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Deterministic Ising Dynamics

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A deterministic cellular automaton rule is presented which simulates the Ising model. On each cell in addition to an Ising spin is a space–time parity bit and a variable playing the role of a momentum conjugate to the spin. The procedure permits study of nonequilibrium phenomena, heat flow, mixing, and time correlations. The algorithm can make full use of multispin coding, thus permitting fast programs involving parallel processing on serial machines.

INTRODUCTION

Numerical simulations of statistical systems have become a major tool in the study of phase transitions and critical phenomena. Monte Carlo and molecular dynamics calculations represent two complimentary schemes for such simulations. In the Monte Carlo approach, one generates a Markov chain of configurations using a pseudo-random number generator. The algorithm is constructed, usually using a principle of detailed balance, so that the ultimate probability of encountering any particular configuration is proportional to the Boltzmann weight. The corresponding temperature is a parameter in the program; indeed, the computer is serving as a thermal reservoir at that temperature.

Molecular dynamics calculations, on the other hand, are an attempt to follow the deterministic evolution of a system under an appropriate microscopic Hamiltonian. This approach makes no use of random numbers, the apparent statistical nature of the whole system arising from the complexity of a large phase space. Such algorithms also do not utilize the temperature as an input parameter. Indeed, its value is found after the by fact using the equipartition of energy among the various degrees of freedom. For example, the average kinetic energy of a given molecule should be $\frac{1}{2}kT$ per degree of freedom.

Recently a simulation algorithm interpolating between the Monte Carlo and molecular dynamics techniques was presented [1]. This microcanonical Monte

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Carlo method consists of taking a random walk on a surface of constant energy. To simplify the process of maintaining the constraint that the energy be constant, one or more additional variables, called demons, serve to transfer energy around the system. These variables play a role analogous to the kinetic energy in molecular dynamics in that their average value gives a handle on the temperature of the system. Two advantages of this approach are that it can be programmed to run an order of magnitude faster than conventional Monte Carlo for discrete systems [2], and it does not require high quality random numbers. In addition, generalizing the scheme to several parameters beyond the "temperature," it provides a method for measuring these parameters. This should prove useful in Monte Carlo renormalization group calculations [3].

In this paper we investigate a variation on this microcanonical scheme as applied to the Ising model. Here, however, the "demon" variables do not move around the lattice, but become an integral part of the system. Each site of the lattice is tied to one such variable, which then plays the role of a momentum conjugate to the corresponding spin. Energy is no longer transferred around the lattice by the demons, but can only flow through the bonds via the intrinsic Ising interaction.

In this way we obtain a deterministic Ising dynamics which exactly conserves the total energy. Any localized region can heat or cool only by the transfer of energy from other parts of the lattice. In this respect [illegible] algorithm differs from the stochastic Ising dynamics presented by Gla[illegible] [illegible]epresented by conventional Metropolis simulation [5]. Indeed, those [illegible] parameter representing the temperature. In essence the Glauber system is [illegible]eat reservoir with which energy can be exchanged. In our case, on the other hand, the temperature is a statistical concept which is only defined by averages, which may be over space, time, or both. Because the temperature of the system is internally determined, heat flow and thermal conductivity can be studied numerically. It is not clear that these concepts have any meaning in a conventional Monte Carlo simulation.

A particular advantage of the present scheme is that it is easily implemented by simple bit manipulation. All variables are small integers and no real numbers are used. From a practical point of view, this means that extremely fast programs using multispin coding are possible [2, 6]. This technique uses bit by bit boolean operations to permit parallel processing on a serial machine. The algorithm is also readily amenable to true parallel processing.

From a conceptual point of view, the approach is able to simulate a heat equation via an algorithm in which all bits used by the computer are of comparable importance. This is in sharp contrast to the use of floating point numbers, wherein the first bit of a word is more important that the last. As the heat equation is a rather generic partial differential equation, the computational advantages of this bit manipulation approach may have considerably wider application (a similar point of view has been expressed in [7]).

