”  $m$  of the system. Assigning a “parity”  $p(\mathbf{k}^{(\pm)}) = \pm 1$  to the remaining  $N - 2^d$   $\mathbf{k}$ -vectors of  $\Gamma^*$  in a convenient way, the residual Brillouin zone can be regrouped into pairs  $(\mathbf{k}^{(+)}, \mathbf{k}^{(-)} = -\mathbf{k}^{(+)})$  of even and odd parity, and the real- and imaginary parts  $\Re \tilde{s}(\mathbf{k}^{(+)})$ ,  $\Im \tilde{s}(\mathbf{k}^{(+)})$  of the positive parity modes can now be taken to represent the remaining  $2 \times (N - 2^d)/2 = N - 2^d$  independent real degrees of freedom in Fourier representation.

However, now that we have abandoned the Ising constraint, the above Ising Hamiltonian has to be complemented by additional terms that guarantee convergence of the related canonical partition function. In fact, if we want to stay inside the Ising universality class, we are forced to pass to the equally well-known  $\phi^4$  model, defined by the Hamiltonian

$$\mathcal{H}[s] = - \sum_{\mathbf{x}, \mathbf{y} \in \Gamma} \frac{J(\mathbf{x} - \mathbf{y})}{2} s(\mathbf{x}) s(\mathbf{y}) + \sum_{\mathbf{x} \in \Gamma} \Phi(s(\mathbf{x})) \quad (4)$$

in which a so-called *on-site potential*

$$\Phi(s) := \frac{\tilde{A}_2}{2} s^2 + \frac{s^4}{4} \quad (5)$$

has been added to the lattice interaction energy. For later convenience, we switch to the dimensionless representation

$$\beta \mathcal{H}[s] = - \sum_{\mathbf{x}, \mathbf{y} \in \Gamma} \frac{K(\mathbf{x} - \mathbf{y})}{2} s(\mathbf{x}) s(\mathbf{y}) + \sum_{\mathbf{x} \in \Gamma} \left( \frac{\tilde{a}_2}{2} s^2(\mathbf{x}) + \frac{\beta}{4} s^4(\mathbf{x}) \right) \quad (6)$$

where  $K(\mathbf{x}) := \beta J(\mathbf{x})$ ,  $a_2 := \beta A_2$  and of course  $\beta = 1/T$ . From the FT point of view, while the harmonic part

$$\beta \mathcal{H}^{(2)}[s] := \frac{1}{2} \sum_{\mathbf{k}} D(\mathbf{k}) \tilde{s}(\mathbf{k}) \tilde{s}(\mathbf{k}^*), \quad D(\mathbf{k}) := \tilde{a}_2 - \tilde{K}(\mathbf{k}) \quad (7)$$

of this Hamiltonian is again readily diagonalizable, the anharmonic part

$$\beta \mathcal{H}^{(4)}[s] = \frac{\beta}{4N} \sum_{\mathbf{k}_1, \dots, \mathbf{k}_4} \tilde{s}(\mathbf{k}_1) \dots \tilde{s}(\mathbf{k}_4) \Delta(\mathbf{k}_1 + \dots + \mathbf{k}_4), \quad (8)$$

of this potential seems to express a “law of conservation of difficulty”, which manifests itself in the appearance of the lattice Kronecker delta

$$\Delta(\mathbf{k}) = \frac{1}{N} \sum_{\mathbf{x} \in \Gamma} e^{i\mathbf{k}\mathbf{x}} = \begin{cases} 1, & \mathbf{k} \in \Gamma_* \\ 0, & \text{else} \end{cases} \quad (9)$$

In other words, to actually compute the energy of configuration encoded in terms of the Fourier amplitudes  $\tilde{s}(\mathbf{k})$ , one must perform a sum over all possible mode contributions belonging to combinations of four representatives of Brillouin zone vectors that add up to a reciprocal lattice vector. Needless to say that even for modest system sizes this represents an enormous number of possibilities that is hopeless to enumerate in practical applications. Clutching at straws, we note that actually a MC simulation does not require to compute the total energy at each move, but only the *energy change* accompanying it (an observation that will nevertheless soon prove to be useful). However, even the total change of  $\beta \mathcal{H}^{(4)}[s]$  under a shift of a single amplitude takes  $O(N^3)$  operations, which means that such computations are out of the question for any serious application. Of course, we could go back to real space by means of the fast Fourier transformation, which is known to be of order  $O(N \ln N)$ , but what advantage would that give us over a “native” real-space algorithm?

