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Fourier Monte Carlo Implementation Guide

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Abstract

The Fourier Monte Carlo algorithm represents a powerful tool to study criticality in lattice spins systems. In particular, the algorithm constitutes an interesting alternative to other simulation approaches for models with microscopic or effective long-ranged interactions. However, due to the somewhat involved implementation of the basic algorithmic machinery, many researchers still refrain from using Fourier Monte Carlo. It is the aim of the present article to lower this barrier. Thus, the basic Fourier Monte Carlo algorithm is presented in great detail with emphasis on providing ready-to-use formulas for the reader's own implementation.

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Keywords: Monte Carlo simulations, lattice spin models, long-ranged interactions, critical phenomena, renormalization group

1. Introduction

Since its introduction [1], the Fourier Monte Carlo (FMC) algorithm has proved to be a valuable tool for successfully tackling a number of problems that had challenged or even defeated previous computational approaches. Examples include the numerical determination of coarse-grained free energies with gradient corrections from a given microscopic Hamiltonian [1], the observation of Fisher renormalized critical exponents in compressible spin models [2], a study of the renormalization group flows in a step-by step numerical implementation of Wilson's momentum shell prescription [3, 4, 5] and the investigation of the universal properties of solid membranes [6]. FMC may not be a general-purpose method. Instead, it should be regarded as a kind of surgical tool that represents a competitive (and sometimes the only feasible) choice for many interesting problems, particularly such involving criticality in systems with microscopic or effective long-ranged interactions (see e.g. Ref. [7]). In fact, the recently discovered [6] simple modification of FMC to effectively suppress critical slowing down [8, 9, 10] promises to promote FMC in the current top league of simulation algorithms from critical behavior.

Yet, even though there is definitely interest in using the machinery of FMC, despite past efforts [11, 12] many potential users found the task of setting up the formulas and working out a concrete implementation to be too painful to seriously consider using it in practice. It is the purpose of the present article to provide ready-to-use formulas and practical implementation tips for FMC, such that this algorithm becomes more convenient to use for a wider range of research groups.

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Listing 1: possible C implementation of parity function $\pi(\boldsymbol{q})$

```
int parity (const int m[dim]){ // integer coordinate array of q
  int d,n;
  for(d=0;d<dim;d++)
    if((n=m[d]%(L/2))) break; // q on d-th coordinate hyperplane or BZ boundary?
  return((n>0)-(n<0));        // return sign of coordinate m[d] mod L/2
}
```

2. Brillouin zone setup

We consider a d-dimensional simple cubic lattice Γ of linear dimension L and lattice constant $a = 1$ with periodic boundary conditions. In what follows we assume L to be even. Let us denote a site of Γ by $\boldsymbol{x} \in \Gamma$, and their total number by $N = L^d$. A configuration φ of a lattice spin model on Γ is nothing but a collection $\{\varphi(\boldsymbol{x}) : \boldsymbol{x} \in \Gamma\}$, where we assume $\varphi(\boldsymbol{x}) \in \mathbb{R}$ for simplicity [13]. In order to employ the Fourier transform, let us start by identifying the set of admissible wave vectors $\tilde{\Gamma} = (2\pi/L) \cdot \mathbb{Z}$ that are compatible with the given lattice data. Obviously, $\tilde{\Gamma}$ contains the so-called reciprocal lattice $\Gamma_* := 2\pi \cdot \mathbb{Z}^d$ of Γ as a subset [14]. The corresponding coset space $\Gamma^* := \tilde{\Gamma}/\Gamma_*$ is known as the (first) Brillouin zone (BZ) of Γ. Its elements, which will be denoted by $[\boldsymbol{q}]$ or simply $\boldsymbol{q}$ and which we shall also call wave vectors, are represented by d-tuples of reals

$$q_i = (2\pi/L)m_i, \qquad m_i \in \{-L/2+1, -L/2+2, \ldots, -1, 0, 1, \ldots, L/2-1, L/2\} \tag{1}$$