Our dynamics is set up formally as a collection of cellular automata [8]. Another cellular automaton dynamics discussed in [9], gave several exact results for a variation on the usual three-dimensional Ising model. The approach presented here

differs in being a totally deterministic and reversible dynamics. Unfortunately the present dynamics does not appear to be exactly solvable even in the one dimensional case.

THE DYNAMICS

For simplicity we discuss a two-dimensional square lattice. The algorithm is readily generalized to any dimension or other lattice structures. Associated with each site i of the lattice are four binary bits. Time evolution is by discrete steps, with the values for the site variables at time-step $t+1$ being uniquely determined from their values and those of their nearest neighbors at time t. The updating rule, described in detail below, thus defines a system of deterministic cellular automata.

The first of the four bits on each site is the Ising spin. Considered as a bit taking the value 0 or 1, we denote this variable by B_i. When we wish to use the multiplicative representation of the Z_2 group, we write this variable as

$$S_i = 2_i B_i - 1 \in \{\pm 1\}. \tag{1}$$

The energy of the Ising model is

$$H_I = \sum_{\{i,j\}} S_i S_j, \tag{2}$$

where the sum is over all nearest neighbor pairs of lattice sites.

The next two bits on each site represent the demon or momentum variable conjugate to the spin. These bits represent a two bit integer taking values from 0 to 3. Denoting these bits by $D_{1,i}$ and $D_{2,i}$, we associate with them the kinetic energy

$$H_K = 4 \sum_i (D_{1,i} + 2D_{2,i}). \tag{3}$$

The factor of 4 is inserted because flipping any spin in Eq. (2) only changes the Ising energy by a multiple of four, and we wish to keep this property for the kinetic term as well. The updating algorithm presented below exactly conserves the total energy

$$H = H_K + H_I. \tag{4}$$

Actually the number of bits representing the momentum variable is arbitrary. From an analytic point of view, it might be simpler to consider an arbitrary positive integer. At the opposite extreme, one could consider only a single bit, although in this case the following dynamics in more than one dimension cannot change an isolated spin completely surrounded by antiparallel neighbors. We feel that keeping two bits is a reasonable compromise because in equilibrium the kinetic

term will be excited with a Boltzmann weight. For temperature near the critical value in the two or three-dimensional models, a two bit demon will be fully excited only a few percent of the time and thus two bits are nearly equivalent to an infinity of them.

The fourth bit associated with each site gives the space–time parity of the site. The sole purpose of this bit is to implement a checkerboard style updating. This is a trivial way of circumventing the result of [10], stating that any cellular automaton rule which updates all spins simultaneously cannot simulate the Ising model. Here at each time step we only consider changing spins on that half of the sites that have a set parity bit. All these parity bits are then inverted for the next time–step. Although we refer to this bit as an extra variable, in practice the computer need not actually be storing its value for each site because of its rather trivial nature.

We now give the dynamical rules for updating the spin and momentum variables. When the parity bit for a step is reset ($=0$) the only change is to invert that bit for the next time–step. On the other hand, if the parity bit is set ($=1$), in addition we use the microcanonical rule of [1]. That is, first, the resulting change in the Ising energy of Eq. (2) upon a flip of the spin S_i is calculated. If this change can be absorbed in the momentum variable associated with the same site in such a manner that the total energy of Eq. (4) is exactly conserved, then both the spin is flipped and the momentum is appropriately changed. If, however, the kinetic term is unable to absorb the energy change, then both the spin and associated momentum remain unchanged.

