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# Thermal conductivity of a kinetic Ising model

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Using a novel extension of the microcanonical Monte Carlo algorithm, we have simulated the behavior of a two-dimensional nearest-neighbor ferromagnetic Ising model in the presence of a temperature gradient. The technique consists of setting the temperatures of boundary spins, while allowing "demons" associated with the other sites to control heat transfer. We demonstrate that our system is in local thermodynamic equilibrium, and compute the thermal conductivity as a function of temperature.

Large-scale Monte Carlo simulations of systems undergoing complex behavior, such as phase transitions, have led to important insights into fundamental processes.[1,2] In many applications, the dynamical behavior of strongly interacting many-body systems is studied by a Monte Carlo simulation of the master equation. Of course, while a Monte Carlo approach allows the treatment of much of the microscopic behavior, important physics is missing in some problems. For example, in the usual Monte Carlo algorithm, the temperature is fixed by the prescribed interaction of a dynamical system with a heat bath. This can be a useful approximation if the time scales over which thermal diffusion occurs are very fast, but in other problems where the dynamical process is *controlled* by local variations in temperature,[3] it is clearly inadequate. Such problems include the calculation of thermal conductivities and pattern formation by dendritic growth. In this Rapid Communication we study such a dynamical Monte Carlo algorithm which allows the study of the effects of thermal fields. As an application of the method, we obtain numerical results for the thermal conductivity as a function of temperature in a many-body system: the two-dimensional Ising model.

The method we use is based on the microcanonical algorithm of Creutz and co-workers,[4,5] which is complementary to the standard Monte Carlo method. This algorithm has usually been used to study equilibrium properties. However, Creutz[6] has shown that the method can be used for dynamical properties, in a qualitative study of thermal conductivity. Here, we extend and generalize his work, and investigate transport properties in a nonequilibrium steady state. Indeed, just as the equilibrium situation permits measurement of thermodynamic quantities, such as the susceptibility, a nonequilibrium steady state makes possible the direct measurement of thermal conductivity and the observation of transport mechanisms.

Our variant of the microcanonical algorithm models the kinetics by using "demons" (analogous to Maxwell's demon) to control the distribution of energy throughout the system. As in the original algorithm, the demons also allow the measurement of temperature, since their individual distributions become Boltzmann type as the Monte Carlo run proceeds. If one demon is used, in thermodynamic equilibrium with a system of $N$ spins, it has $(1/N)$th of the total energy, so that the situation approximates a microcanonical ensemble with a single temperature. Here, however, we shall use one demon *per* spin, which allows us to monitor *local* temperature fields. In either case, a demon permits flipping of a spin with which it is in contact either if it receives energy thereby, or if it is able to provide sufficient energy for the flip to take place. Thus, the total energy of the spins plus demons is conserved, but over short length and time scales there can be local fluctuations of the energy of the spins, which give rise to thermal diffusion. Thus, the order parameter is nonconserved, but it is coupled to a conserved field, the energy. This is called model $C$ in critical dynamics.[7]

To be explicit, the Hamiltonian we have studied is the two-dimensional ferromagnetic Ising model: $H = -J \times \sum_{\langle ij \rangle} \sigma_i \sigma_j$, where $J$ is the interaction constant, the sums run over distinct nearest-neighbor pairs and the spins take on a value of $\sigma_i = \pm 1$. Our calculations were carried out on a $96 \times 96$ square lattice, which is of sufficient size to represent well the second-order phase transition.[5] Tests were also done on lattices of other sizes. A nonequilibrium steady state was prepared by fixing the temperatures of the top and bottom boundaries: demons there permitted flips if they received energy and permitted energetically unfavorable flips with Boltzmann probabilities. In this manner, a boundary spin is placed in contact with a heat bath as if it were part of a canonical ensemble: Its transition probabilities are those of the Metropolis algorithm.[1] Periodic boundary conditions were used in the transverse direction. We started each run by setting the total energy of the interior spins to a value corresponding to a temperature intermediate between those of the boundaries. The system was then annealed until the temperature profile became stable, before data was taken.