The reflection $\boldsymbol{q} \to -\boldsymbol{q}$ defined on $\tilde{\Gamma}$ leaves Γ_* invariant and thus induces an involution $* : \Gamma^* \to \Gamma^*$, $\boldsymbol{q} \mapsto \boldsymbol{q}^*$. The subset

$$\Gamma^0 := \{q_i = (2\pi/L)m_i,\ m_i \in \{0, L/2\}\} \quad \subset \Gamma^* \tag{2}$$

is invariant under $*$ and will be called the set of high-symmetry vectors. Since $*^2 = \mathbf{I}$, all other vectors $\boldsymbol{q} \in \Gamma^* \backslash \Gamma^0$ can be grouped in pairs $(\boldsymbol{q}, \boldsymbol{q}^*)$. A order of such a pair can be defined by a convenient parity function $\pi(\boldsymbol{q})$, which should be zero for all vectors of Γ^0 and ± 1 for all others, such that

$$\Gamma^* = \Gamma^0 \cup \Gamma^+ \cup \Gamma^- \tag{3}$$

where, of course, $\Gamma^\pm = \{\boldsymbol{q} \in \Gamma^* : \pi(\boldsymbol{q}) = \pm 1\}$. For instance, in C we might write code like that in Listing 1.

The foundation of the discrete Fourier transform on Γ is provided by the basic formulas [14]

$$\frac{1}{N}\sum_{\boldsymbol{q}\in\Gamma^*} e^{\pm i\boldsymbol{q}\boldsymbol{x}} = \delta_{\boldsymbol{x},\boldsymbol{0}}, \qquad \frac{1}{N}\sum_{\boldsymbol{x}\in\Gamma} e^{\pm i\boldsymbol{q}\boldsymbol{x}} = \Delta_\Gamma(\boldsymbol{q}) := \begin{cases} 1, & \boldsymbol{q} \in \Gamma_* \\ 0, & \text{else} \end{cases} \tag{4}$$

where we have introduced the lattice delta function $\Delta_\Gamma(\boldsymbol{q})$ as a periodic generalization of the ordinary Kronecker delta. The relations (4) immediately allow to conclude that there is a one-to-one correspondence

$$\varphi(\boldsymbol{x}) \equiv \frac{1}{N}\sum_{\boldsymbol{q}\in\Gamma^*} \tilde{\varphi}(\boldsymbol{q}) e^{i\boldsymbol{q}\boldsymbol{x}}, \qquad \tilde{\varphi}(\boldsymbol{q}) \equiv \sum_{\boldsymbol{x}\in\Gamma} \varphi(\boldsymbol{x}) e^{-i\boldsymbol{q}\boldsymbol{x}} \tag{5}$$

between the representations of a microstate of the system by the set of real field-values $\varphi(\boldsymbol{x})$ and one given by the collection of Fourier amplitudes $\tilde{\varphi}(\boldsymbol{q})$. Note that, in contrast to other conventions found in the literature, our normalization is asymmetric. The advantage of normalizing the discrete Fourier transforms in this way is twofold. First of all, note that with this convention the Fourier amplitudes $\tilde{\varphi}(\boldsymbol{q})$ are extensive, which, usually being conjugate to an external field that is intensive, is quite natural. Second, it turns out that in the FMC algorithm, upon rescaling the bare coupling constants by powers of $1/N$ (see below), it allows to eliminate all explicit appearances of N from the energy calculations. Moreover, this normalization is very convenient when comparing formulas to those derived from a continuum formulation.

If the field $\varphi(\boldsymbol{x})$ were complex-valued, then, of course, all real and imaginary parts of the amplitudes $\tilde{\varphi}(\boldsymbol{q})$ can be regarded as constituting its $2N$ real degrees of freedom. Since, however, $\varphi(\boldsymbol{x})$ is assumed to be real-valued, the relations

$$\tilde{\varphi}(\boldsymbol{q}^*) = \tilde{\varphi}^*(\boldsymbol{q}), \qquad \boldsymbol{q} \in \Gamma^* \tag{6}$$

from which it follows that in particular

$$\tilde{\varphi}^*(\boldsymbol{h}) = \tilde{\varphi}(\boldsymbol{h}), \qquad \boldsymbol{h} \in \Gamma^0 \tag{7}$$

express the resulting redundancy in terms of its Fourier amplitudes. In this case, however, we can employ the above parity-induced partition (3) to conveniently organize the actual independent degrees of freedom, according to which we only need to keep track of the sets of real numbers

$$\{\varphi(\boldsymbol{h}) : \ \boldsymbol{h} \in \Gamma^0\} \qquad \text{and} \qquad \{\Re\varphi(\boldsymbol{q}), \Im\varphi(\boldsymbol{q}) : \ \boldsymbol{q} \in \Gamma^+\} \tag{8}$$

Since on a simple cubic d-dimensional lattice there are 2^d vectors of parity zero, the first set constitutes 2^d real numbers. On the other hand, inspection of Listing 1 reveals that there are exactly $N - 2^d$ vectors of nonzero parity, and therefore $(N - 2^d)/2$ ones with positive parity, such that the second set contains $N - 2^d$ reals. Together, both sets therefore hold a total of N real degrees of freedom as it should be.