As discussed in [1], on a large system the values of the kinetic variable should become exponentially distributed with the Boltzmann weight corresponding to the temperature $T=1/\beta$ of the system. Thus we expect

$$P(E_i) \propto \exp(-4\beta E_i), \tag{5}$$

where we define $E_i = D_{1,i} + 2D_{2,i}$. Thus the expectation value of E_i gives a means of measuring the system temperature

$$\langle E_i \rangle = \sum_{n=0}^{3} n e^{-4\beta} \Big/ \sum_{n=0}^{3} e^{-4\beta}. \tag{6}$$

This relation is easily inverted to find β. The expectation value in Eq. (6) can be taken either over time or some spatial region or both.

Because of the checkerboard updating implemented with the parity bits, the algorithm requires two time–steps to give every spin of the lattice a chance to change. Thus in comparison to ordinary Monte Carlo simulations, two steps correspond to one full sweep over the system variables.

We close this section by noting that in addition to being deterministic, this dynamics is reversible. A simple inversion of all parity bits between two time–steps will reverse the evolution and send the system exactly backwards through the initial sequence of configurations. This inversion of parity bits amounts to hitting either the red or the black squares of the checkerboard updating procedure twice in a row.

Some Experiments

We now discuss several simple numerical experiments done on the two dimensional model. We use a fully multispin coded program on a CDC 7600 computer. As this uses 60 bit words, we keep our lattice of size 120 in one dimension so that a given row of the lattice occupies two words. In the following we make the other dimension 120 as well. We always work with periodic boundary conditions.

A first question is whether the model actually succeeds in reproducing the Ising model. Figure 1 shows the results of several runs in the vicinity of the critical point of the model. Here we plot the nearest neighbor correlation as a function of the inverse temperature. The points are the results of simulations with the deterministic dynamics and the curve represents the exact solution on an infinite lattice. The simulations represent the average over the last 18,000 of 20,000 time-steps. For initial conditions we took all spins ordered and all momenta as zero except for the second bit of all those lying on sites of even parity. The latter bits were initially set to unity randomly with a given probability for each run. If this probability is a fraction with a denominator which is a power of two, this initial setting of bits can be easily accomplished with logical operations on random words. In Fig. 1 the statistical errors on the measured points are comparable to the size of the dots. Note that the data agree well with the exact solution except near the critical point at $\beta = \frac{1}{2}\log(1+\sqrt{2}) = 0.44068$. Here finite size effects are presumably coming into play.

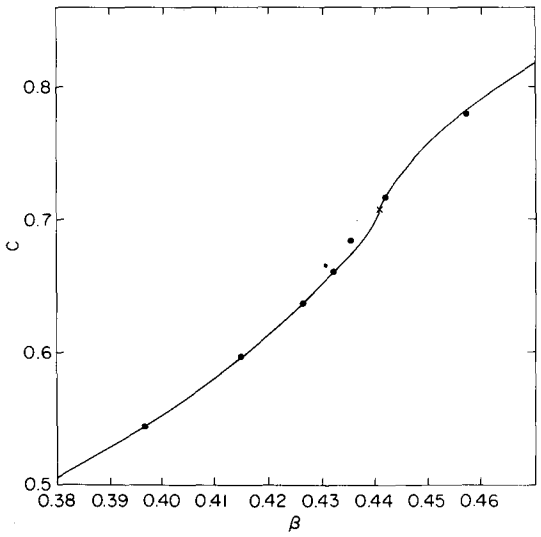

FIG. 1. The nearest neighbor correlation as a function of inverse temperature for the two-dimensional Ising model. The solid line is the exact solution for an infinite lattice and the points are from simulations using the deterministic dynamcis on a 120×120 site lattice. The cross indicates the critical temperature and coupling.

We now turn to some experiments which conventional Monte Carlo could not do. In Fig. 2 we show the relaxation of a system where the initial energy distribution was not uniform. Here we initialized the lattice as above except on rows 31 to 90 the probability of setting second momenta bits on even sites was $\frac{3}{4}$ and on the remaining rows it was $\frac{1}{2}$. Thus the middle half of the lattice contained more energy per site, corresponding to a higher initial temperature. In Fig. 2 the profile of the temperature is plotted at various times. Each point is obtained from the expectation of the momentum variables averaged over five rows and 500 time-steps. For the average over the first 500 steps we see that the lattice center is substantially hotter than the edges. (Actually because the lattice is periodic, there is no true edge.) As time evolves, this temperature peak diffuses away. By 4000 iterations the initial peak is beginning to dissolve into the fluctuations in the local temperature.

