



REVERSIBLE ISING DYNAMICS

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ABSTRACT

I discuss a reversible deterministic dynamics for Ising spins. The algorithm is a variation of microcanonical Monte Carlo techniques and is easily implemented with simple bit manipulation. This provides fast programs to study non-equilibrium phenomena such as heat flow.

In this talk I will consider a variation on the microcanonical Monte Carlo algorithm that I discussed in last year's lattice gauge conference at Argonne. I introduced the present model in a recent preprint, to which you should refer for more details.

The microcanonical Monte Carlo method combines features of conventional Monte Carlo simulations of the Boltzmann distribution and molecular dynamics calculations. The algorithm involves the use of one or more auxiliary variables, called "demons," to transfer energy between the various degrees of freedom of a statistical system. In this way the combined energy of the system and the demons is held exactly constant. While this method can be useful for determining couplings in Monte Carlo renormalization group studies, its main virtue appears to be that for discrete systems, such as the Ising model, it can be programmed to run an order of magnitude faster than conventional Monte Carlo algorithms.

Here I wish to consider these demon variables more seriously as a part of the system. I will have one such variable for each site of an Ising lattice. This will then play the role of a momentum conjugate to the corresponding Ising spin. While still serving as temporary storage places for the lattice energy, the momenta can no longer

transfer energy from one site to another. Instead, energy can only flow through the lattice bonds via the Ising interaction.

In this dynamics, as in molecular dynamics, temperature is a stochastic concept. The energies of the immobile demons fluctuate according to the Boltzmann distribution. The temperature is defined by inverting this distribution as observed on averages over a region of space or time, or both.

Before proceeding to a detailed description of the microscopic rules, let me discuss the obvious question of whether the dynamics is ergodic. Indeed, it is easily shown not to be. The algorithm commutes with translations of the lattice. Thus any state which is periodic will remain so. Of course, conventional molecular dynamics simulations have similar symmetries. The fraction of states with such symmetries should become insignificant as the volume of the system goes to infinity. It would, however, be interesting to know if the dynamics has any more subtle symmetries which can seriously further limit ergodicity.

For simplicity I will consider the two dimensional model for the remainder of the talk. On each site of the lattice are four bits. The first of these is simply the Ising spin $S_i \in \{\pm 1\}$. associated with these spins is the energy

$$H_i = \sum_{\{ij\}} S_i S_j \quad (1)$$

where the sum is over all nearest neighbors. The next two bits on each site form a two bit integer $D_{2,i}, D_{1,i}$ ($D_{j,i} \in \{0,1\}$) representing the momentum conjugate to the spins. They are associated with the kinetic energy

$$H_K = 4 \sum_i (D_{1,i} + 2 D_{2,i}). \quad (2)$$

The factor of 4 is inserted because flipping any spin in eq. (2) only changes the Ising energy by a multiple of 4, and we wish to keep this property for the kinetic term as well. The fourth bit on each site is its space-time parity. This is used to implement a checkerboard updating without violating the definition of cellular automata. At each

time step we only consider changes of spins on that half of the sites that have a set parity bit. All parity bits are inverted for the next time step. Because of the rather trivial nature of this fourth bit, its value need not actually be stored.

The updating rule for this system is the microcanonical rule of ref. (1) on all spins with set parity bits. The resulting change in the Ising energy associated with the flip of a given spin is calculated. If this change can be absorbed by the kinetic variable on that site, then the spin is flipped and the corresponding change in the momentum made. Otherwise, the spin and its momentum retain their old values. Note that the dynamics is exactly reversed by an extra inversion of the parity bits. Hitting the red squares of our checkerboard twice returns the lattice to its original state.

Temperatures are determined from the distribution of kinetic energies. In particular, we expect

$$P(E_i) \propto \exp(-4 \beta E_i). \quad (3)$$

where I have defined $E_i = D_{1,i} + 2 D_{2,i}$ and $\beta = 1/T$. Thus the average value of E_i can be easily inverted to give the temperature.

Note that this dynamics is constructed so that the total energy

$$H = H_I + H_K \quad (4)$$

is exactly conserved. The only way the energy can flow around the lattice is through the bonds. Although the algorithm can simulate the equilibrium Ising model, it is not particularly good for this. In particular, we will see that a state with an initially non-uniform energy distribution can take a long time to equilibrate if the heat must flow long distances. On the other hand, the procedure allows numerical experiments which cannot be done with conventional Monte Carlo; in particular, one can study this heat flow.