After these preparations, we may proceed to rewrite a given model Hamiltonian (9) in terms of Fourier amplitudes. In the following we will study lattice φ^4 types of model. The prototypical Hamiltonian we exemplify here is that of the nearest-neighbor φ^4 model [13]

$$\mathcal{H}[\varphi] = \frac{D}{2}\sum_{\langle \boldsymbol{xy}\rangle}(\varphi(\boldsymbol{x}) - \varphi(\boldsymbol{y}))^2 + \frac{A}{2}\sum_{\boldsymbol{x}\in\Gamma}\varphi^2(\boldsymbol{x}) + \frac{B}{4}\sum_{\boldsymbol{x}\in\Gamma}\varphi^4(\boldsymbol{x}) \tag{9}$$

We work out its Fourier representation, starting with the second summand. The more mathematically oriented reader will immediately recognize the simple relation

$$\frac{A}{2}\sum_{\boldsymbol{x}\in\Gamma}\varphi^2(\boldsymbol{x}) = \frac{A}{2N}\sum_{\boldsymbol{q}\in\Gamma^*}\tilde{\varphi}(\boldsymbol{q})\tilde{\varphi}(\boldsymbol{q}^*) = \frac{A}{2N}\sum_{\boldsymbol{q}\in\Gamma^*}|\tilde{\varphi}(\boldsymbol{q})|^2 \tag{10}$$

which immediately follows from inserting the definition (5) and employing the relations (4), as a form of Parseval's theorem [15]. Using similar manipulations, one also readily derives

$$\frac{D}{2}\sum_{<\boldsymbol{xy}>}[\varphi(\boldsymbol{x}) - \varphi(\boldsymbol{y})]^2 = \frac{D}{2N}\sum_{\boldsymbol{q}}\sum_{\mu=1}^{d} 4\sin^2(q_\mu/2)|\tilde{\varphi}(\boldsymbol{q})|^2 \tag{11}$$

for the first term of (9). The fact that both (10) and 11 are diagonal in terms of $\tilde{\varphi}(\boldsymbol{q})$ is a consequence of the translational invariance and harmonicity of the original terms in the Hamiltonian (9). The central issue of the FMC algorithm is how to deal with the remaining anharmonic fourth order contribution. In a naive straightforward approach similar to the above, we would obtain the expression

$$\frac{B}{4}\sum_{\boldsymbol{x}\in\Gamma}\varphi^4(\boldsymbol{x}) = \frac{B}{4N^4}\sum_{\boldsymbol{q}_1\ldots\boldsymbol{q}_4\in\Gamma^*}\tilde{\varphi}(\boldsymbol{q}_1)\ldots\tilde{\varphi}(\boldsymbol{q}_4)\sum_{\boldsymbol{x}\in\Gamma}e^{i(\boldsymbol{q}_1+\ldots+\boldsymbol{q}_4)\boldsymbol{x}} = \frac{B}{4N^3}\sum_{\boldsymbol{q}_1\ldots\boldsymbol{q}_4\in\Gamma^*}\tilde{\varphi}(\boldsymbol{q}_1)\ldots\tilde{\varphi}(\boldsymbol{q}_4)\Delta_\Gamma(\boldsymbol{q}_1+\ldots+\boldsymbol{q}_4) \tag{12}$$

in which all products of Fourier amplitudes, whose $\boldsymbol{q}$-vectors sum up to give a reciprocal vector, contribute to the last sum. The resulting combinatorial complexity seems intractable from the angle of simulations. Instead, let us consider the auxiliary field $\varphi^2(\boldsymbol{x})$ of *squared* amplitudes of our original field. As a field in its own right, $\varphi^2(\boldsymbol{x})$ has the Fourier representation

