The Ising Model with Hybrid Monte Carlo

Johann Ostmeyer,[1] Evan Berkowitz,[2,3] Thomas Luu,[2] Marcus Petschlies,[1] and Ferenc Pittler[4]

[1] *Helmholtz-Institut für Strahlen- und Kernphysik, Rheinische Friedrich-Wilhelms-Universität Bonn, 53012 Bonn Germany*
[2] *Institut für Kernphysik & Institute for Advanced Simulation, Forschungszentrum Jülich, 54245 Jülich Germany*
[3] *Maryland Center for Fundamental Physics, University of Maryland, College Park 20742, USA*
[4] *Computation-based Science and Technology Research Center, The Cyprus Institute, 20 Kavafi Street, 2121 Nicosia, Cyprus*

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The Ising model is a simple statistical model for ferromagnetism. There are analytic solutions for low dimensions and very efficient Monte Carlo methods, such as cluster algorithms, for simulating this model in special cases. However most approaches do not generalise to arbitrary lattices and couplings. We present a formalism that allows one to apply Hybrid Monte Carlo (HMC) simulations to the Ising model, demonstrating how a system with discrete degrees of freedom can be simulated with continuous variables. Because of the flexibility of HMC, our formalism is easily generalizable to arbitrary modifications of the model, creating a route to leverage advanced algorithms such as shift preconditioners and multi-level methods, developed in conjunction with HMC.

I. INTRODUCTION

The Ising model is a simple model of ferromagnetism and exhibits a phase transition in dimensions $d \geq 2$. Analytic solutions determining the critical temperature and magnetization are known for $d = 1$ and 2 [1], and in large dimensions the model serves as an exemplary test bed for application of mean-field techniques. It is also a popular starting point for the discussion of the renormalization group and calculation of critical exponents.

In many cases systems that are seemingly disparate can be mapped into the Ising model with slight modification. Examples include certain neural networks [2, 3], percolation [4–6], ice melt ponds in the arctic [7], financial markets [8–10], and population segregation in urban areas[11, 12], to name a few. In short, the applicability of the Ising model goes well beyond its intended goal of describing ferromagnetic behavior. Furthermore, it serves as an important pedagogical tool—any serious student of statistical/condensed matter physics as well as field theory should be well versed in the Ising model.

The pedagogical utility of the Ising model extends into numerics as well. Stochastic lattice methods and the Markov-chain Monte-Carlo (MCMC) concept are routinely introduced via application to the Ising model. Examples range from the simple Metropolis-Hastings algorithm to more advanced cluster routines, such as Swendsen-Wang [13] and Wolff [14] and the worm algorithm of Prokof'ev and Svistunov [15]. Because so much is known of the Ising model, it also serves as a standard test bed for novel algorithms. Machine learning (ML) techniques were recently applied to the Ising model to aid in identification of phase transitions and order parameters [16–20].

A common feature of the algorithms mentioned above is that they are well suited for systems with discrete internal spaces, which of course includes the Ising model. For continuous degrees of freedom the hybrid Monte Carlo (HMC) algorithm[21] is instead the standard workhorse. Lattice quantum chromodynamics (LQCD) calculations, for example, rely strongly on HMC. Certain applications in condensed matter physics now also routinely use HMC[22–24]. Furthermore, algorithms related to preconditioning and multi-level integration have greatly extended the efficacy and utility of HMC. With the need to sample posterior distributions in so-called big data applications, HMC has become widespread even beyond scientific applications.

It is natural to ask, then, how to apply the numerically-efficient HMC to the broadly-applicable Ising model. At first glance, the Ising model's discrete variables pose an obstacle for smoothly integrating the Hamiltonian equations of motion to arrive at a new proposal. We hope this paper serves a pedagogical function, as a nice platform for introducing both HMC and the Ising model, and a clarifying function, demonstrating how HMC can be leveraged for models with discrete internal spaces.

So, for pedagogical reasons, our implementation of HMC is the simplest 'vanilla' version. As such, it does not compete well, in the numerical sense, with the more advanced cluster algorithms mentioned above. However, it seems likely that by leveraging the structure of the Ising model one could find a competitive HMC-based algorithm, but we leave such investigations for the future.

