A projection method for statics and dynamics of lattice spin systems

M. Kolesik,1,2 M. A. Novotny,1 and P. A. Rikvold1,3
1 Supercomputer Computations Research Institute, Florida State University, Tallahassee, Florida 32306-4130
2 Institute of Physics, Slovak Academy of Sciences, Dábravská cesta 9, 84228 Bratislava, Slovak Republic
3 Center for Materials Research and Technology, and Department of Physics, Florida State University, Tallahassee, Florida
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A method based on Monte Carlo sampling of the probability flows projected onto the subspace of one or more slow variables is proposed for investigation of dynamic and static properties of lattice spin systems. We illustrate the method by applying it, with projection onto the order-parameter subspace, to the three-dimensional 3-state Potts model in equilibrium and to metastable decay in a three-dimensional 3-state kinetic Potts model.

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The widespread use of computer simulations in many fields of physics presents a constant challenge to develop new, faster, and more efficient algorithms. Here we describe a method to study dynamic and static properties of spin lattice systems. It is based on Monte Carlo sampling of the probability flow projected onto the subspace of one or more slow variables. Here we use the order parameter. The projected information is subsequently used to reconstruct dynamic and/or static quantities. This idea was first explored by Schulman [1], and a similar approach for the dynamics of metastable decay was developed by Lee et al. [2] and in Ref. [3]. The present work extends these developments. We show how appropriately sampled projected probability flows can be utilized to investigate static probability distributions, as well as the dynamics of spin systems. The method is illustrated for three cases. The first two deal with three-dimensional, three-state Potts models in equilibrium. The ferromagnetic model at its transition temperature is considered in order to explain, for a generic situation, the basics of the method. This model is of interest also in lattice-gauge theory [4]. Next, the antiferromagnetic model below its critical temperature is included to show an unusual example of the phase structure. Although only intended as an illustration, these results greatly elucidate previous Monte Carlo observations of a medium-temperature phase in this model [5]. Our third example concerns the application to the dynamics of metastable decay in the 3-dimensional 3-state kinetic ferromagnetic Potts model, which can be regarded as an extension of the Ising model approximation for extremely anisotropic magnetic systems [6]. We demonstrate the strength of the method by measuring metastable lifetimes in a region of weak fields, where direct simulations are not feasible.

Consider a 3-state Potts model with the Hamiltonian $H = -J \sum_{\langle i,j \rangle} \delta(\sigma_i, \sigma_j)$ where $\sigma_i \in \{0, 1, 2\}$ is the “spin” at lattice site $i$, and the summation runs over all nearest-neighbor pairs on a simple-cubic lattice. Macroscopically, the system is characterized by the concentrations $\{n_0, n_1, n_2\}$, $\sum n_i = 1$, of spins in the three states. These triples are mapped into an equilateral triangle representing the order-parameter space. In Figs. 1 and 2, the projection of a point onto the axis extending from the $i$-th corner gives the concentration $n_i$.

Consider a simulation using a Monte Carlo method with local updates at randomly chosen sites. At any given moment, the spins can be divided into classes specified by the state $\sigma$ of the spin and by the numbers $\{a, b, 6-a-b\}$ of its neighbors in the states $\{0, 1, 2\}$. Let $p^{\sigma\sigma'}(n_0, n_1, n_2)$ be the average equilibrium population of spins in the class $\{\sigma, a, b\}$, conditional on the total concentrations $n_i$ of spins in state $i$. Further, denote by $p^{\sigma\sigma'}_{ab}$ the probability that a spin in the class $\{\sigma, a, b\}$ will flip to the state $\sigma'$ when visited by the updating algorithm.

The central objects of the proposed method are the global flip rates $v^{\sigma\sigma'}(n_0, n_1, n_2)$:

$$v^{\sigma\sigma'}(n_0, n_1, n_2) = \sum_{ab} c^{\sigma\sigma'}_{ab}(n_0, n_1, n_2) p^{\sigma\sigma'}_{ab}.$$  \hspace{1cm} (1)

They define an ideal aggregate Markov process on the order-parameter space $\{(n_0, n_1, n_2)\}$. This process gives an exact equilibrium aggregated probability density $P(n_0, n_1, n_2)$, which can be calculated from the detailed-balance condition $P(n_0 + 1, n_1, n_2) = p^{\sigma\sigma'}_{ab}(n_0, n_1, n_2) v^{\sigma\sigma'}_{ab}(n_0, n_1, n_2)$ plus analogous equations for the other transitions.