$$\varphi^2(\boldsymbol{x}) = \frac{1}{N}\sum_{\boldsymbol{Q}\in\Gamma^*}\widetilde{(\varphi^2)}(\boldsymbol{Q})e^{i\boldsymbol{Q}\boldsymbol{x}}, \qquad \widetilde{(\varphi)^2}(\boldsymbol{Q}) = \sum_{\boldsymbol{x}\in\Gamma}\varphi^2(\boldsymbol{x})e^{-i\boldsymbol{Q}\boldsymbol{x}} \tag{13}$$

where the capitalization $\boldsymbol{Q}$ indicates that $\boldsymbol{Q}$ originates from the sum of two possibly "smaller" wave vectors $\boldsymbol{q}_1, \boldsymbol{q}_2$, a fact that will become of importance once we will have introduced a cutoff Λ in Γ^* (see below). Quite trivially, Parseval's identity gives once more

$$\frac{B}{4}\sum_{\boldsymbol{x}\in\Gamma}\varphi^4(\boldsymbol{x}) = \sum_{\boldsymbol{x}\in\Gamma}(\varphi^2(\boldsymbol{x}))^2 = \frac{B}{4N}\sum_{\boldsymbol{Q}\in\Gamma^*}\widetilde{(\varphi^2)}(\boldsymbol{Q})\widetilde{(\varphi^2)}(\boldsymbol{Q}^*) \tag{14}$$

i.e. the sum is again diagonal, albeit not in terms of the amplitudes $\tilde{\varphi}(\boldsymbol{q})$ but in terms of the amplitudes $\widetilde{(\varphi^2)}(\boldsymbol{Q})$. Of course, since $\varphi^2(\boldsymbol{x})$ is completely determined by $\varphi(\boldsymbol{x})$, we can express its Fourier amplitudes by the set of $\tilde{\varphi}(\boldsymbol{q})$ as

$$\begin{aligned}\widetilde{(\varphi^2)}(\boldsymbol{Q}) &= \sum_{\boldsymbol{x}\in\Gamma}\varphi^2(\boldsymbol{x})e^{-i\boldsymbol{Q}\boldsymbol{x}} = \frac{1}{N^2}\sum_{\boldsymbol{p},\boldsymbol{q}\in\Gamma^*}\tilde{\varphi}(\boldsymbol{p})\tilde{\varphi}(\boldsymbol{q})\sum_{\boldsymbol{x}\in\Gamma}e^{i(\boldsymbol{p}+\boldsymbol{q}-\boldsymbol{Q})\boldsymbol{x}} = \frac{1}{N}\sum_{\boldsymbol{p},\boldsymbol{q}\in\Gamma^*}\tilde{\varphi}(\boldsymbol{p})\tilde{\varphi}(\boldsymbol{q})\Delta_\Gamma\left(\boldsymbol{p}+\boldsymbol{q}-\boldsymbol{Q}\right)\\ &= \frac{1}{N}\sum_{\boldsymbol{p}\in\Gamma^*}\tilde{\varphi}(\boldsymbol{p})\tilde{\varphi}([\boldsymbol{Q}+\boldsymbol{p}^*])\end{aligned} \tag{15}$$

As explained above, the coset notation $[\boldsymbol{Q}+\boldsymbol{p}^*]$ implies that if the sum of wave vectors $\boldsymbol{Q}+\boldsymbol{p}^* \in \tilde{\Gamma}$ happens to fall outside of the boundary of the first Brillouin zone Γ^*, it needs to be "folded back" to the zone by subtracting a suitable reciprocal vector $\boldsymbol{G} \in \Gamma_*$. If we define

$$\tilde{S}(\boldsymbol{Q}) := N \times \widetilde{(\varphi^2)}(\boldsymbol{Q}) = \sum_{\boldsymbol{p}\in\Gamma^*}\tilde{\varphi}(\boldsymbol{p})\tilde{\varphi}([\boldsymbol{Q}+\boldsymbol{p}^*]) \tag{16}$$

such that $\tilde{S}(\boldsymbol{Q}) \sim N^2$, then

$$\frac{B}{4}\sum_{\boldsymbol{x}\in\Gamma}\varphi^4(\boldsymbol{x}) = \frac{B}{4N^3}\sum_{\boldsymbol{Q}\in\Gamma^*}\tilde{S}(\boldsymbol{Q})\tilde{S}(\boldsymbol{Q}^*) \tag{17}$$

