Monte Carlo simulation in Fourier space

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Abstract

In the context of solving the long-standing problem of computing Landau–Ginzburg free energies including gradient corrections for the $\phi^4$ model, we recently introduced a new Monte Carlo algorithm for lattice spin systems based exclusively on Fourier amplitudes of the underlying spin configurations [A. Tröster, Phys. Rev. B 76 (2007) 012402]. In the present paper we shall provide additional information on the motivation, main ideas and constructions underlying the algorithm. Also we discuss important details of its construction with emphasis on an analysis of its scaling behavior with system size.

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Nowadays computer simulations play an overwhelmingly important role in modern physics. The reasons for this fact are manifold. On the one hand, current research often deals with highly nonlinear problems where analytical solutions or satisfying approximations are prohibitively difficult to find. On the other hand, the focus might also be on systems involving a large number of interacting particles, and even for comparatively simple interaction types, these systems are again analytically intractable. In statistical mechanics, researchers have suffered for a long time from the fact that only a small number of non-trivial models allow for analytic solutions (for a comprehensive review see [1]), which, while most of them describe only rather exotic or artificial cases or are limited to low dimensions, nevertheless frequently reveal an impressive complexity.

Most approaches to simulate models of Statistical Mechanics on a computer can roughly be classified as being of the Molecular Dynamics or Monte Carlo (MC) type. We assume the reader to be familiar with the general concepts of computer simulations and refer the novice reader to literature [2,3]. In particular, MC simulations are well suited to study lattice models [4], for which there exist numerous types of algorithms. As a survey of the literature reveals, as a rule these simulations are implemented in real space. To be specific, consider the case of lattice spin models. Constructing such a model involves defining a $d$-dimensional host Bravais lattice $\Gamma$, with sites $x$ populated by so-called generalized “spins” $s(x)$ that can take on values from a (finite or infinite) fixed set of possible values. Next, a Hamiltonian $H$ is defined, which maps each particular spin configuration $s := \{s(P)\}$ in an extensive way onto a real-valued energy $H[s]$ bound from below. Once these ingredients are known and an ensemble (e.g., canonical or microcanonical) is chosen, MC simulations can be undertaken. The actual algorithm that is used in such a simulation then roughly depends on two major choices:

(i) The construction rule(s) for the random walk in configuration space.
(ii) The rule for accepting/rejecting a newly generated configuration.

Let us make the popular choice of the so-called Metropolis algorithm [4] for (ii). As to (i), this usually still leaves us with a considerable freedom in generating MC “moves” (i.e. defining—in a randomized way—a new trial configuration starting from the currently existing configuration). It thus comes as no surprise that the study (applicability, strengths and weaknesses, implementation and performance optimization) of the resulting MC algorithms continue to be under investigation up to date.

There are certain problems, however, that seem to refuse to give in to any attempt to design a prescription that leads to a satisfactory MC algorithm based on real space MC moves.
This may be due to different reasons. For instance, the system may be subject to constraints that severely restrict the choice of admissible MC moves. As a good example of such a situation, consider the various attempts to perform a coarse graining (CG) of spin models in real space. Starting from a microscopic Hamiltonian defined on, say, a simple cubic $d$-dimensional lattice $\Gamma^*$ of size $L^d$ with periodic boundary conditions, a homogeneity constraint on some length scale $l$ much larger than the lattice constant $a$ is imposed on the system. Then, one tries to average out small wavelength fluctuations to obtain an effective coarse grained Hamiltonian. In real space, one might try to approach the problem by dividing a given lattice into smaller sublattices and performing the statistical by averaging over all spins inside the subcells while imposing a uniform total magnetization of all subcells during the course of the simulation [5–9]. An obvious disadvantage of such an approach is the limited choice of possible CG length scales $l$ that are commensurate with respect to $L$ and the periodic boundary conditions. This problem is particularly disturbing in applications where one is interested in a “floating” homogeneity constraint. For instance, one might want to identify the CG length scale $\xi(T)$ of the bulk system. The resulting constrained free energies are of interest if fast Fourier transformation, an algorithm which is of the order $O(N \log N)$, is used to convert real space MC moves into shifts of Fourier amplitudes, the computational effort for a single MC step may actually turn out to be $O(N^2)$ because of an unfavorable structure of the underlying Hamiltonian. As a prominent example, we mention phase transitions with elastic couplings, whose long interaction range are well known to alter the behavior of phase transitions in a profound way [11]. To be more explicit, consider the theory of compressible Ising models, which has been studied intensively (see, e.g., Refs. [12–17]; a nice historical summary of their discussion, spanning over several decades up to recent times, can be found in [18]). One way to approach the problem is the following. Consider a spin model coupled to an elastic Hamiltonian which is harmonic in the strains. Integrating out the elastic degrees of freedom, one is left with an effective Hamiltonian, in which the original elastic interaction, which is long range in nature, is formally cast into a Landau–Ginzburg type Hamiltonian, whose coupling constants show a nontrivial wave-vector dependence [19]. It is only in the special case of cubic systems with elastic isotropy that the resulting effective Hamiltonian can be reformulated in terms of real space configurations in a manageable way.