In fig. (1) I show the results of a particular experiment of this type. Here the energy distribution of the initial lattice was not uniform; rather, the center half of the lattice was hotter than the remainder. The figure shows the temperature distribution as a function of distance through the lattice for varying times after the

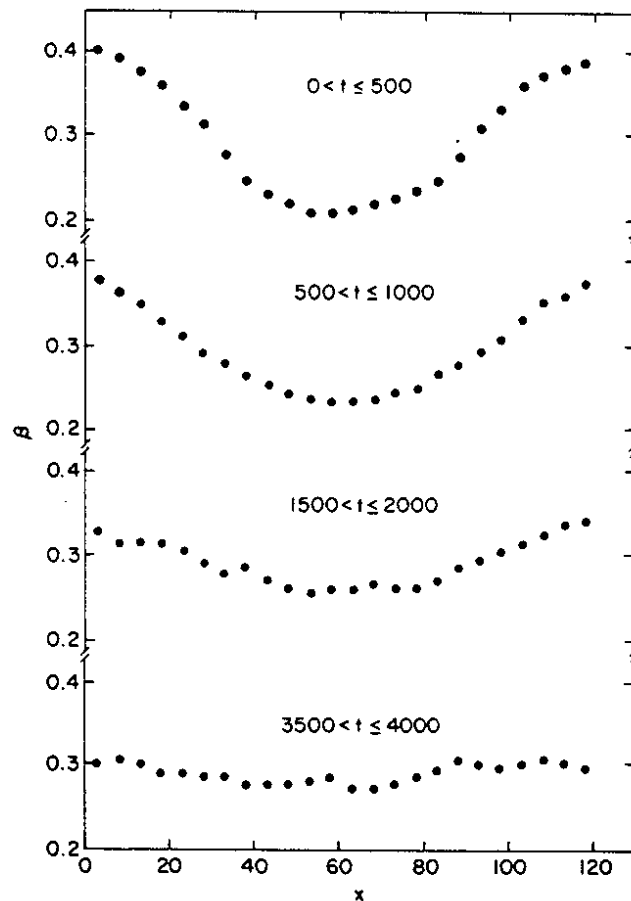


Fig. 1 The evolution of a thermal bump on a 120×120 lattice. The points are the temperature on a given row as obtained from an average over the given time range.

initial configuration. Note that the thermal peak gradually diffuses away and by 4000 iterations it is beginning to dissolve into thermal fluctuations. Thus we are studying a diffusion equation where the computer is only doing simple bit manipulations.

In fig. (2) I show the steady-state thermal profile of a periodic 120 by 120 lattice where heat is added to row 1 (=row 121) after each update and heat is simultaneously removed from row 61. In this experiment the heat was flowing at an average rate Q of 0.016 units per time step per site. Using the linear slope of 0.0055 for small beta in figure 4, we find the thermal conductivity at high temperatures behaves as