This paper is organized as follows. In Section II we review the Ising model. We describe how one can transform the Ising model, which resides in a discrete spin space, into a model residing in a continuous space by introducing an auxiliary field and integrating out the spin degrees of freedom. The numerical stability of such a transformation is not trivial[1], and we describe the conditions for maintaining stability. With our continuous space defined, we show in

[1] Such stability considerations have been egregiously ignored in the past.

Section III how to simulate the system with HMC. Such a discussion of course includes a cursory description of the HMC algorithm. In Section IV we show how to calculate observables within this continuous space, since quantities such as magnetization or average energy are originally defined in terms of spin degrees of freedom which are no longer present. We also provide numerical results of key observables, demonstrating proof-of-principle. We conclude in Section V.

II. FORMALISM

The Ising model on a lattice with N sites is described by the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} s_i s_j - \sum_i h_i s_i \tag{1}$$

$$= -\frac{1}{2} J s^\top K s - h \cdot s \tag{2}$$

where $s_i = \pm 1$ are the spins on sites $i = 1, \ldots, N$, J the coupling between neighbouring spins (denoted by $\langle i, j \rangle$), h_i is the local external magnetic field, and the $^\top$ superscript denotes the transpose. We also define the symmetric connectivity matrix K containing the information about the nearest neighbour couplings. The factor $\frac{1}{2}$ on the nearest-neighbor term (2) accounts for the double counting of neighbour pairs that arises from making K symmetric. If h is constant we write

$$h = h_0 \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} . \tag{3}$$

We assume a constant coupling for simplicity in this work. The same formalism developed here can however be applied for site-dependent couplings as well. In this case we simply have to replace the matrix JK by the full coupling matrix.

The partition sum over all spin configurations $\{s_i\} \equiv \{s_i \,|\, i = 1, \ldots, N\}$

$$Z = \sum_{\{s_i\}=\pm 1} \mathrm{e}^{-\beta H} \tag{4}$$

with the inverse temperature β is impractical to compute directly for large lattices because the number of terms increases exponentially, providing the motivation for Monte Carlo methods. Our goal is to rewrite Z in terms of a continuous variable so that molecular dynamics (MD) becomes applicable. The usual way to eliminate the discrete degrees of freedom and replace them by continuous ones is via the Hubbard-Stratonovich (HS) transformation. For a positive definite matrix $A \in \mathbb{R}^{N \times N}$ and some vector $v \in \mathbb{R}^N$, the HS relation reads

$$\mathrm{e}^{\frac{1}{2} v^\top A v} = \frac{1}{\sqrt{\det A \, (2\pi)^N}} \int_{-\infty}^{\infty} \left[\prod_{i=1}^{N} \mathrm{d}\phi_i \right] \mathrm{e}^{-\frac{1}{2} \phi^\top A^{-1} \phi + v \cdot \phi} \tag{5}$$

where we integrate over an *auxiliary field* ϕ. The argument of the exponent has been linearized in v. In our case the matrix $J'K$ with

$$J' \coloneqq \beta J \tag{6}$$

takes the place of A in the expression above. However, $J'K$ is not positive definite in general, nor is $-J'K$. The eigenvalues λ of K are distributed in the interval

$$\lambda \in [-n, n] \tag{7}$$

where n is the maximal number of nearest neighbours a site can have. In the thermodynamic limit $N \to \infty$ the spectrum becomes continuous and all values in the interval are reached. Thus the HS transformation is not stable: the Gaussian integral with negative eigenvalues does not converge.

We have to modify the connectivity matrix in such a way that we can apply the HS transformation. Therefore we introduce a constant shift C to the K matrix,

$$\tilde{K} \coloneqq K + C \, \mathbb{1}, \tag{8}$$

where C has to have the same sign as J', by adding and subtracting the corresponding term in the Hamiltonian. Now $\tilde{K}$ has the same eigenspectrum as K, but shifted by C. Thus if we choose $|C| > n$, $J'\tilde{K}$ is positive definite. We will take such a choice for granted from now on. For variable coupling the interval (7) might have to be adjusted, but the eigenspectrum remains bounded from below, so C can be chosen large enough to make $J'\tilde{K}$ positive definite.