But if the use of real space algorithms for such systems is troubled by so many difficulties, why not use the real and imaginary parts of the discrete Fourier amplitudes $\tilde{s}(k)$ as the basic MC variables? Taking the example of Ising spins, we quickly realize that this idea, which is suggested by the above survey, is plagued by another problem. To understand what the trouble is requires some technical and notational preparations. To start with, we introduce the reciprocal lattice $\Gamma^* \subset \mathbb{R}^d$ of our original (direct) lattice $\Gamma$. Finite computer storage demands that the direct lattice $\Gamma$ is finite, and certain boundary conditions must be imposed, which we chose to be periodic in this work. Let $\tilde{\Gamma}$ denote the space of all $k$-vectors that are consistent with these boundary conditions. The corresponding (first) Brillouin zone of the lattice is the space $\Gamma^* := \tilde{\Gamma}/\Gamma$, of all equivalence classes of such $k$-vectors up to addition of reciprocal vectors. Reflection $k \mapsto -k$ about the origin of $\tilde{\Gamma}$ induces a well-defined map $k \rightarrow k^*$ on $\Gamma^*$. Now we define

$$s(x) = \frac{1}{\sqrt{N}} \sum_{k \in \Gamma^*} \tilde{s}(k)e^{ikx},$$

(1)

$$\tilde{s}(k) = \frac{1}{\sqrt{N}} \sum_{x \in \Gamma} s(x)e^{-ikx}.$$  

(2)

If the spins $s(x)$ are only required to be real-valued, these formulas imply that their amplitudes must satisfy the constraints $\tilde{s}(k^*) = \tilde{s}(-k^*)$, $k \in \Gamma^*$, and so are not directly independent from one another. However, in fact it is always possible to choose a certain subset set of $k$-vectors from $\Gamma^*$ related to a corresponding set of $N$ independent real amplitudes parameterizing each configuration of the system. $2d$ of them are given by the purely real amplitudes $\tilde{s}(h)$ corresponding to the $2d$ distinct “high-symmetry vectors” $h \in \Gamma^*$ with the property that $h^* = h$. In particular, $h = 0$ corresponds to the real-valued zero mode $\tilde{s}(0) = \sqrt{N/m}$, where $m$ is the average magnetization of the system. The remaining $N - 2d$ $k$-vectors of $\Gamma^*$ can be arbitrarily divided into pairs $(k^+, k^-) = (-k^+)$ of some suitably de-
fined even and odd “parity” \( p(k^{(\pm)}) = \pm 1 \). The real and imaginary parts \( \Re \tilde{s}(k^{(\pm)}) \), \( \Im \tilde{s}(k^{(\pm)}) \) of the positive parity modes can now be taken to represent the residual \( 2 \times (N - 2^d)/2 = N - 2^d \) independent real degrees of freedom in Fourier representation.

Compared to real-valued spins, actual Ising spins \( s(x) \) have to satisfy the much more rigid set of \( N \) constraints \( \delta^2 s(x) = 1 \) \( \forall x \in \varGamma \), from which it follows that, e.g., \( N = \sum_{x \in \varGamma} \delta^2 s(k) \delta^2 s(k^*) \). This, however, implies that individual Fourier amplitudes of Ising spins fail to constitute independent degrees of freedom and in particular cannot be shifted independently from one another during the course of a MC simulation.

What can we do about this? Inside the Ising universality class, the above parametrization considerations strongly suggest that this problem could be avoided by allowing for real-valued spins \( s(x) \in \mathbb{R} \) as MC variables. However, to stabilize the energy, we now have to add anharmonic polynomial terms to the Hamiltonians. A well-known representative of the Ising universality class obtained in this way is the so-called \( \phi^4 \) model with Hamiltonian

\[
\mathcal{H} = -\frac{1}{2} \sum_{x,y} J(x-y) s(x) s(y) + \frac{A_2}{2} \sum_x \delta^2 s(x) + \frac{s^4(s)}{4}.
\]

(3)