Of special importance are the zeroes of the “drift functions” $v^{\sigma\sigma'} - v^{\sigma'\sigma}$, since they determine the extremal points of the probability densities. For the statics of the Potts model, we restrict ourselves to these zero loci.

We simulated the ferromagnetic model ($J = 1$) at its first-order phase transition temperature $T = 1.81618$ for a $20^3$ lattice. Flip-rate histograms were binned using $2^{14}$ equilateral triangles covering the whole order-parameter triangle, and $10^6$ configurations were typically generated. Figure 3(a) shows a schematic picture of the drift in one of the three directions. Its zero locus consists of two parts. The first one is the symmetry axis of the triangle, and the second is a symmetric arc. We only show...
a portion of the arc, since the statistics become insufficient far from the probability density maxima. Flows in different directions are related by rotations of $2\pi/3$. All three zero loci are superimposed in Fig. 1(b). Where three loci corresponding to different directions intersect, the probability density has a stationary point. There are three stable extrema $S_i$, corresponding to the three ordered phases. The three points $U_i$ are saddle points, and the center of the triangle represents the stable, disordered phase. This example shows how one identifies candidates for stable phases from the intersections of the drift-function zero loci.

![FIG. 1. (a): Zeros of the drift $v_{12} - v_{21}$ in the $1 \leftrightarrow 2$ direction for the 3-dimensional 3-state Potts ferromagnet. Light solid lines are stable loci, while dashed lines are unstable. Heavy arrows indicate the direction of the probability flow. (b): Zero loci for the three directions superimposed. See text for a full description.](image)

Next, we turn to the antiferromagnetic Potts model ($J=-1$). Because of the sublattice-symmetry breaking, we sampled the flip rates for each sublattice separately. Figure 2 shows the union of the zero loci of the drift functions in all three directions. As in the ferromagnetic case, for each direction there is the symmetry induced straight line (triangle axis) and a nontrivial part, which is here a closed curve. The closed-curve parts of the zero loci have several interesting properties:

1. The closed loci for the three different directions are identical and can be accurately parameterized by

$$\{m \cos t + r \cos 2t, m \sin t - r \sin 2t\}, \ t \in (0, 2\pi). \tag{2}$$

2. Positions of the sublattices on this curve are correlated in such a way that their distance (sublattice magnetization difference $|AB| = 2m$ in Fig. 2) is constant.

3. There are finite-size effects in the diameter and shape of the curve, but there is no sign that it separates into three distinct components.

We stress that the only observed deviations from these properties are numerical uncertainties on the order of the discreteness of the order-parameter space. On lattices smaller than $32^3$, we sampled complete flip-rate histograms as in the ferromagnetic case. On larger lattices, we only measured flip rates at isolated points of the order-parameter space (typically $5 \times 10^4$ configurations). The data were then interpolated and used to find the roots of the drift functions. In this way, we could confirm the above observations, even with lattices as large as $64^3$, by measuring flip rates only in the vicinity of the expected zero locus. In fact, having located two points we can predict the rest with an accuracy suggesting that the parameterization of Eq. (2) may be exact.

![FIG. 2. Zero locus of the drift functions $v_{\sigma\sigma'} - v_{\sigma'\sigma}$ of the 3-dimensional 3-state Potts antiferromagnet at $T = 1.0J$. The dashed sections of the triangle axes are unstable in directions perpendicular to the axes. The solid parts are stable. The closed, solid curve is stable in all three directions. This curve, obtained for a $64^3$ lattice, represents the degenerate maximum of the probability density of a sublattice location in the order-parameter space.](image)
have added a term describing the interaction with the external field $H$. With this choice of the external field, the model can be regarded as an extension of the kinetic Ising model, which can serve as an approximation for nanoscale ferromagnets [3]. The third spin state of the present model can mimic local magnetization “perpendicular” to the external field and allows for “finite anisotropy.” The Glauber dynamics with updates at randomly chosen sites is used throughout the rest of the paper. Time is measured in Monte Carlo Steps per Spin (MCSS).