It seems that the above obstacles have prevented Fourier MC simulations until recently. What is the way out? Given some thought, the question arises if – by clever storing, tabulating and bookkeeping of certain information on the present configuration – it would be possible to reduce the number of operations necessary to calculate energy changes, possibly at the expense of some additional memory consumption. Indeed, for each given spin configuration  $s = \{s(\mathbf{x})\}_{\mathbf{x} \in \Gamma}$ , consider the associated *squared* spin configuration

$$\mathbf{S} \equiv \{S(\mathbf{x})\}_{\mathbf{x} \in \Gamma} := \{s^2(\mathbf{x})\}_{\mathbf{x} \in \Gamma} \quad (10)$$

In the case of Ising spins,  $\mathbf{S}$  would of course be trivial. However, for real-valued spins,  $\mathbf{S}$  can be thought of a special (non-negative) spin distribution on the lattice. As such, we can also define its Fourier transform in a standard way:

$$\tilde{S}(\mathbf{k}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{x} \in \Gamma} S(\mathbf{x}) e^{-i\mathbf{k}\mathbf{x}}, \quad S(\mathbf{x}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in \Gamma^*} \tilde{S}(\mathbf{k}) e^{+i\mathbf{k}\mathbf{x}}. \quad (11)$$

Inserting the Fourier transform for  $s(\mathbf{x})$ , an easy calculation now yields the relation

$$\tilde{S}(\mathbf{q}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in \Gamma^*} \tilde{s}(\mathbf{k}) \tilde{s}(\mathbf{q} + \mathbf{k}^*) \quad (12)$$

between  $\tilde{S}(\mathbf{q})$  and  $\tilde{s}(\mathbf{k})$ , where we used the important orthogonality relations

$$\sum_{\mathbf{x} \in \Gamma} e^{\pm i\mathbf{x}\mathbf{k}} = N \delta_{\mathbf{k}, \mathbf{0}}, \quad \sum_{\mathbf{k} \in \Gamma^*} e^{\pm i\mathbf{x}\mathbf{k}} = N \delta_{\mathbf{x}, \mathbf{0}} \quad (13)$$

and the notation  $[\mathbf{q} + \mathbf{k}^*] \in \Gamma^*$  to denote the member of the Brillouin zone equivalent to the vector  $\mathbf{q} - \mathbf{k}$  up to a reciprocal vector. The reason for introducing  $\mathbf{S}$  is simple. Observe the trivial fact that  $s^4(\mathbf{x}) = (s^2(\mathbf{x}))^2 = S^2(\mathbf{x})$ . But then Parseval’s theorem implies that  $\sum_{\mathbf{x} \in \Gamma} s^4(\mathbf{x})$  is *diagonal in terms of the amplitudes*  $\tilde{S}(\mathbf{k})$ :

$$\sum_{\mathbf{x} \in \Gamma} s^4(\mathbf{x}) = \sum_{\mathbf{x} \in \Gamma} S^2(\mathbf{x}) = \sum_{\mathbf{k} \in \Gamma^*} \tilde{S}(\mathbf{k}) \tilde{S}(\mathbf{k}^*) \quad (14)$$

In which way does this help? Suppose that we choose one of the “original” spin amplitudes,  $\tilde{s}(\mathbf{k}_0)$ , say, and shift it by a certain complex number  $\epsilon$ . Of course, we must then shift  $\tilde{s}(\mathbf{k}_0^*)$  by the complex conjugate value  $\epsilon^*$ , such that the actual effect on this “move” on the total configuration of Fourier amplitudes is

$$\delta \tilde{s}(\mathbf{k}) := \epsilon \delta_{\mathbf{k}, \mathbf{k}_0} + \epsilon^* \delta_{\mathbf{k}, \mathbf{k}_0^*}, \quad \mathbf{k}_0 \in \Gamma_s^* \quad (15)$$

As an easy calculation shows, under such a move the modes of the squared spin configuration  $\mathbf{S}$  then change according to

$$\begin{aligned} \delta \tilde{S}(\mathbf{q}) = & \frac{1}{\sqrt{N}} \left( 2\epsilon \tilde{s}([\mathbf{q} - \mathbf{k}_0]) + 2\epsilon^* \tilde{s}([\mathbf{q} + \mathbf{k}_0]) \right. \\ & \left. + \epsilon^2 \delta_{[\mathbf{q}-2\mathbf{k}_0], \mathbf{0}} + 2|\epsilon|^2 \delta_{\mathbf{q}, \mathbf{0}} + \epsilon^{*2} \delta_{[\mathbf{q}+2\mathbf{k}_0], \mathbf{0}} \right) \end{aligned} \quad (16)$$

and we note that for each given vector  $\mathbf{q}$  this takes just  $O(1)$  operations to compute. But in computing the change

$$\delta \mathcal{H}_4 = \sum_{\mathbf{q} \in \Gamma_s^*} \delta \mathcal{H}_4(\mathbf{q}) \quad (17)$$