As promised, we are now able to eliminate all the cumbersome powers of N from our formulas by absorbing them into the rescaled coupling constants

$$D_N := \frac{D}{N}, \qquad A_N := \frac{A}{N}, \qquad B_N := \frac{B}{N^3} \tag{18}$$

and arrive at

$$\mathcal{H}[\varphi] = \frac{1}{2}\sum_{\boldsymbol{q}\in\Gamma^*}\tilde{D}_N(\boldsymbol{q})|\tilde{\varphi}(\boldsymbol{q})|^2 + \frac{B_N}{4}\sum_{\boldsymbol{Q}\in\Gamma^*}|\tilde{S}(\boldsymbol{Q})|^2 \tag{19}$$

where the generalized dispersion $\tilde{D}_N(\boldsymbol{q})$ for nearest neighbor interaction is

$$\tilde{D}_N(\boldsymbol{q}) = A_N + D_N\sum_{\mu=1}^{d}4\sin^2\left(\frac{aq_\mu}{2}\right) \tag{20}$$

Obviously $\tilde{D}_N(\boldsymbol{q}^*) = \tilde{D}_N(\boldsymbol{q})$ is real-valued.

3. Working with subsets of the Brillouin zone

Eqs. (16) and (19) contain an order of N terms and so represent a quite expensive way to calculate the total energy. In Monte Carlo (MC), however, it is not the total energy itself that needs to be calculated from scratch at every move, but only the energy *change*. Nevertheless, as we shall see below, calculating this change takes the same order of operations as the number of wave vectors that is involved. In terms of computational effort, this indicates that for lattice Hamiltonians like (9) with short-ranged interaction, the resulting algorithm is certainly inferior to

algorithms based on simple direct lattice moves. For studying criticality in systems with long-ranged interactions, on the other hand, this is a completely different story, since then the calculation of the lattice interaction terms may take $O(N^2)$ operations in a direct lattice setting, while the calculation of energy changes still requires $O(N)$ operations. In contrast, the effort to determine these energy changes in FMC is independent of the actual range of interactions, since the Fourier-transformed lattice interaction will result in a dispersion term similar to that of (19) and (20), which is diagonal in the space of Fourier amplitudes, the only requirement being that the lattice interaction is translation-invariant, which is usually guaranteed. For Coulombic interactions, even an Ewald summation procedure in reciprocal space is available [16, 17]. Thus, if we tabulate the resulting dispersion function $\tilde{D}_N(\boldsymbol{q})$ at the start-up phase of the simulation, harmonic energy changes are therefore readily computed (concrete formulas are provided below).

At this point we would still be left with $O(N)$ operations required to calculate energy changes with FMC. This, however, is only true as long as the number of wave vectors involved in the problem at hand is equal to the number of lattice sites N. A central advantage of FMC is, however, that it is designed to allow to study the behavior of the system when only modes parametrized by a chosen subset $\mathcal{B}^* \subset \Gamma^*$ of the full Brillouin zone are allowed to participate in the simulation. For consistency we should demand that $\mathcal{B}^*$ is invariant under the $*$-operation.

- One type of such subset is defined by introducing a wave vector cutoffs Λ, i.e. setting

$$\mathcal{B}^* = \mathcal{B}^*(\Lambda) = \{\boldsymbol{q} \in \Gamma^* : -\Lambda \le q_i \le \Lambda\} \tag{21}$$

  While a spherical cutoff can also be introduced, for our purposes the cubic cutoff geometry implied by (21) turns out to be more convenient. In fact, parametrizing $\Lambda = \Lambda(l)$ by an integer $0 < l < L/2$ as $\Lambda(l) = 2\pi l/L$, we can just as well write

$$\mathcal{B}^* = \mathcal{B}^*(l) = \{\boldsymbol{q} = (2\pi/L)(m_i, \ldots, m_d) \in \Gamma^* : -l \le l_i \le l\} \tag{22}$$

  In terms of trying to accomplish the task of computing the full partition function of the system, all "fast" modes $\tilde{\varphi}(\boldsymbol{q})$ for wave vectors $\boldsymbol{q} \notin \mathcal{B}^*(\Lambda)$ can be thought of "having already been integrated out" at the expense of leaving an *effective* Hamiltonian governing the behavior of the remaining "slow" modes. In other words, as long as we are not interested in microscopic specifics of our system but only in its universal asymptotic behavior at long wavelengths, we are free to choose a convenient effective (Landau-Ginzburg) Hamiltonian from the appropriate universality class subject to a convenient cutoff Λ. For small Λ, the number $|\mathcal{B}^*|$ of residual wave vectors participating in such a simulation will then be considerable smaller than the original number of lattice sites N. Conversely stated, since π resembles the lattice cutoff corresponding the zone boundary of the original lattice, then the introduction of a cutoff $\Lambda(l)$ amounts to effectively simulating a system with a linear size $\pi/\Lambda(l) = L/2l$ larger than the original one.