We now consider placing a heat source and a heat sink in the lattice. For this

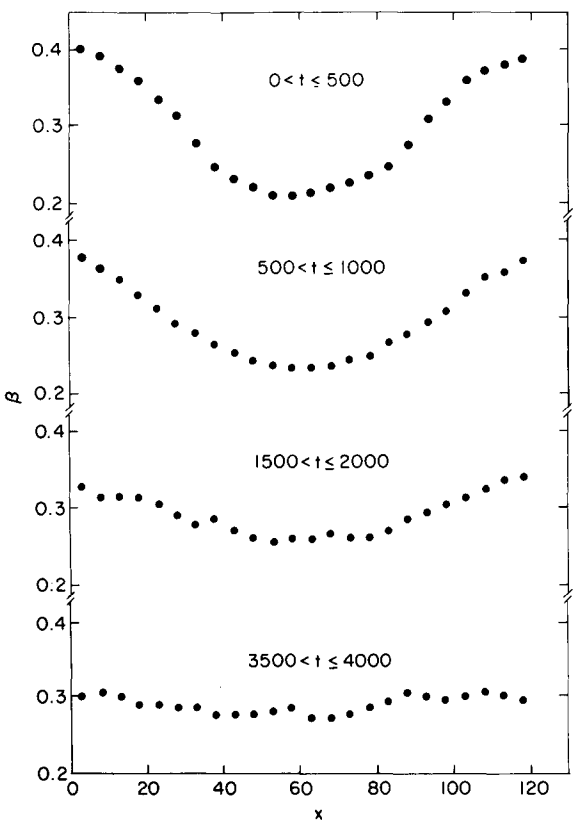

FIG. 2. The evolution of a thermal bump. The initial condition is described in the text. The top points represent the thermal profile averaged over the first 500 time-steps. Descending in the figure, we show $500 < t \leqslant 1000$, $1500 < t \leqslant 2000$, and $3500 < t \leqslant 4000$.

experiment, after each two time–steps we randomize the first bit of all momentum variables on even sites in the first row of the lattice. This effectively couples this row to a high temperature heat source. At the same time we remove heat from row 61 by setting all the momenta on this row to zero. For our initial lattice we procede as before and set all spins and momenta to zero except the second bits of the momenta on even sites, which are set to one with probability $\frac{1}{2}$. In Fig. 3 we show the amount of heat entering and leaving the lattice as a function of time. The quantity plotted here is the change in the energy H per time–step and per spin in the source or the sink row. Each point is an average over 1000 time steps and is divided by two to correct for the two directions heat can flow around our periodic lattice. Note that after 10,000 updates the inflowing and outflowing heats match. Figure 4 shows the final steady state temperature profile as obtained by averaging the momenta in each row over 1000 updates after an initial 19,000.

From the slope in Fig. 4 we can determine a thermal conductivity. We define K by

$$Q = -K\,\Delta T/\Delta x. \tag{7}$$

Here x is the distance through the lattice and Q is the heat flow entering row 1 per spin and per update. Note from the figure that in the high temperature region β is nearly linear in the distance through the lattice. This slope is approximately 0.0055 units in beta per lattice row. From Fig. 3 we see that the heat is flowing at a rate of about 0.016 units per time–step per site. Thus we obtain

$$K \approx 3\beta^2 \tag{8}$$

for the thermal conductivity in the high temperature region. The increase in slope in Fig. 4 as the temperature drops indicates a rapid decrease in the conductivity as the