of the quartic contribution to the Hamiltonian, we only need to work out

$$\delta \mathcal{H}_4(\mathbf{q}) = \frac{1}{4} \left[ \tilde{S}(\mathbf{q}^*) \delta \tilde{S}(\mathbf{q}) + \delta \tilde{S}(\mathbf{q}^*) \tilde{S}(\mathbf{q}) + \delta \tilde{S}(\mathbf{q}^*) \delta \tilde{S}(\mathbf{q}) \right] \quad (18)$$

for each  $\mathbf{q}$ , which adds up to  $O(N)$  operations altogether to compute the energy change resulting from the anharmonic part of the Hamiltonian. We are thus left with computing the shift of the harmonic part of the Hamiltonian under a move of type (15). For this, we easily obtain

$$\delta \mathcal{H}_2 = 2\tilde{D}(\mathbf{k}_0) \left[ \Re(\epsilon \tilde{s}(\mathbf{k}_0^*)) + (\Re \epsilon)^2 \delta_{\mathbf{k}_0, \mathbf{k}_0^*} + \left(1 - \delta_{\mathbf{k}_0, \mathbf{k}_0^*}\right) \frac{|\epsilon|^2}{2} \right] \quad (19)$$

It is also clear that the above algorithm is ergodic and satisfies detailed balance [10].

### 3. Scope and Limits

Summarizing the given line of arguments, for the  $\phi^4$ -model we succeeded in constructing an algorithm which is based exclusively on the use of Fourier amplitudes and requires at most  $O(N)$  steps for each move. The  $\phi^4$  model and its properties are very well known. Does our algorithm allow for generalizations? In fact, the above ideas are easily modified to cover more general cases. For instance, a corresponding algorithm can obviously be constructed for a fourth order term of the “*generalized squared-square*” structure

$$\mathcal{H}^{(4)} \sim \sum_{\mathbf{k}} A_4(\mathbf{k}) \tilde{F}(\mathbf{k}) \tilde{F}(-\mathbf{k}) \quad (20)$$

with

$$\tilde{F}(\mathbf{k}) \sim \sum_{\mathbf{q}} R(\mathbf{p}, \mathbf{q}) \tilde{s}(\mathbf{q}) \tilde{s}(\mathbf{k} - \mathbf{q}) \quad (21)$$

Also, fourth order terms built from products of multicomponent order parameters of any prescribed internal symmetry pose no problem in principle.

On the other hand, we should stress that the presence of a sixth (or higher) order term of type  $\sum_x s^6(x)$  presents a serious obstacle to the present algorithm, as its updates under MC moves of type (15) require up to  $O(N^2)$  operations. Somewhat related is the mentioned impossibility to apply it to strict Ising systems, which is quite regrettable as this also excludes applications to rigid or compressible lattice gas models. However, the Ising model results might be recovered from  $\phi^4$  simulations in the order-disorder limit  $J \rightarrow 0$  after proper rescaling of spins (cf. Ref. [5]).

### 4. Subspaces of the Brillouin zone

So, let's compare. As many existing algorithms show, locality in real space often allows for algorithms which are even  $O(1)$ , while long-range interactions may require an effort of  $O(N)$ . Obviously, at least for systems with short

range interactions, our Fourier MC algorithm is likely to be outperformed by standard real-space methods. So, what is it actually good for?

As noted in the introduction, the algorithm really begins to show its advantages when applied to problems where summations are not running over all  $\mathbf{k} \in \Gamma^*$  but are confined to certain subspaces of the Brillouin zone. In other words, there are certain problems for which only those amplitudes  $\tilde{s}(\mathbf{k})$ , whose  $\mathbf{k}$ -vectors are inside a given subspace  $\Gamma_s^* = \{\mathbf{k}_1, \dots, \mathbf{k}_{n_s}\}$ , which we will call the “active” part of the Brillouin zone, are allowed to take on nonzero values during the course of the simulation. Of course, the structure of this set depends on the problem under investigation. In concrete applications, however,  $\Gamma_s^*$  will usually be chosen to be  $*$ -invariant.

In what follows,  $n_s = |\Gamma_s^*| \leq N$  will denote the number of vectors of  $\Gamma_s^*$ . The alert reader will notice that passing from  $s$  to  $S$  will introduce additional  $\mathbf{k}$ -vectors to the problem, since  $S$  may display variations on a shorter length scale than  $s$  (think of  $\sin^2 x$  as compared to  $\sin x$ ). Therefore, the number  $n_S = |\Gamma_S^*|$  of  $\mathbf{k}$ -vectors belonging to the set

$$\Gamma_S^* = \{[\mathbf{p} + \mathbf{q}^*] : \mathbf{p}, \mathbf{q} \in \Gamma_s^*\} \quad (22)$$

may be considerably larger than  $n_s$  and even reach  $n_S = N$  while  $n_s < N$ . Nevertheless, if  $\Gamma_s$  is “small” enough, i.e.  $n_s \ll N$ , we may also have  $n_S \ll N$ . In particular, this can be the case in problems where a *cutoff*  $\Lambda$  is defined in the Brillouin zone. Let us thus suppose that indeed  $n_S \ll N$ , and review the construction of our algorithm. For the convenience of the reader, we summarize the logic of the complete algorithm as well as the number of required operations at each step in the following pseudocode chart:

**procedure** INITIALIZATION:

Initialize  $\tilde{s}(\mathbf{k})$ ;

Initialize  $\tilde{S}(\mathbf{q})$  using Eqn. (12);

▷  $O(n_s n_S)$  operations, required only once

**end procedure**

**procedure** FOURIERMETROPOLIS

**repeat**

Generate move (15);

Calculate  $\Delta\mathcal{H}_2$ ;

▷  $O(1)$  operations

Initialize  $\Delta E = \Delta\mathcal{H}_2$ ;

**for** ( $i = 1$ ;  $i \leq n_S$ ;  $i++$ ) **do**

▷  $O(n_S)$  operations

Calculate  $\delta\tilde{S}(\mathbf{q}_i)$

▷  $O(1)$  operations

Add  $\Delta E += \Delta\mathcal{H}_4(\mathbf{q}_i)$ ;

▷  $O(1)$  operations

**end for**

accept=StandardMetropolisRule( $\Delta E$ );

**if** accept **then**

Update  $\tilde{s}(\mathbf{k}) += \delta\tilde{s}(\mathbf{k})$ ;

▷  $O(1)$  operations

**for** ( $i = 1$ ;  $i \leq n_S$ ;  $i++$ ) **do**

▷  $O(n_S)$  operations

Update  $\tilde{S}(\mathbf{q}_i) += \delta\tilde{S}(\mathbf{q}_i)$ ;

**end for**

**end if**

**until** done

**end procedure**

Finally, let us comment on the memory requirements of the algorithm. Storage of the amplitudes  $\tilde{s}(\mathbf{k})$  requires an array of  $n_s$  complex numbers. The array  $\tilde{S}(\mathbf{k})$  hosts another  $n_S$  complex numbers, so altogether we get away with storage space for less than  $2N$  complex numbers. However, to speed up the algorithm, one may generally need to set up lookup tables to compute the Brillouin zone vectors  $[\mathbf{p} + \mathbf{q}]$  corresponding to  $\mathbf{p} + \mathbf{q}$  up to addition of a reciprocal lattice vector, implying a memory consumption of  $n_s \times n_S \leq N^2$  integers. Also, assuming the structure (20), (21), performance considerations might suggest to also tabulate the values of the coupling constants  $R(\mathbf{p}, \mathbf{q})$ , consuming a similar amount of storage space.

#### 4.1. Coarse Graining

In principle, there are two promising classes of systems, to which our method can be applied, and which are intimately related to each other: *coarse grained* and *critical* systems. Suppose that there is a phase transition in the system, where one of the modes  $\tilde{s}(\mathbf{k}_c)$  becomes unstable under the change of a “driving field”, e.g. temperature. For simplicity, we will assume  $\mathbf{k}_c = \mathbf{0}$ . The modes surrounding our critical mode  $\tilde{s}(\mathbf{0})$  correspond to long wavelength fluctuations, and it is well known that the critical behavior of this transition is dominated by these modes.

Suppose we switch on an external field  $H(\mathbf{x})$  linearly coupled to  $s(\mathbf{x})$  by considering the Hamiltonian

$$\begin{aligned} \beta\mathcal{H}[s, \mathbf{h}] = & - \sum_{\mathbf{x}, \mathbf{y} \in \Gamma} \frac{K(\mathbf{x} - \mathbf{y})}{2} s(\mathbf{x})s(\mathbf{y}) + \sum_{\mathbf{x} \in \Gamma} \left( \frac{\tilde{a}_2}{2} s^2(\mathbf{x}) + \frac{\beta}{4} s^4(\mathbf{x}) \right) \\ & - \sum_{\mathbf{x} \in \Gamma} h(\mathbf{x})s(\mathbf{x}) \end{aligned} \quad (23)$$

where  $h(\mathbf{x}) = \beta H(\mathbf{x})$  denotes the dimensionless counterpart of  $H(\mathbf{x})$ , which also parametrizes the corresponding canonical partition function

$$Z[\mathbf{h}] := \int \mathcal{D}s \, e^{-\beta\mathcal{H}[s, \mathbf{h}]}, \quad \int \mathcal{D}s := \int_{-\infty}^{\infty} \prod_{\mathbf{x} \in \Gamma} ds(\mathbf{x}) \quad (24)$$