- Another important application of FMC concerns coarse-grained systems, in which one wants to integrate over a "momentum shell"

$$\mathcal{B}^* = \mathcal{B}^*(\Lambda, \Lambda_0) = \{\boldsymbol{q} \in \Gamma^* : \Lambda \le |q_i| \le \Lambda_0\} \tag{23}$$

  where, of course, $\Lambda < \Lambda_0$ (the terminology is inspired by quantum field theory). Similar to (22), this subset of the Brillouin zone can be parametrized as

$$\mathcal{B}^* = \mathcal{B}^*(l, l_0) = \{\boldsymbol{q} = (2\pi/L)(m_i, \ldots, m_d) \in \Gamma^* : l \le |l_i| \le l_0\} \tag{24}$$

  Such momentum shells are encountered, for instance, in calculations of renormalization group transformations following Wilson's momentum shell prescription [3, 4, 5].

In a practical implementation of FMC it is important to recognize that, being composed of sums of two wave vectors taken from $\mathcal{B}^*$, the wave vectors $\boldsymbol{Q}$ parametrizing the array of amplitudes $\tilde{S}(\boldsymbol{Q})$ will generally *not* be elements of the set $\mathcal{B}$ but rather of the larger set

$$C^* := \{\boldsymbol{q} + \boldsymbol{p} : \boldsymbol{q}, \boldsymbol{p} \in \mathcal{B}^*\} \quad \supset \mathcal{B}^* \tag{25}$$

Thus, in a critical simulation of a long-range interacting system, the cutoff Λ must indeed be chosen much smaller than $\pi/2$ in order to really gain an advantage over a real space implementation.

Apart from these considerations, a further and in fact major advantage of FMC in the simulation of critical systems is, however, the collective nature of its move set (as opposed to the local move set suggested by direct lattice algorithms), and the possibility to dramatically reduce or even remove critical slowing down by optimizing the step widths of amplitude shifts separately for each wave vector [6].

For convenience, we finally introduce the notation

$$\mathcal{B}^p := \mathcal{B}^* \cap \Gamma^p, \qquad C^p := C^* \cap \Gamma^p, \qquad p = 0, \pm \tag{26}$$

Of course, all the above formulas, which were defined with respect to the full BZ, can be appropriately restricted to the subspaces $\mathcal{B}^*, C^*$ simply by declaring $\tilde{\varphi}(\boldsymbol{q}) \equiv 0$ if $\boldsymbol{q} \notin \mathcal{B}^*$ and $\tilde{S}(\boldsymbol{Q}) \equiv 0$ for $\boldsymbol{Q} \notin C^*$.

Dependent on the chosen cutoff geometry for the problem at hand, $\mathcal{B}^*$ and C^* may often contain the zone center zero vector $\boldsymbol{h} = \boldsymbol{0}$ (known as the so-called Γ point in spectroscopy [14, 18]), but exclude the remaining high-symmetry vectors from Γ^0. As some of the formulas for computing energy changes turn out to be slightly different for MC shifts of real modes as opposed to complex ones, it turns out to be convenient to organize the arrays $\tilde{\varphi}(\boldsymbol{q})$ and $\tilde{S}(\boldsymbol{Q})$ as follows. In a C style array declared as **double** complex* phi, we would, of course, place $\tilde{\varphi}(\boldsymbol{q} = \boldsymbol{0})$ at index 0, followed by all values of the complex modes for vectors $\boldsymbol{q} \in \mathcal{B}^*$ of positive parity in a convenient order (for instance, partially ordered by increasing size $|\boldsymbol{q}|$), eventually adding the modes belonging to the remaining high-symmetry vectors $\boldsymbol{h} \in \mathcal{B}^0$ in case they are needed.