Now we can apply the HS transformation to the partition sum

$$Z = \sum_{\{s_i\}=\pm 1} \mathrm{e}^{\frac{1}{2}\beta J s^\top \tilde{K} s - \frac{1}{2}\beta J C s^2 + \beta h \cdot s} \tag{9}$$

$$= \mathrm{e}^{-\frac{1}{2}J'CN} \sum_{\{s_i\}=\pm 1} \mathrm{e}^{\frac{1}{2}J' s^\top \tilde{K} s + h' \cdot s} \tag{10}$$

$$= \mathrm{e}^{-\frac{1}{2}J'CN} \sum_{\{s_i\}=\pm 1} \frac{1}{\sqrt{\det \tilde{K}\,(2\pi J')^N}} \int_{-\infty}^{\infty} \left[\prod_{i=1}^{N} \mathrm{d}\phi_i\right] \mathrm{e}^{-\frac{1}{2J'}\phi^\top \tilde{K}^{-1}\phi + (h'+\phi)\cdot s} \tag{11}$$

$$= \frac{\mathrm{e}^{-\frac{1}{2}J'CN}}{\sqrt{\det \tilde{K}\,(2\pi J')^N}} \int_{-\infty}^{\infty} \left[\prod_{i=1}^{N} \mathrm{d}\phi_i\right] \mathrm{e}^{-\frac{1}{2J'}\phi^\top \tilde{K}^{-1}\phi} \left[\prod_{i=1}^{N} 2\cosh\left(h'_i + \phi_i\right)\right] \tag{12}$$

$$= 2^N \frac{\mathrm{e}^{-\frac{1}{2}J'CN}}{\sqrt{\det \tilde{K}\,(2\pi J')^N}} \int_{-\infty}^{\infty} \left[\prod_{i=1}^{N} \mathrm{d}\phi_i\right] \mathrm{e}^{-\frac{1}{2J'}\phi^\top \tilde{K}^{-1}\phi + \sum_i \log\cosh\left(h'_i+\phi_i\right)} \tag{13}$$

where we used in (10) that $s_i^2 = 1$ for all i and defined $h' \coloneqq \beta h$ analogously to (6). In (11) we performed the HS transformation and in (12) we explicitly evaluated the sum over all the now-independent s_i, thereby integrating out the spins. After rewriting the cosh term in (13) we are left with an effective action that can be used to perform HMC calculations. However, we do not recommend using this form directly, as it needs a matrix inversion.

Instead, let us perform the substitution

$$\phi = \sqrt{J'}\tilde{K}\psi - h' \tag{14}$$

with the functional determinant $\sqrt{J'}^N \det \tilde{K}$. This allows us to get rid of the inverse of $\tilde{K}$ in the variable part of the partition sum

$$Z = \sqrt{\left(\tfrac{2}{\pi}\right)^N \det \tilde{K}}\, \mathrm{e}^{-\frac{1}{2}J'CN} \int_{-\infty}^{\infty} \left[\prod_{i=1}^{N} \mathrm{d}\psi_i\right] \mathrm{e}^{-\frac{1}{2}\psi^\top \tilde{K}\psi + \frac{1}{\sqrt{J'}}\psi\cdot h' - \frac{1}{2J'}h'^\top \tilde{K}^{-1} h' + \sum_i \log\cosh\left(\sqrt{J'}\left(\tilde{K}\psi\right)_i\right)}. \tag{15}$$

The only left over term involving an inversion remains in the constant $h'^\top \tilde{K}^{-1} h'$. Fortunately this does not need to be calculated during HMC simulations. We do need it, however, for the calculation of some observables, such as the magnetisation (27), and for this purpose it can be calculated once without any need for updates.

A further simplification can be achieved when the magnetic field is constant (3) and every lattice site has the same number of nearest neighbours n_0. Then we find that

$$\tilde{K} h' = (n_0 + C)\, h' \tag{16}$$

and thus

$$h'^\top \tilde{K}^{-1} h' = h'^\top \frac{1}{n_0 + C} h' = \frac{N}{n_0 + C} h_0'^2 . \tag{17}$$