An essential quantity related to metastability is the lifetime $\tau$, defined as follows. All spins are initialized in state 0, the temperature $T < T_c$ is fixed, and an external magnetic field $H$ favoring state 1 and disfavoring state 0 is applied. The field does not interact with spins in state 2. This initial state is metastable and decays through the nucleation and subsequent growth of stable-phase droplets. The average time needed to reach a configuration with half of the system in the stable phase is $\tau$.

The difficulty is that realistic models, subjected to “experimentally reasonable” magnetic fields, have lifetimes which are extremely long in terms of the Monte Carlo time. Here we describe a significant extension of the method proposed in Refs. [1–3]. This allows us to obtain lifetimes in experimentally reasonable magnetic fields, have lifetimes which are extremely long in terms of the Monte Carlo time. Here we describe a significant extension of the method proposed in Refs. [1–3]. This allows us to obtain lifetimes in arbitrarily weak fields without prohibitively lengthy simulations.

The projected flip rates are defined, as in the static case, in terms of the normalized spin-class populations $c_{ab}^\sigma (n)$ and flipping probabilities $p_{ab}^\sigma$: 

$$g(n) = \sum_{ab, \sigma \neq 1} c_{ab}^\sigma (n) \ p_{ab}^\sigma , \ s(n) = \sum_{ab, \sigma \neq 1} c_{ab}^\sigma (n) \ p_{ab}^\sigma .$$  

We parameterize $g$ and $s$ only by the total number $n$ of spins in state 1, thus projecting the population data onto a one-dimensional histogram. The rates $g$ and $s$ correspond to growth and shrinkage of the stable phase. They depend on the external field and on the way the configurations are generated, as explained below.

The flip rates are used to map the metastable-decay dynamics onto a one-dimensional absorbing Markov chain. We assign to all configurations with $n$ overturned spins a single state $n$ in the chain. The one-dimensional dynamics is given by the flip rates. From state $n$ we have the probability $g(n)$ of jumping to state $n + 1$, the probability $s(n)$ of jumping to $n - 1$, and the probability $1 - s(n) - g(n)$ of remaining in the current state. This random walk starts at $n = 0$ and terminates when it reaches $n = N$, corresponding to a stopping criterion which we chose to be $N = V/2$, with $V$ the volume of the system. Using standard methods from the theory of absorbing Markov chains [3], we obtain the mean lifetime $\tau$ and the total average time $h(n)$ (measured in MCSS, with $h(N) = 0$) spent by the random walker in the state $n$ as

$$\tau = \sum_{n=0}^{N-1} h(n) , \ h(n - 1) = \frac{V^{-1} + s(n) h(n)}{g(n - 1)} .$$  

How accurately these formulas reproduce the lifetime depends on how the class populations are sampled. One option is to sample them in zero external field in an equilibrium ensemble with conserved order parameter for each needed value of $n$. Such data can be used to estimate the lifetime in very weak fields, but in strong fields it is underestimated because the class populations near the top of the free-energy barrier are not reproduced well by the equilibrium ensemble.

The simple but important improvement presented here is the way the class populations are measured. At any time, the system is only allowed to have $n$, the number of spins in the stable phase, larger than a time-dependent lower bound, $n_{\text{min}}$. Simulation starts with $n_{\text{min}}(t=0) = -1$, and $n_{\text{min}}$ is increased slowly. The class populations $c_{ab}^\sigma$ are sampled during this forced-escape simulation with an applied external field and are subsequently used to calculate the lifetime from Eqs. (3,4).

Why does this work? Consider first the limit of zero forcing speed ($n_{\text{min}} = -1$ at all times). One starts a simulation by releasing a “random walker” from the initial state. When the walker reaches the absorbing state, one starts a new run and repeats the whole process until $N_{\text{esc}}$ escapes from metastability are realized. One can imagine that each walker generates an oriented “world line.” Therefore, an “equation of continuity” holds for each $n < N$: $N_{n\rightarrow n+1} = N_{\text{esc}} + N_{n+1\rightarrow n}$ with $N_{i\rightarrow j}$ the number of transitions between the subspaces with $i$ and $j$ overturned spins. It is straightforward to express this equality in terms of the transition probabilities and class populations as generated by the simulation. One obtains a relation for $h(n)$ equivalent to Eq. (4). Thus, if the forcing is infinitely slow, Eqs. (3,4) give the exact $\tau$.