The array **double** complex* S is organized similarly. As Formula (16) shows, each single step in sums generating this array from the array of values $\tilde{\eta}(\boldsymbol{q})$ requires to add pairs of vectors $\boldsymbol{p}^* \in \mathcal{B}^*$ and $\boldsymbol{Q} \in C^+$, and so does each FMC move (see formulas (36) and (37) below). One may therefore consider tabulating these sums and keeping the resulting 2-dimensional index table, which we may declare as **int** **vsum, in memory during the simulation. In a practical FMC study, one frequently studies the system with fixed lattice size and cutoff but at various values of the coupling constants and initializations of the array $\tilde{\varphi}(\boldsymbol{q})$. These choices neither affect the table **vsum nor any of the other Brillouin zone data. Efficient use of CPU time therefore suggests to store this invariant structural information on the Brillouin zone (total numbers of vectors in $\mathcal{B}^0, \mathcal{B}^+, C^0, C^+$ and their integer coordinate values) together with this index table in a binary file, which is the read into memory at each start-up of an actual simulation run.

4. Formulas for energy changes under Fourier Monte Carlo moves

In FMC, the basic MC move consists of the following steps:

- Draw a wave vector $\boldsymbol{k} \in \mathcal{B}^*$ at random.
- If $\boldsymbol{k} \equiv \boldsymbol{h} \in \mathcal{B}^0$, draw a real number r from an interval $[-\rho(\boldsymbol{h}), \rho(\boldsymbol{h})]$ and shift

$$\tilde{\varphi}(\boldsymbol{q}) \to \tilde{\varphi}(\boldsymbol{q}) + r\delta_{\boldsymbol{q},\boldsymbol{h}} \tag{27}$$

- If $\boldsymbol{k} \in \mathcal{B}^\pm$, draw a complex number ϵ from an circle of radius $\rho(\boldsymbol{k})$ in the complex plane and shift

$$\tilde{\varphi}(\boldsymbol{q}) \to \tilde{\varphi}(\boldsymbol{q}) + \epsilon\delta_{\boldsymbol{q},\boldsymbol{k}} + \epsilon^*\delta_{\boldsymbol{q},\boldsymbol{k}^*} \tag{28}$$

  (in a practical implementation, we will only need the case $\boldsymbol{k} \in \mathcal{B}^+$, but (28) is more convenient for proving the formulas below).

4.1. Harmonic energy shift

We split the harmonic part of the Hamiltonian into the separate contributions of real and complex modes as

$$E_2 \equiv \frac{1}{2}\sum_{\boldsymbol{q}\in\mathcal{B}^*} \tilde{D}_N(\boldsymbol{q})|\tilde{\varphi}(\boldsymbol{q})|^2 = \frac{1}{2}\sum_{\boldsymbol{h}\in\mathcal{B}^0} \tilde{D}_N(\boldsymbol{h})\tilde{\varphi}^2(\boldsymbol{h}) + \sum_{\boldsymbol{q}\in\mathcal{B}^+} \tilde{D}_N(\boldsymbol{q})|\tilde{\varphi}(\boldsymbol{q})|^2 \tag{29}$$

A shift

$$\tilde{\varphi}(\boldsymbol{q}) \to \tilde{\varphi}(\boldsymbol{q}) + r\delta_{\boldsymbol{q},\boldsymbol{h}}, \qquad r \in \mathbb{R},\ \boldsymbol{h}^* = \boldsymbol{h} \tag{30}$$

of a real-valued mode then induces a change $\delta E_2 := E_2' - E_2$ of the harmonic energy

$$\delta E_2 = \frac{1}{2} D_N(\boldsymbol{h})(\tilde{\varphi}(\boldsymbol{h}) + r)^2 - \frac{1}{2} D_N(\boldsymbol{h})\tilde{\varphi}^2(\boldsymbol{h}) = D_N(\boldsymbol{h})\left[r\tilde{\varphi}(\boldsymbol{h}) + r^2/2\right] = D_N(\boldsymbol{h})\left[r\varphi(\boldsymbol{h}) + r^2/2\right] \tag{31}$$