$$K \sim 3\beta^2 \quad (5)$$

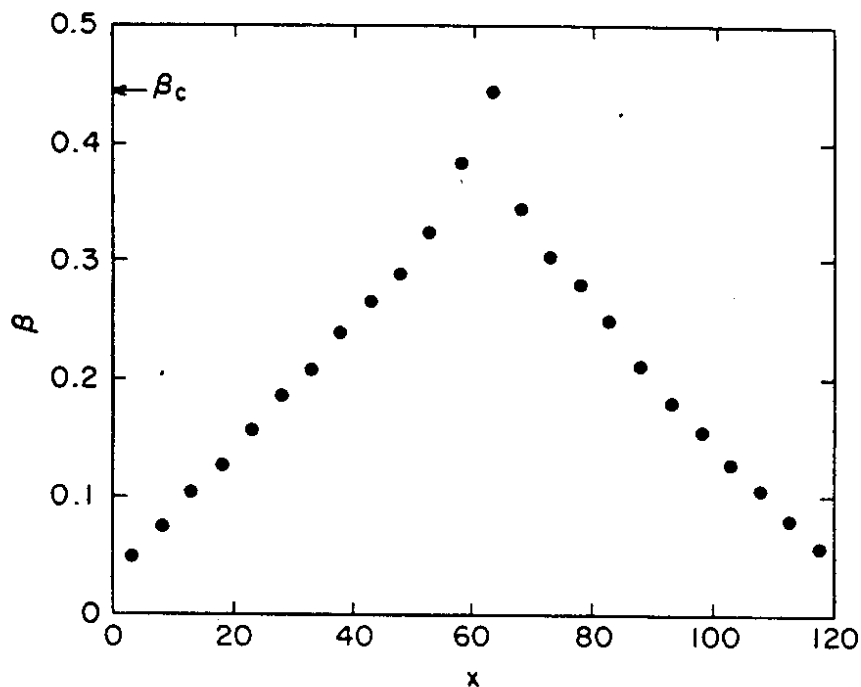


Fig. 2 The steady state thermal profile of a periodic 120×120 lattice heated at row 1 and cooled at row 61.

where K is defined in terms of the heat flow Q by

$$Q = -K \delta T / \delta x. \quad (6)$$

The slope in figure 2 increases rapidly as the critical temperature of the Ising model is approached. This indicates a sharp decrease of the thermal conductivity; indeed, in the ordered phase of this model, the thermal conductivity becomes extremely small, making convergence of this dynamics quite slow.

A good dynamics for statistical treatment should give a path through phase space which is quite sensitive to small disturbances. For our discrete Ising system, the correlation between the spins on two lattices gives a simple definition of a distance between two configurations. In fig. (3) I show the evolution of this correlation when the two lattices initially differ only in the value of a single spin. The correlation is plotted versus the square of the time to give a straight line at short times. This behavior is due to a region of decorrelated spins growing with time linearly in dimension about

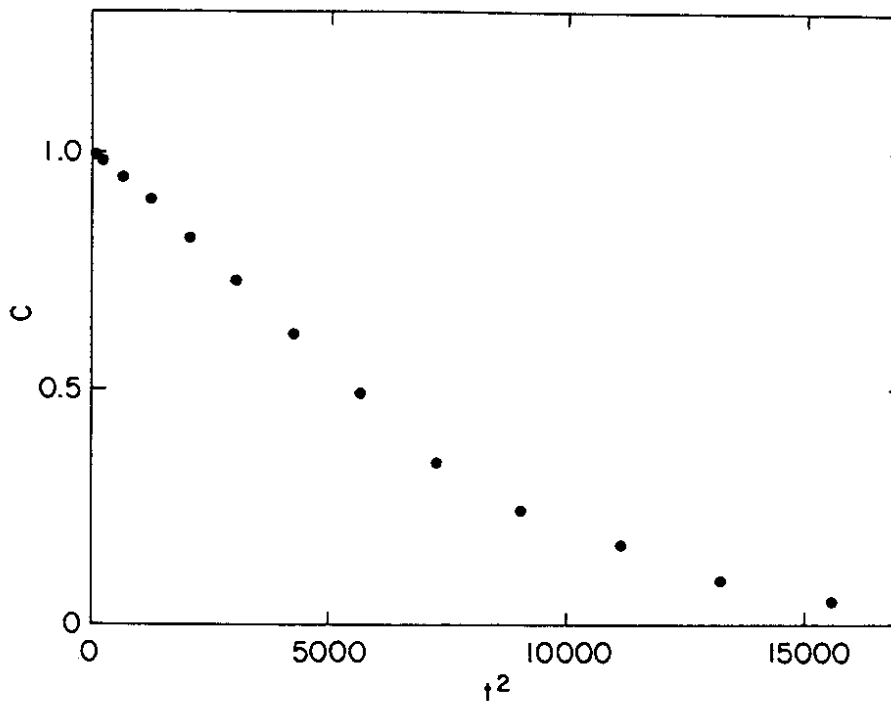


Fig. 3 As a function of time squared, the correlation between two lattices initially differing only in the value of a single spin. The quantity C represents the expectation of a spin on the first lattice times the corresponding spin on the second. The average inverse temperature of the lattices is $\beta = 0.409$.

the initial disturbed spin. An interesting experiment that I have not done is to see if this decorrelated region assumes a circular shape as it grows.

To conclude, I have presented a simple dynamics which is able to simulate a heat equation via an algorithm in which all bits used by the computer are of comparable importance. As the heat equation is a rather generic partial differential equation, the computational advantages of this bit manipulation may have considerably wider application⁴.

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