III. HMC

Hybrid Monte Carlo requires introducing a fictitious time and conjugate momenta, integrating current field configurations according to Hamiltonian equations of motion to make a Metropolis proposal. The effective action for the auxiliary field ψ (15) can be used to derive a Hamiltonian by adding conjugate momenta p,

$$\mathcal{H} = \frac{1}{2}p^2 + \frac{1}{2}\psi^\top \tilde{K}\psi - \frac{1}{\sqrt{J'}}\psi \cdot h' - \sum_i \log\cosh\left(\sqrt{J'}\left(\tilde{K}\psi\right)_i\right) \tag{18}$$

with the equations of motion (EOM)

$$\dot{\psi} = \frac{\partial \mathcal{H}}{\partial p} = p \tag{19}$$

$$\dot{p} = -\frac{\partial \mathcal{H}}{\partial \psi} = -\tilde{K}\psi + \frac{1}{\sqrt{J'}}h' + \sqrt{J'}\tilde{K}\tanh\left(\sqrt{J'}\tilde{K}\psi\right) \tag{20}$$

where the tanh is understood element-wise.

Thus one can employ the hybrid Monte Carlo (HMC) algorithm. Starting with some initial ψ configuration, p is sampled according to a Gaussian distribution $\mathrm{e}^{-\frac{1}{2}p^2}$. The EOM are integrated to derive a new configuration. The integration of the differential equations is performed by a symmetric symplectic integrator (we use leap-frog here, but more efficient schemes can be applied). The new configuration is accepted with the Metropolis-Hastings probability $\min\left(1, \mathrm{e}^{-\Delta\mathcal{H}}\right)$ in order to maintain detailed balance despite inexact numerical integration; $\Delta\mathcal{H} = \mathcal{H}_{\text{new}} - \mathcal{H}_{\text{old}}$ is the corresponding energy difference.

After some thermalization a number N_{cf} of configurations $\{\psi^n\}$ is created and the estimator of an observable $O(\psi)$

$$\overline{O} = \frac{1}{N_{\text{cf}}}\sum_{n=1}^{N_{\text{cf}}} O(\psi^n) \tag{21}$$

converges to the expectation value

$$\langle O\rangle = \frac{1}{Z}\sqrt{\left(\tfrac{2}{\pi}\right)^N \det\tilde{K}}\,\mathrm{e}^{-\frac{1}{2}J'CN}\int_{-\infty}^{\infty}\left[\prod_{i=1}^{N}\mathrm{d}\psi_i\right] O(\psi)\,\mathrm{e}^{-\frac{1}{2}\psi^\top\tilde{K}\psi + \frac{1}{\sqrt{J'}}\psi\cdot h' - \frac{1}{2J'}h'^\top\tilde{K}^{-1}h' + \sum_i \log\cosh\left(\sqrt{J'}\left(\tilde{K}\psi\right)_i\right)} \tag{22}$$

as the ensemble size $N_{\text{cf}} \to \infty$.

Not much time has been spent on the tuning of C during this work. We expect that the choice of C can influence the speed of the simulations. Clear is that $|C|$ must not be chosen too large because in the limit $|C| \to \infty$ the Hamiltonian can be approximated by

$$\frac{1}{C}\mathcal{H} = \frac{1}{2}\psi^2 - \sqrt{J'}\sum_i |\psi_i| + \mathcal{O}\left(C^{-1}\right) \tag{23}$$

with the minima

$$\psi_i = \pm\sqrt{J'}. \tag{24}$$

Any deviation from a minimum is enhanced by the factor of C and is thus frozen out for large $|C|$. This reproduces the original discrete Ising model up to normalisation factors. Plainly the HMC breaks down in this case. As the limit is approached, the values for the ψ_i become confined to smaller and smaller regions. The result is that HMC simulations can get stuck in local minima and the time series is no longer ergodic. From now on we use $|C| = n + 10^{-5}$.

A large coupling (at low temperature) J' introduces an ergodicity problem as well. This case however is less problematic because there are only two regions with a domain wall between them; the region with all $\psi_i > 0$ and the region with all $\psi_i < 0$. The ergodicity issue is alleviated by proposing a global sign flip and performing a Metropolis accept/reject step every couple of trajectories, similar to that proposed in [24].