If  $h(\mathbf{x})$  is spatially inhomogeneous, information on all the spatial correlations of spins at sites  $\mathbf{x}_i$  can be obtained in terms of the connected correlation functions, which are generated by successive derivatives of  $\ln Z[\mathbf{h}]$  with respect to the field values  $h(\mathbf{x}_i)$ . However, according to the above reasoning, to explore the long-range critical behavior, it suffices to study the effect of (small amplitude) fields  $h(\mathbf{x})$  containing *only long wavelength* variations. In other words, to study long range phenomena near a phase transition only fields whose wavelength exceeds some minimal length scale  $l$  need to be considered. In terms of the Fourier spectrum of  $h(\mathbf{x})$ , this amounts to assuming a cutoff  $\Lambda = 2\pi/l$  such that  $\tilde{h}(\mathbf{k}) = 0$  for  $|\mathbf{k}| > \Lambda$ , i.e. we now assume that

$$h(\mathbf{x}) \equiv \frac{1}{\sqrt{N}} \sum_{|\mathbf{k}| \leq \Lambda} h(\mathbf{k}) e^{i\mathbf{k}\mathbf{x}} \quad (25)$$

Through the bilinear coupling of  $h(\mathbf{x})$  and  $s(\mathbf{x})$ , this immediately leads to a subdivision of any given spin configuration  $s(\mathbf{x})$  into a “slow” (i.e. long wavelength) part

$$\eta(\mathbf{x}) := \frac{1}{\sqrt{N}} \sum_{|\mathbf{k}| \leq \Lambda} s(\mathbf{k}) e^{i\mathbf{k}\mathbf{x}} \quad (26)$$

which still couples to  $h(\mathbf{x})$ , and a remaining “fast” part

$$\varphi(\mathbf{x}) := s(\mathbf{x}) - \eta(\mathbf{x}) \quad (27)$$

This offers the opportunity to perform a partial trace over the fast modes, i.e. integrate out the modes  $\tilde{s}(\mathbf{k})$  of the canonical partition function  $Z[\mathbf{h}] = \int \mathcal{D}s \, e^{-\beta\mathcal{H}[s, \mathbf{h}]}$  with the guarantee that the coefficients of the remaining effective Hamiltonian  $H^{(L,l)}[\eta]$  for the slow modes, defined by

$$Z[\mathbf{h}] \equiv e^{-\beta N u_0} \int \mathcal{D}\eta \, e^{-\beta H^{(L,l)}[\eta] + \sum_{|\mathbf{k}| \leq \Lambda} \tilde{h}(\mathbf{k}) \tilde{\eta}(\mathbf{k}^*)} \quad (28)$$

are still *independent of the external field*  $h(\mathbf{x})$ . This remaining effective Hamiltonian, which thus results from thermally averaging out the effect of short-range fluctuations, is called the *coarse grained* Hamiltonian of the original system at scale  $l$  and will be denoted by  $H^{(L,l)}[\eta]$ . By applying to general symmetry considerations [6] one can show that it must

be of the form

$$\begin{aligned} \beta H^{(L,I)}[\eta] = & \frac{1}{2} \sum_{\mathbf{k}} u_2^{(L,I)}(\mathbf{k}) \tilde{\eta}(\mathbf{k}) \tilde{\eta}(\mathbf{k}^*) \\ & + \frac{1}{4N} \sum_{\mathbf{k}_1, \dots, \mathbf{k}_4} u_4^{(L,I)}(\mathbf{k}_1, \dots, \mathbf{k}_4) \tilde{\eta}(\mathbf{k}_1) \dots \tilde{\eta}(\mathbf{k}_4) \Delta_{\Gamma} \left( \sum_{i=1}^4 \mathbf{k}_i \right) \\ & + \frac{1}{6N^2} \sum_{\mathbf{k}_1, \dots, \mathbf{k}_6} u_6^{(L,I)}(\mathbf{k}_1, \dots, \mathbf{k}_6) \tilde{\eta}(\mathbf{k}_1) \dots \tilde{\eta}(\mathbf{k}_6) \Delta_{\Gamma} \left( \sum_{i=1}^6 \mathbf{k}_i \right) \\ & + \dots \end{aligned} \quad (29)$$

where the coefficients  $u_i^{(L,I)}$  can be assumed to be symmetric in their arguments. The reader will note that our Fourier Monte Carlo approach is tailor-made to tackle this kind of problem, in which the above “small” subspace of the Brillouin zone  $\Gamma_s^*$  is identified as  $\Gamma_s^* = \{\mathbf{k} \in \Gamma^* : |\mathbf{k}_i| > \Lambda, i = 1, \dots, d\}$ .