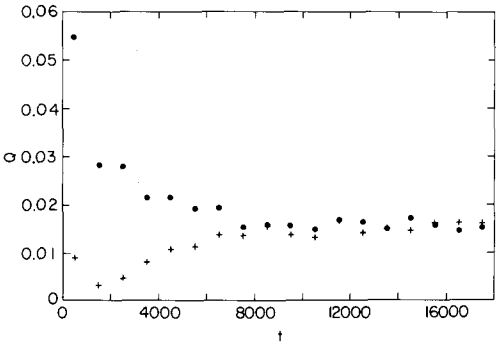

FIG. 3. For the hear flow experiment described in the text, the solid points represent the heat per spin and per time–step entering row 1 and the pluses represent the heat leaving row 61, both plotted as a function of time.

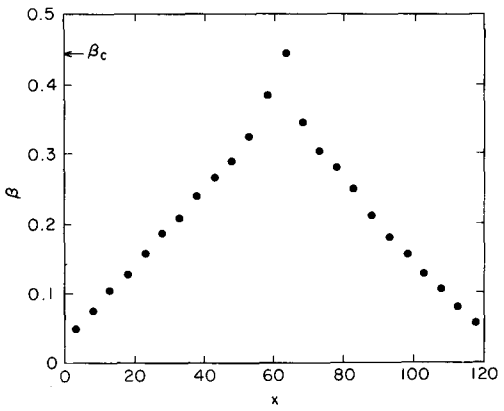

FIG. 4. The steady state thermal profile of a 120×120 lattice heated at row 1 and cooled at row 61.

critical temperature is approached. Indeed, we have found that this conductivity becomes quite small and difficult to measure below the critical point. It would be interesting to have some theoretical predictions for the behavior of this quantity at high and low temperatures.

Given any dynamical rule for evolution, one can ask for correlations between the dynamical variables at different times. In Fig. 5 we show the correlation between a spin and itself at a later time as a function of the time difference. Each plotted point is an average over the lattice and over 5000 time-steps after an initial 1000 to equilibrate. To obtain this average, we used the trick [11] of using two lattices where the second is obtained by doing some number of iterations on the first. The two lattices are then each updated independently and repeatedly compared. This technique allows one to accumulate high statistics on lattices separated by a large number of time steps but without storing a large number of intermediate lattices. Note that the falloff of the correlation with time is initially quite rapid, while eventually a simple exponential behavior sets in. In this figure two values of beta are shown. As might be naively expected, the run closer to the critical point has the longer decorrelation time.

A good dynamics for studying statistical phenomena should give a path through phase-space which is quite sensitive to small disturbances. Indeed, if two trajectories start near one another, they should rapidly diverge from each other if statistical results are to be independent of initial conditions. This mixing phenomenon is easily studied with the dynamics considered here. The correlation between the spins on two lattices gives a simple definition of a distance between two configurations. In Fig. 6 we show the evolution of the correlation between two lattices which initially differ only by one spin being flipped. After an initial 1000 time-steps to get a single lattice into equilibrium, all of its spins and moment are copied into a second lattice. Exactly one spin in this second lattice is then flipped.