Similar straightforward manipulations show that a shift

$$\tilde{\varphi}(\boldsymbol{k}) \to \tilde{\varphi}(\boldsymbol{k}) + \epsilon\delta_{\boldsymbol{k},\boldsymbol{k}_0} + \epsilon^*\delta_{\boldsymbol{k},\boldsymbol{k}_0^*} \tag{32}$$

of a *complex* mode results in a change

$$\delta E_2 = D_N(\boldsymbol{k}_0)\left[\epsilon^*\varphi(\boldsymbol{k}_0) + \epsilon\varphi(\boldsymbol{k}_0^*) + |\epsilon|^2\right] = D_N(\boldsymbol{k}_0)\left\{2\Re\left[\epsilon^*\varphi(\boldsymbol{k}_0)\right] + |\epsilon|^2\right\} \tag{33}$$

4.2. Anharmonic energy shift

Similar to the harmonic energy contribution, we can separate

$$E_4 \equiv \frac{B_N}{4}\sum_{\boldsymbol{Q}\in C^*} |\tilde{S}(\boldsymbol{Q})|^2 = \frac{B_N}{4}\sum_{\boldsymbol{H}\in C^0} |\tilde{S}(\boldsymbol{H})|^2 + \frac{B_N}{2}\sum_{\boldsymbol{Q}\in C^+} |\tilde{S}(\boldsymbol{Q})|^2 \tag{34}$$

A shift $\tilde{S} \to \tilde{S} + \delta\tilde{S}$ induces a change $\delta E_4 = E_4' - E_4$ of

$$\delta E_4 = \frac{B_N}{4}\sum_{\boldsymbol{H}\in C^0}\left[(\delta\tilde{S}(\boldsymbol{H}))^2 + 2\tilde{S}(\boldsymbol{H})\delta\tilde{S}(\boldsymbol{H})\right] + \frac{B_N}{2}\sum_{\boldsymbol{Q}\in C^+}\left[\delta\tilde{S}(\boldsymbol{Q})\delta\tilde{S}(\boldsymbol{Q}^*) + \tilde{S}(\boldsymbol{Q})\delta\tilde{S}(\boldsymbol{Q}^*) + \delta\tilde{S}(\boldsymbol{Q})\tilde{S}(\boldsymbol{Q}^*)\right] \tag{35}$$

Thus, it remains to calculate the changes $\delta\tilde{S}(\boldsymbol{H})$, $\boldsymbol{H} \in C^0$ and $\delta\tilde{S}(\boldsymbol{Q})$, $\boldsymbol{Q} \in C^+$. Actually the formulas turn out to be identical for both cases. Under a shift of type (27) of a real mode $\tilde{\varphi}(\boldsymbol{h})$, it is easy to see that

$$\delta\tilde{S}(\boldsymbol{Q}) = 2r\tilde{\varphi}([\boldsymbol{Q} + \boldsymbol{h}]) + r^2\delta_{\boldsymbol{Q},\boldsymbol{0}} \tag{36}$$

In contrast, a somewhat longer but equally easy calculation shows that shifting a complex mode $\tilde{\varphi}(\boldsymbol{k})$ according to (28) yields a change

$$\delta\tilde{S}(\boldsymbol{Q}) = 2\epsilon\tilde{\varphi}([\boldsymbol{Q} + \boldsymbol{k}^*]) + 2\epsilon^*\tilde{\varphi}([\boldsymbol{Q} + \boldsymbol{k}]) + \epsilon^2\delta_{\boldsymbol{Q},[2\boldsymbol{k}]} + 2|\epsilon|^2\delta_{\boldsymbol{Q},\boldsymbol{0}} + (\epsilon^*)^2\delta_{\boldsymbol{Q},[2\boldsymbol{k}^*]} \tag{37}$$

Formulas (31), (33) and (35)–(37) are all we need in order to calculate the energy changes under MC moves of type (27) and (28). Based on these formulas, it is then straight forward to implement a standard Metropolis MC scheme.

To debug the resulting implementation, the author recommends to implement FMC for the simple nearest neighbor φ^4 model defined by Eqn. (9) without any cutoff restrictions, and to compare the resulting values for the total energies, energy changes and so on with those of its "native" implementation on the direct lattice, which is a trivial thing to do in comparison. In addition, after each single MC move, to detect errors in the code it is highly recommended to constantly monitor and compare the configurations of the fields $\tilde{\varphi}(\boldsymbol{k})$ and $\varphi(\boldsymbol{x})$ and the resulting configurations $\tilde{S}(\boldsymbol{Q})$ and $\varphi^2(\boldsymbol{x})$ generated by both codes during the test phase of an implementation of FMC by utilizing the discrete Fourier transformation formulas listed above.

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