It remains to determine the “relevant” part of the coefficients  $u_{2n}^{(L,I)}$  from simulation. In the case of a standard  $\phi^4$  theory in 3 dimensions, we are interested in the so-called *Landau–Ginzburg Hamiltonian*

$$\begin{aligned} \beta H_{LG}^{(L,I)}[\eta] = & \frac{1}{2} \sum_{\mathbf{k}} (D_0^{(L,I)} k^2 + A_2^{(L,I)}) \tilde{\eta}(\mathbf{k}) \tilde{\eta}(\mathbf{k}^*) \\ & + \frac{A_4^{(L,I)}}{4N} \sum_{\mathbf{k}_1, \dots, \mathbf{k}_4} \tilde{\eta}(\mathbf{k}_1) \dots \tilde{\eta}(\mathbf{k}_4) \Delta_{\Gamma} \left( \sum_{i=1}^4 \mathbf{k}_i \right) \\ & + \frac{A_6^{(L,I)}}{6N^2} \sum_{\mathbf{k}_1, \dots, \mathbf{k}_6} \tilde{\eta}(\mathbf{k}_1) \dots \tilde{\eta}(\mathbf{k}_6) \Delta_{\Gamma} \left( \sum_{i=1}^6 \mathbf{k}_i \right) + \dots \end{aligned} \quad (30)$$

which only retains a  $\mathbf{k}$ -dependence  $u_2^{(L,I)}(\mathbf{k}) \approx A_2^{(L,I)} + D_0^{(L,I)} k^2$  up to quadratic order on the harmonic part of the potential, whereas any  $\mathbf{k}$ -dependence of the other coefficient functions  $u_{2n}^{(L,I)}(\mathbf{k}_1, \dots, \mathbf{k}_6) \approx A_{2n}^{(L,I)}$ ,  $n = 2, 3, \dots$  is completely neglected. To determine these, one can perform simulations at “special” configurations of the surviving slow modes as we now discuss.

To compute the homogeneous coefficients  $u_2^{(L,I)}(\mathbf{0}), u_4^{(L,I)}(\mathbf{0}, \dots, \mathbf{0}), u_6^{(L,I)}(\mathbf{0}, \dots, \mathbf{0}), \dots$ , one performs a series of simulations, summing over the fast modes while setting all the slow modes except the “central” homogeneous mode  $\tilde{\eta}(\mathbf{0})$  identically to zero. The logarithm of the resulting probability distribution  $P_0(\tilde{\eta}_0)$  for this mode is then fitted to a polynomial, which allows to extract the above coefficients as fit parameters. Since the resulting potentials will be of a  $\phi^4$  type with possibly high central barrier, these simulations are most conveniently performed using a thermal Wang-Landau algorithm [5, 7, 8, 9]. Figure 1 gives a 2d sketch of the mode configurations labelled by the corresponding vectors in the Brillouin zone. Generalizing this idea to  $\mathbf{k} \neq \mathbf{0}$ , we consider configurations where only the real part  $r = \Re \tilde{\eta}(\pm \mathbf{k})$  of a single pair of slow modes is allowed to be different from zero (cf. Fig. 2 for 2d sketches of mode configurations labelled by the corresponding vectors in the Brillouin zone, which illustrate the configurations taken for determining the dispersion along the (10)-direction).

Just like for the zero mode, we can then compute the corresponding probability distribution, which we denote by  $P_{\mathbf{k}}(r)$ . This function is again fitted to a polynomial in the variable  $r$ , whose curvature at zero gives the corresponding value  $u_2^{(L,I)}(\mathbf{k})$ . Doing this for various  $\mathbf{k}$ -vectors thus allows to reconstruct the full quadratic dispersion term. For the example of a simple  $\phi^4$ -theory, details and results of this approach can be found in Ref. [10].

#### 4.2. Critical systems

Investigation of critical behavior are in a sense complementary to coarse graining problems, as they require to integrate out the long-range fluctuations. In comparison to real-space approaches, we note several points which should elucidate the circumstances under which our method should be valuable:

- Long-range but translationally invariant lattice interactions may be diagonalized by the Fourier transform; their study is thus inexpensive in the Fourier MC method.