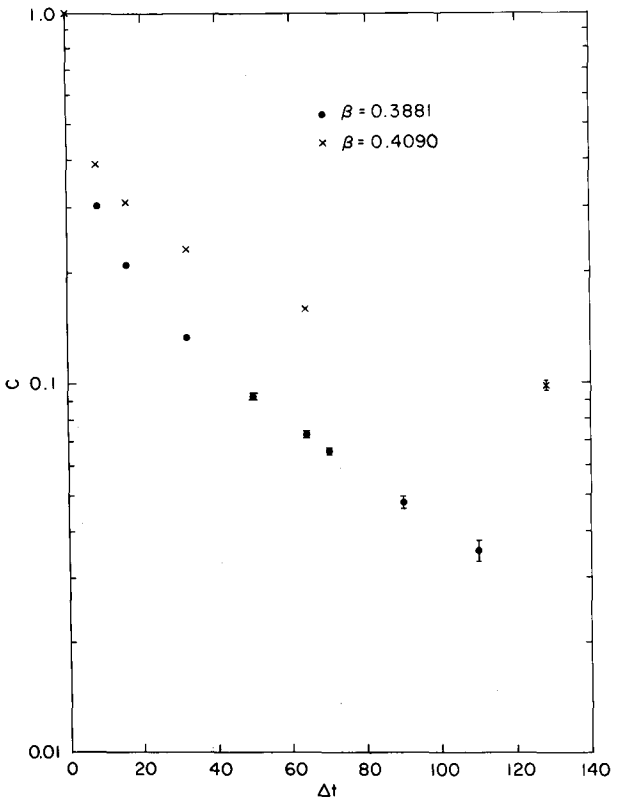

FIG. 5. The temporal correlation of a spin with itself as a function of the time between measurements. The solid points represent a lattice with $\beta = 0.3881$ and the crosses, $\beta = 0.4090$.

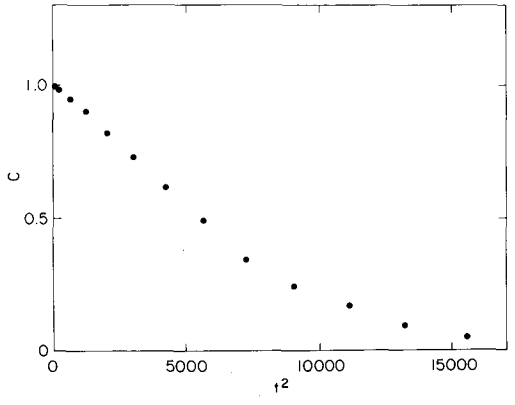

FIG. 6. As a function of time squared, the correlation between two lattices initially differing only in the value of a single spin. The quantity C represents the expectation of a spin on the first lattice times the corresponding spin on the second. The lattices are at $\beta = 0.4090$.

Finally, both lattices are subjected to the dynamics of this paper and compared. The points represent the correlation between corresponding spins in the two lattices; the measurements are averaged over 20 time–steps.

In Fig. 6 we have plotted the data versus t^2. This gives rise to a linear behavior at short times. To understand this, note that any disturbance can propagate into the lattice by at most one spacing in any unit time interval. Thus there is a "speed of light" or maximum velocity with which the effects of any disturbance can propagate. This means that the maximum dimension which can possibly be affected by our initial spin flip grows linearly with time. As our lattice is two dimensional, the volume included in this dimension grows with t^2. The observed behavior indicates that the disturbance we have introduced indeed grows at a constant velocity, although this speed appears to be somewhat less than the maximum possible of one site per update. This velocity is related to the Lyapunov exponent mentioned in [8]. With the model in d dimensions, this argument suggests that the initial behavior of this correlation will be linear in t^d.

Concluding Remark

We have presented a simple dynamical system which simulates the Ising model. An obvious question is whether this dynamics is ergodic. Indeed, it is easy to show that it is not. The rules for temporal evolution are symmetric under certain translations of the entire lattice and its momentum variables. This includes translations in any single coordinate direction by a multiple of two spacings, or a simultaneous translation in two directions by an odd number of sites in each. In addition the dynamics is symmetric to an inversion of all the lattice spins. Thus, if we start with a lattice configuration which is symmetric under any combination of such symmetries, it will remain so. Of course, conventional molecular dynamics calculations can have similar symmetries. For a generic continuous system, configurations carrying a preserved symmetry will represent a set of measure zero in the entire volume of phase–space. With a finite volume Ising system such configurations necessarily represent a finite part of the discrete phase–space, but this fraction should become insignificant as the volume goes to infinity. It would be interesting to know if this dynamics possesses further hidden symmetries beyond those mentioned above.

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