Ironically, by employing this idea we only seem to have traded one problem for another. As is well known, the quadratic part of the Hamiltonian can be diagonalized by Fourier transformation. Fourier-transforming the quartic contribution to the Hamiltonian, however, results in

\[
\sum_x s^4(x) = \frac{1}{N} \sum_{k_1, \ldots, k_4} \tilde{s}(k_1) \cdots \tilde{s}(k_4) \delta_{k_1 + \cdots + k_4}.
\]

(4)

where \([p]\) denotes the unique vector of the Brillouin zone \( \varGamma^* \) obtained from the vector \( p \in \varGamma \) by addition of a suitably chosen reciprocal vector, and we abbreviate the \( d \)-dimensional Kronecker delta by \( \delta_k = \delta_{k_0} \). Thus, the computation of the energy of a particular configuration is complicated by an intricate matching condition of four-tuples \( k_1, \ldots, k_4 \) of \( k \)-vectors. In what follows we let \( \varGamma^* \times \varGamma^* = \{k_1, \ldots, k_n_2 \} \) denote the “active” part of the Brillouin zone, i.e. the subset of all those \( k \)-vectors of the Brillouin zone, whose accompanying Fourier amplitudes \( \tilde{s}(k) \) 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, \( \varGamma^* \times \varGamma^* \) will usually be chosen to be \( \ast \)-invariant. We would like to take advantage of the fact that while the number of lattice sites \( N \) is still the same, in concrete applications the total number \( n_s = |\varGamma^*| \leq N \) of active vectors may be much smaller than \( N \), for instance, if there is a cutoff \( \Lambda \) defined in the Brillouin zone.

Under a move of type (8), this expression changes to

\[
\Delta \mathcal{H}_2 = 2 \tilde{D}(k_0) \left[ (\Re \tilde{s}(k_0^2)) + (\Im s)^2 \delta_{k_0,k_0^*} + (1 - \delta_{k_0,k_0^*}) \frac{|e|^2}{2} \right].
\]

(11)

To compute the change

\[
\delta \mathcal{H}_4 = \sum_{q \in \varGamma^*_S} \delta \mathcal{H}_4(q)
\]

(12)

of the quartic contribution to the Hamiltonian, where

It is only recently that we have discovered a loophole in this zoo of obstacles [10]. In fact, the basic ideas are disarmingly simple. First, we observe that \( s^4(x) = (s^2(x))^2 \). Therefore, introducing the squared spin field \( S(x) := s^2(x) \), we write

\[
\sum_x s^4(x) = \sum_x S^2(x) = \sum_q \tilde{s}(q) \tilde{S}(q^*)
\]

(5)

which is obviously diagonal in terms of the modes

\[
\tilde{s}(q) = \frac{1}{\sqrt{N}} \sum_x S(x) e^{-iqx} = \frac{1}{\sqrt{N}} \sum_k \tilde{s}(k) \tilde{s}([q + k^*]).
\]

(6)

Note that squaring \( s(x) \) may introduce additional \( k \)-vectors into a given problem, as the wavelength spectrum of a squared spin field generally involves shorter wavelengths, forcing us to define an accompanying new \( \ast \)-invariant subset \( \varGamma^*_S = \{q_1, \ldots, q_{n_S} \} \) of the first Brillouin zone. From (6) we expect

\[
0 \leq n_s \leq n_S \leq N
\]

(7)

since a simulation usually involves the zero mode \( \tilde{s}(0) \) proportional to the magnetization of the system.

Next, we remind ourselves of the fact that in order to generate a Markov chain using the Metropolis rule, it is only required to compute the energy changes accompanying the transition between consecutive spin configurations. In our MC algorithm, these basic moves will be of the type \( [\tilde{s}(k)]_{k \in \varGamma^*} \rightarrow [\tilde{s}(k)]_{k \in \varGamma^*} + \delta \tilde{s}(k)_{k \in \varGamma^*} \). For each move, a vector \( k_0 \) is drawn randomly from the active part of the Brillouin zone, a complex number \( e \) is chosen randomly from some circle of fixed finite radius around zero in the complex plane, and we set

\[
\delta \tilde{s}(k) := e \delta_{k,k_0} + e^* \delta_{k,k_0^*}, \quad k_0 \in \varGamma^*_S.
\]

(8)

The resulting algorithm is ergodic and obeys detailed balance.