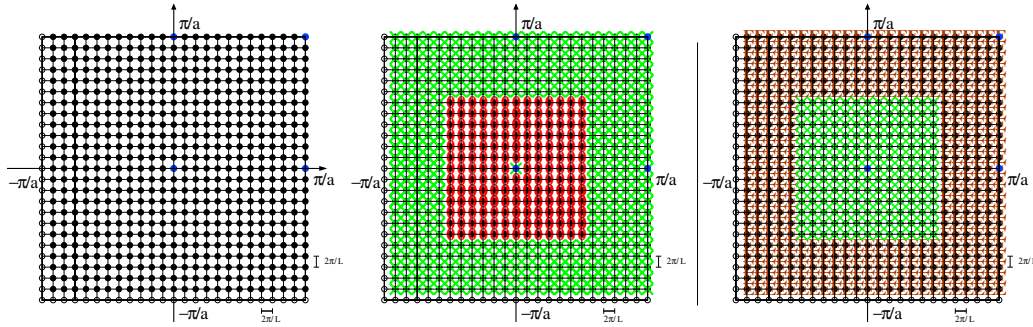


Figure 1: (a) Sketch of the Brillouin zone of a two-dimensional simple cubic lattice. Blue dots  $\bullet$  denote high-symmetry vectors  $\mathbf{k} = \mathbf{k}^*$  corresponding to real-valued Fourier modes, open circles  $\circ$  symbolize  $\mathbf{k}$ -vectors outside of the Brillouin zone that are equivalent to boundary vectors up to addition of a reciprocal vector. (b) Sketch of the corresponding simulation scheme used to calculate the homogeneous (“Landau”) part of the Landau-Ginzburg potential. Red zeros  $0$  denote  $\mathbf{k}$ -vectors, whose corresponding modes  $\tilde{\eta}(\mathbf{k})$  are kept zero, while green crosses  $\times$  denote  $\mathbf{k}$ -vectors whose accompanying modes are allowed to fluctuate during the simulation. (c) Simulation scheme for critical systems governed by an effective coarse-grained Hamiltonian. Again, green crosses  $\times$  correspond to fluctuating modes, whereas brown letters  $E$  correspond to  $\mathbf{k}$ -vectors of modes, whose contribution to the partition function is implicitly included in the temperature dependence of the effective Hamiltonian.

- Not surprisingly, in critical systems the RG-relevant part of the couplings, which determine the long-range properties of the system, are usually found to be conveniently expressed in a Fourier representation, which are often related to the “bare” values of macroscopically known observables. However, real-space algorithms are unable to take advantage of these “minimal” Hamiltonians, but usually start with a purely microscopic model.
- To obtain reliable information on the behavior of modes near  $\mathbf{k} = \mathbf{0}$  from simulation, one must go to large linear system sizes  $L$ . In principle, in combination with finite size scaling (FSS), this basic difficulty of simulating critical systems can be overcome. However, also FSS only gives reliable results if the available system sizes exceed a certain threshold. For instance, to distinguish a weak first order transition with “pseudocritical” behavior, in which the correlation length  $\xi(T) \leq \xi_{\max}$  may become large but nevertheless remains finite for all temperatures, from a true second order one, one must go to system sizes  $L > \xi_{\max}$ . For real-space algorithms starting from a microscopic Hamiltonian this can turn out to be prohibitively difficult, as the number of MC variables grows like  $L^d$ . However, with our present approach we can deal with this as follows.

Instead of the full microscopic Hamiltonian, we choose a minimal effective (“Landau–Ginzburg”) Hamiltonian which contains nothing but the relevant couplings required for the problem, together with a  $\mathbf{k}$ -vector cutoff  $\Lambda$ . As we explained above, this Hamiltonian can be regarded as a coarse-grained microscopic Hamiltonian, resulting from averaging out all Fourier modes corresponding to  $\mathbf{k}$ -vectors outside this cutoff. The actual simulation therefore involves all modes inside the cutoff. Choosing  $\Lambda$  small enough, the density of  $\mathbf{k}$ -vectors can now be increased without increasing the total number of MC variables. But as the discrete Brillouin zone of a finite cubic lattice of linear size  $La$  is again a cubic lattice with lattice constant  $a^* = \frac{2\pi}{La}$ , increasing the density of  $\mathbf{k}$ -vectors is just equivalent to going to larger system sizes  $L$ . Fig. 1(c) shows a sketch of the resulting simulation scheme.

## 5. Finite Size Scaling for Cutoff Systems

We add a remark on the proper construction of FSS for Fourier MC simulations. As pointed out above, Fourier MC usually involves a cutoff  $\Lambda$  in the Brillouin zone. Now the very idea of FSS is to compare and relate the behavior of systems of different linear system size, and as we pointed out in the previous section, increasing  $L$  corresponds to increasing the density of  $\mathbf{k}$ -vectors. From these simple considerations it is clear that FSS for cutoff systems will only work if the Brillouin zone subvolumes inside and outside the cutoff are similar, containing strictly the same fraction of vectors inside and outside the cutoff. But this requirement also puts restrictions on the geometry of the cutoff. In fact, assume that we naively pick a spherical cutoff  $|\mathbf{k}| \leq \Lambda$  as implied by sloppy notation above. Then, due to the

discreteness of the mesh of  $\mathbf{k}$ -vectors for finite systems, at different linear sizes  $L$  we will generally not find *exactly* the same fraction of  $\mathbf{k}$ -vectors inside this spherical cutoff. The resulting discreteness error is observed to be large enough to completely ruin FSS; for instance, the 3d Ising Binder cumulants fail to cross at a common intersection point etc. Our advice therefore is to choose a cutoff geometry that is compatible with the symmetry of the Brillouin zone.