Now, if the rate of increase of $n_{\text{min}}$ is nonzero but sufficiently small, the system always produces nearly the “correct” configurations as if there were no forcing. While deep in the metastable free-energy well, forcing prevents the system from returning to $n \leq n_{\text{min}}$, but it still allows it to thermalize and generate metastable configurations with $n$ at and slightly above $n_{\text{min}}$. As $n_{\text{min}}$ increases, the procedure scans the configurations along the escape path from metastability. When $n_{\text{min}}$ approaches the top of the free-energy barrier, the system has a better chance to escape, and the stable phase grows too quickly to equilibrate. There is nothing to prevent escape, because there is no upper bound on $n$ which would cause unwanted thermalization. The system is free to escape through natural nonequilibrium configurations.

To approach the slow-forcing limit in practice, one performs a series of measurements and determines a value of $dn_{\text{min}}/dt$ below which the estimated lifetime is insensitive to the choice of $dn_{\text{min}}/dt$. We expect such forcing speed to be related to the inverse equilibration time for states deep in the metastable well. Another computationally important aspect is to obtain sufficient statistics for the forced escapes, since the class-population data tend to
be noisy at and beyond the top of the free-energy barrier. Here, we measured about $10^3$ escapes at rates up to $dn_{\text{min}}/dt \approx 10^{-3} \text{MCSS}^{-1}$.

![Figure 3](image)

**FIG. 3.** The metastable lifetime of a 3-dimensional 3-state kinetic Potts ferromagnet as a function of the magnetic field for two system sizes at $T \approx 0.55T_c$. Symbols □ and ◊ are simulation results (with error bars smaller than the symbol size), and lines connect the points (+) calculated from the class-population data sampled by the forced-escape method. The inset shows a comparison of the measured (circles) and calculated (line) relative standard deviation of the lifetime.

Figure 3 shows a comparison between the lifetimes obtained from direct simulations and those calculated with the forced-escape method. The agreement is excellent for lifetimes in the whole region accessible to direct simulations. Moreover, the forced escape method can provide lifetime estimates deep in the region of weak fields, where direct simulation is practically impossible. We emphasize that having measured the class populations, one can utilize them to calculate lifetimes for an arbitrary local dynamic with random updates. We can e.g. calculate what the lifetimes would be if we used the Metropolis instead of the Glauber dynamic simply by replacing the flip probabilities $p^a_{\text{G}}$. Although different dynamics produce different flip rates, the class-populations remain close to local equilibrium and are therefore similar for all dynamics that obey detailed balance.

In a similar way as the average lifetime $\tau$, one can use the flip rates to calculate higher moments of the lifetime probability distribution [13]. The inset in Fig. 3 shows the relative standard deviation $\Delta \tau/\tau$ as a function of the field. Despite the fact that the higher moments, unlike the mean lifetime, are only approximate even in the slow-forcing limit, the agreement between the directly simulated results and those based on the forced-escape method (solid line) is good. We believe this is because the relevant Markov chains are nearly weakly lumpable with respect the states along the escape from metastability. For a quantitative description of the form of $\tau$ and $\Delta \tau/\tau$, see Refs. [8] and [13].

In summary, we propose a new method to study the dynamic and static properties of lattice spin systems. It consists in Monte Carlo sampling of the spin-class populations in a projected subspace. These are subsequently used to calculate the spin-flip rates. In the static case, the knowledge of the flip rates is equivalent to the information contained in the probability density. However, the accuracy of the method is much better than with direct distribution sampling. We have demonstrated this on the example of the 3-state antiferromagnetic Potts model. The flip rates can be also utilized to obtain dynamic characteristics of the systems, such as lifetimes, in very weak fields where ordinary simulations are not feasible. Although the resulting dynamic is only an approximation, it provides accurate estimates. The detailed information about the class populations enables one to calculate the lifetime for an arbitrary dynamic with updates at randomly chosen sites, independently of the dynamic used during the data sampling.

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