Turning to the quadratic part of the \( \phi^4 \) Hamiltonian, we introduce the Fourier transform of the lattice interaction

\[
\tilde{j}(k) = \sum_{x \in \varGamma^*} J(x) e^{i k x}.
\]

(9)

If \( J(x) \) is symmetric under inversion, \( J(k) = J(k^*) = J^*(k) \) is real. Combining both quadratic contributions, the harmonic part of the Hamiltonian takes the form

\[
\mathcal{H}_2 = \frac{1}{2} \sum_k \tilde{D}(k) \tilde{s}(k) \tilde{s}(k^*), \quad \tilde{D}(k) := \tilde{A}_2 - \tilde{j}(k).
\]

(10)

Under a move of type (8), this expression changes to

\[
\Delta \mathcal{H}_2 = 2 \tilde{D}(k_0) \left[ (\Re \tilde{s}(k_0^2)) + (\Im s)^2 \delta_{k_0,k_0^*} + (1 - \delta_{k_0,k_0^*}) \frac{|e|^2}{2} \right]
\]

(11)
\[ \delta \mathcal{H}_4(q) = \frac{1}{4} \left[ \hat{S}(q^*) \delta \hat{S}(q) + \delta \hat{S}(q^*) \hat{S}(q) + \delta \hat{S}(q^*) \delta \hat{S}(q) \right] \]  

(13)

It remains to determine the shifts \( \delta \hat{S}(q) \) induced by (8). A short calculation yields

\[ \delta \hat{S}(q) = \frac{1}{\sqrt{N}} \left( 2e^{i\langle(q-k_0)\rangle} + 2e^{i\langle(q+k_0)\rangle} \right) 
+ e^2 \delta |q-2k_0,0| + 2|e|^2 \delta_{q,0} + e^2 \delta_{q+2k_0,0}. \]  

(14)

To check the order of the number of operations necessary to perform the resulting Fourier MC algorithm for the \( \phi^4 \) model, we take a look at the following pseudocode summary of the bare minimal algorithm:

**procedure** **INITIALIZATION:**
- Initialize \( \hat{s}(k) \);
- Initialize \( \hat{S}(q) \) using Eq. (6);

\[ \triangleright O(n_s n_3) \) operations, required only once

**end procedure**

**procedure** **FOURIERMETROPOLIS**

```
repeat
  Generate move (8);
  Calculate \( \Delta \mathcal{H}_2 \); \( \triangleright O(1) \) operations
  for \( i = 1; i \leq n_s; i++ \) do
    Calculate \( \delta \hat{S}(q_i) \); \( \triangleright O(1) \) operations
    Add \( \Delta E_+ = \Delta \mathcal{H}_4(q_i) \); \( \triangleright O(1) \) operations
  end for
  accept StandardMetropolisRule(\( \Delta E \));
  if accept then
    Update \( \hat{s}(k_i) + = \delta \hat{s}(k_i) \); \( \triangleright O(1) \) operations
    for \( i = 1; i \leq n_s; i++ \) do
      Update \( \hat{S}(q_i) + = \delta \hat{S}(q_i) \); \( \triangleright O(1) \) operations
    end for
  end if
until done
```

**end procedure**

We thus conclude that the resulting algorithm is of the order \( O(n_s) \ll O(N) \). Thus, at least for the \( \phi^4 \)-model, our approach, which is exclusively based on the use of the nonzero Fourier amplitudes involved in the setup of a particular problem without making any reference to the real space configurations, represents a major advantage over other attempts. In particular, this is true for situations where the subspace \( \Gamma^*_s \) of the Brillouin zone that hosts the nonzero modes of the problem, is much smaller than the full Brillouin zone \( \Gamma^* \), such that \( n_s, n_3 \ll N \). Remembering that \( \left(L/2\pi\right)^d \) represents the density of \( k \)-vectors in \( \Gamma^* \), on choosing a suitable small enough subset \( \Gamma^*_s \) of active vectors, we conclude that it is possible to considerable stretch the limits of possible linear system sizes \( L \).

We recently applied the above algorithm to calculate Landau–Ginzburg free energies for the \( \phi^4 \) model in \( d = 3 \) including gradient corrections [10], a problem which, despite the familiarity of the \( \phi^4 \) model and the Ising universality class, had been computationally intractable before [20]. In these simulations, partition functions were calculated by summing over all Fourier amplitudes outside a particular cutoff \( A \). The converse situation occurs in simulations where an effective (e.g., Landau–Ginzburg) Hamiltonian is prescribed, and the summation is performed over all modes inside the cutoff, focusing on the system’s critical behavior. In passing we note that for both types of simulations, finite size scaling theory also becomes available if one properly rescales the subsets \( \Gamma^*_s \) for various \( L \) accordingly [10]. At the moment, for the case of compressible \( \phi^4 \) models, such simulations are under way in our laboratory.

**References**

[19] See, e.g., formula (5.2) of Ref. [14].