For a simple cubic lattice, a proper cutoff should thus also be cubic, i.e.  $|k_i| \leq \Lambda$ . Parametrizing  $\Lambda(l) = \frac{2\pi l}{aL}$ ,  $l = 1, 2, \dots, L/2$ , we observe that out of a total of  $N = L^d$  vectors,  $(2l + 1)^d$  vectors will be located inside the cutoff. We conclude that the set of systems characterized by the pairs  $(L, l)$  falls into separate classes labelled by a common value of the fraction

$$\sigma := \frac{L}{2l + 1} \quad (31)$$

Enumerating these pairs to lowest order in the total lattice size  $L$ , we look for families that contain at least four such pairs at moderate system sizes. The following two families appear to be particularly convenient:

$$\sigma = 2 : \quad (L, l) = \{(6, 1), (10, 2), (14, 3), (18, 4), (22, 5), (26, 6), (30, 7), \dots\} \quad (32)$$

$$\sigma = 4 : \quad (L, l) = \{(12, 1), (20, 2), (28, 3), (36, 4), \dots\} \quad (33)$$

Since a value of  $\sigma$  corresponds to a subcube of the Brillouin zone of relative volume fraction  $1/\sigma^d$  of the Brillouin zone, the  $(\sigma = 4)$ -family is well-suited for the study of critical systems at relatively small cutoff while allowing for relatively large linear system sizes  $L$ . However, in special cases, other choices might also be useful. Comparison of results obtained for different  $\sigma$ -families can serve as a consistency check of results.

As an illustration of such a FSS in presence of a cutoff, we refer to our recent paper [11]. In this work, the critical behavior of a  $\phi^4$ -model coupled to harmonic elastic degrees of freedom of the underlying lattice is studied using the above effective Hamiltonian approach for system families corresponding to  $(\sigma = 4)$ .

## 6. Conclusion and Outlook

As we have explained in great detail in this overview, as it stands, our Fourier MC algorithm is certainly not a universal tool. Rather, it is superior to other existing algorithms in certain specialized cases that are inaccessible otherwise or at least extremely tedious to tackle. Such examples include coarse graining problems, compressible lattice models with accompanying long-range strain-mediated interactions and elastic membranes. Also, our algorithm may be applied to explicitly computing RG flows of coupling constants following Wilson's momentum shell RG prescription.

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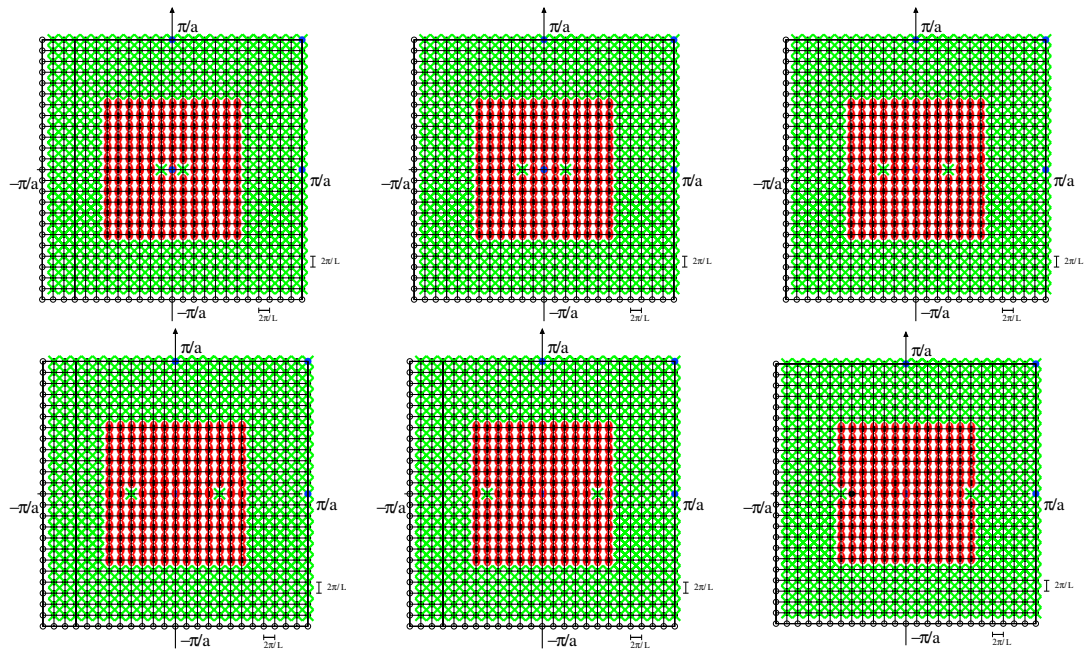


Figure 2: (a)-(f) Sketch of the simulation scheme used to calculate the dispersion part of the Landau-Ginzburg potential for  $k \parallel$  (10). Symbols as in Fig. 1.