IV. RESULTS

Let us again assume constant external field with strength h_0 (3). Then the expectation value of the average magnetisation and energy per site read

$$\langle m\rangle = \frac{1}{NZ}\frac{\partial Z}{\partial h'} \tag{25}$$

$$= \frac{1}{N}\left\langle \frac{1}{\sqrt{J'}}\sum_i \psi_i - \frac{N}{n_0 + C}\frac{h'_0}{J'}\right\rangle \tag{26}$$

$$= \frac{\langle\psi\rangle}{\sqrt{J'}} - \frac{1}{n_0 + C}\frac{h'_0}{J'}, \tag{27}$$

$$\langle\beta\varepsilon\rangle = -\frac{\beta}{NZ}\frac{\partial Z}{\partial\beta} \tag{28}$$

$$= \frac{1}{2}CJ' + \frac{1}{n_0 + C}\frac{{h'_0}^2}{2J'} - \frac{h'_0}{2\sqrt{J'}}\langle\psi\rangle - \frac{\sqrt{J'}}{2N}\left\langle\left(\tilde{K}\psi\right)\cdot\tanh\left(\sqrt{J'}\tilde{K}\psi\right)\right\rangle \tag{29}$$

where $\langle\psi\rangle = \langle\psi_i\rangle$ for any site i due to translation invariance. Any other physical observables can be derived in the same way. For example, higher-point correlation functions like spin-spin correlators may be derived by functionally differentiating with respect to a site-dependent h_i (without the simplification of constant external field (17)). We stress here that, although C appears in observables (as in the magnetization (27) and energy density (29)), the results are independent of C—its value only influences the convergence rate.

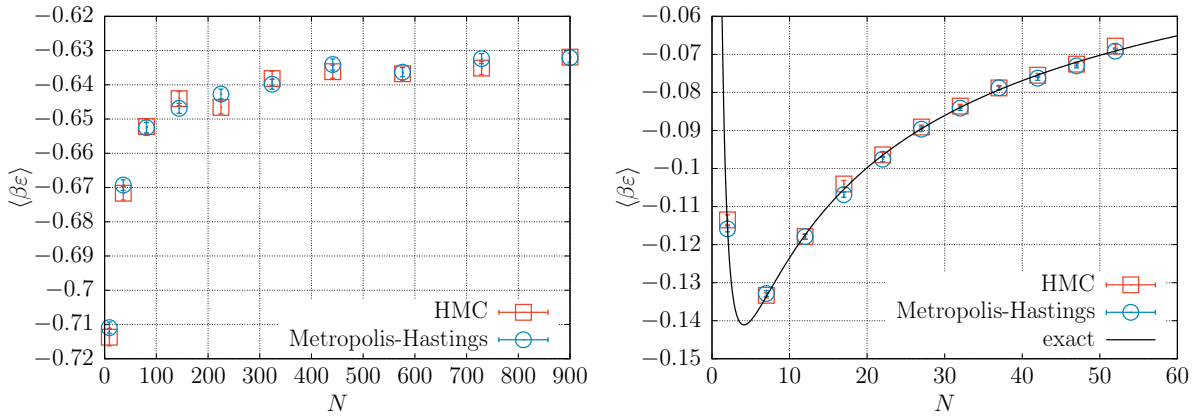

Figure 1. Expectation value of the energy per site for the two dimensional periodic square lattice (left) and the lattice with all-to-all coupling (right) for the HMC and the Metropolis-Hastings algorithms at critical coupling and $h = 0$ with lattice sizes N.

In Figure 1 we demonstrate that the HMC algorithm indeed produces correct results. The left panel shows the average energy per site at the critical point [1] of the two-dimensional square lattice with periodic boundary conditions. The results from the HMC simulations[2] are compared to the results obtained via the local Metropolis-Hastings algorithm with the same number N_{cf} of sweeps (a sweep consists of N spin flip proposals). We not only find that the results are compatible, but also that the errors are comparable. The right panel shows the average energy per site in the case where the coupling is no longer nearest neighbor, but the extreme opposite with all-to-all couplings. This "infinite-range" Ising model [25] has analytic solutions for physical observables as a function of the number of lattice sites N which we show for the case of the average energy (black line). Our numerical results agree very well with the exact result.

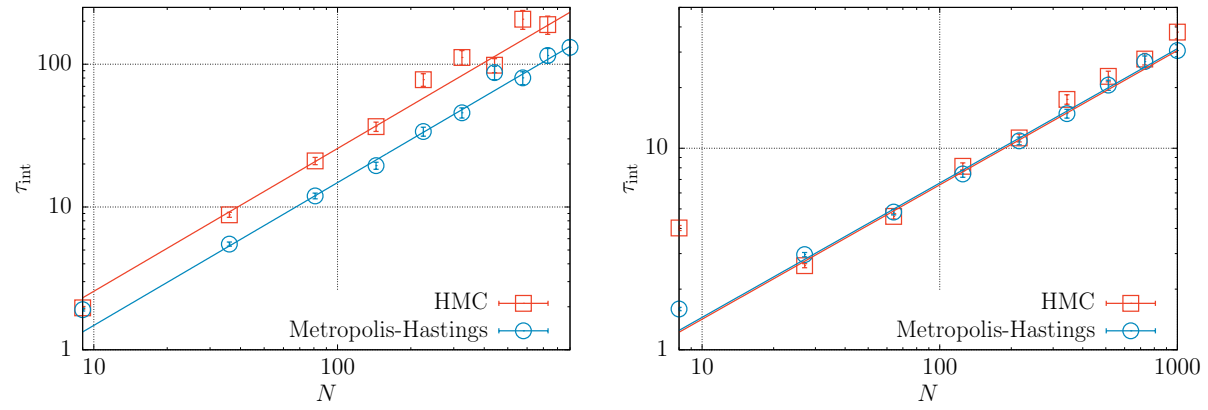

Figure 2. Integrated autocorrelation time of $|m|$ for the HMC and the Metropolis-Hastings algorithms at critical coupling and $h = 0$ for the $d = 2$ (left) and $d = 3$ (right) dimensional periodic square lattice with size N. The lines are fits of the form $\tau_{\text{int}} = \alpha N^{\frac{2}{d}}$ for $N > 10$.

Since it is not the aim of this work to present physical results, but rather to introduce an alternative formulation for simulating the Ising model and generalizations thereof, we do not compute other observables explicitly, nor do

[2] The number of integration steps per trajectory has been set to $\log N$. It turns out that this yields acceptance rates between 70% and 80% for a broad range of lattice sizes and dimensions.

we investigate their dependence on other parameters. On the other hand it is not sufficient that the algorithm in principle produces correct results—we must also investigate its efficiency. A good measure for the efficiency is the severity of *critical slowing down*—that the integrated autocorrelation time[3] τ_{int} diverges at the critical point as some power γ of the system size $\tau_{\text{int}} \propto N^{\gamma}$. One could expect that, being a global update algorithm, the HMC does not suffer as much from critical slowing down as Metropolis-Hastings. Figure 2 however shows that both algorithms have dynamic exponent $z \equiv d\gamma \approx 2$ in $d = 2$ and $d = 3$ dimensions (see Ref. [27] and references within for a discussion of the critical coupling and exponents in $d = 3$). Still one has to keep in mind that a Metropolis-Hastings sweep takes less time than an HMC trajectory and the HMC trajectories become logarithmically longer as N grows.

V. CONCLUSION

In this paper we showed how to apply the HMC algorithm to the Ising model, thereby successfully applying an algorithm that uses continuous state variables to a system with discrete degrees of freedom. We find that the HMC algorithm generalises the Ising model very well to arbitrary geometries without much effort. It has been presented here in the most simple form. In this simple form the HMC is an extremely inefficient algorithm if applied to the Ising model. Although more flexible than the most efficient methods, such as cluster algorithms, it loses as compared even to the Metropolis-Hastings algorithm. The coefficient by which the Metropolis-Hastings algorithm surpasses the HMC decreases with dimension, so that HMC might be preferable in case of an extremely high number of nearest neighbours—in the case of less local coupling, for example.

Moreover, for physical systems that suffer from sign problems, one may hope to leverage complex Langevin, Lefschetz thimble, or other contour-optimizing methods (for a dramatically incomplete set of examples, consider, respectively, Ref. [28, 29], Refs. [30–32], and Refs. [33–35] and references therein). The formulation in terms of continuous variables presented here is well-suited for these methods, while the methods that deal directly with the original discrete variables such as the Metropolis-Hastings, cluster, and worm algorithms, for example, are non-starters. In that sense, our exact reformulation and HMC method can be seen as the first step towards solving otherwise-intractable problems.

The HMC algorithm could be optimised by more efficient integrators and different choices of C, just to name the most obvious possibilities. Many more methods have been developed to improve HMC performance and it is expected that some of them could also speed up the Ising model.

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