For temperatures above $T_c$, the system was annealed for $3 \times 10^4$ Monte Carlo steps per spin (MCS's), and then time averaged over further periods of $10^4$ MCS's. The particular temperature profile chosen had a high-temperature boundary at $T \approx 8.8 T_c$, while the low-temperature boundary was at $T \approx 1.05 T_c$, where $T_c \approx 2.269J$. Figure 1 shows the derivative of the inverse-temperature $(1/T = \beta)$ profile obtained from the averages of 10 independent runs. Each data point is also averaged over the energy distributions of the demons in a

 

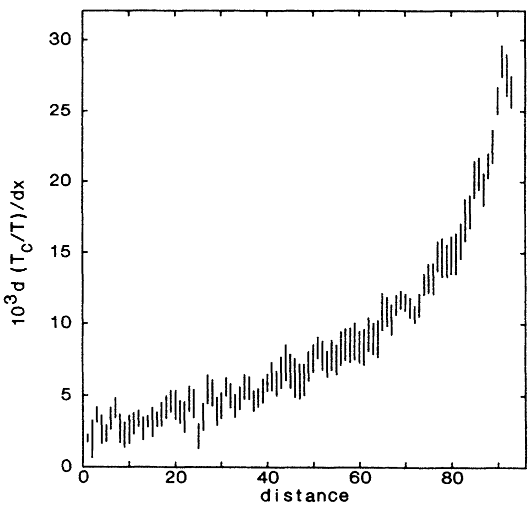


FIG. 1. $d(T_c/T)/dx$ vs $x$ for a system whose boundaries are kept at $T \approx 8.8T_c$ (left-hand side) and $T \approx 1.05T_c$ (right-hand side). Error bars are due to thermodynamic temperature fluctuations, as discussed in the text. The conductivity is calculated by measuring the heat flux through the system.

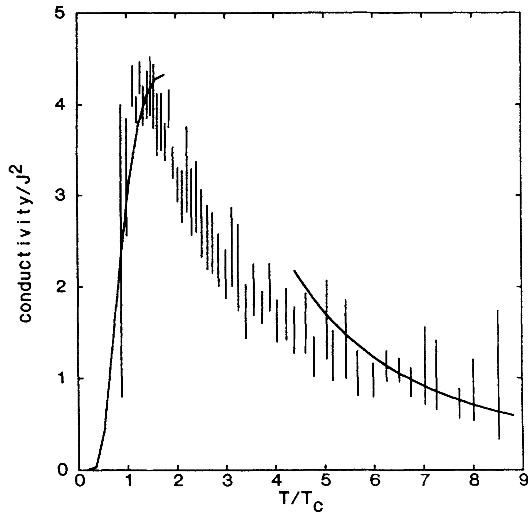


FIG. 2. $\kappa/J^2$ vs $T/T_c$. Solid lines are high- and low-temperature expansion results.

transverse row. The profile in Fig. 1 shows significant curvature, implying that the thermal conductivity varies strongly with temperature. This result is consistent with original qualitative results of Creutz.[6] The errors result from measured fluctuations in $\beta$ and are discussed in detail below.

To calculate the thermal conductivity $\kappa$, we monitored the heat flux $Q$ in the system. This is the average change in the energy of a boundary spin per MCS. When the system had reached local equilibrium, the energies taken up and released, respectively, at the two boundaries agreed within $Q$'s measured 5% statistical fluctuation. Results for $\kappa$ as a function of $T$, using the measured value of the heat flux and the temperature profile of Fig. 1, are given in Fig. 2.

Also shown in Fig. 2 are representative values for $T < T_c$: The data given are for $T = 0.98T_c$ and $T = 0.90T_c$. Approximately $5\times10^4$ MCS's were required to reach a steady state for boundaries held at $T \approx 0.99T_c$ and $T \approx 0.7T_c$. Following this, 10 runs of the same duration were done to produce reasonable statistics for the energy flow. Further discussion of these results is given below.

The data in the high-$T$ limit can be understood using the Green-Kubo relation,[8]

$$\kappa = \frac{1}{T^2}\int d\mathbf{r}\int dt \langle j_x(\mathbf{r},t) j_x(0,0)\rangle ,$$

where a current $j_x(\mathbf{r},t)$ carries energy in the $x$ direction at position $\mathbf{r}$ and at time $t$. The angular brackets represent an ensemble average, and Boltzmann's constant has been set to unity. The expression simplifies, if the correlation length and correlation time are small (as is the case at high or low temperatures), to

$$\kappa \approx \frac{4a^2}{\tau}\frac{\langle \varepsilon^2\rangle}{T^2} ,$$

where $a$ is the bond length, $\tau$ is the time interval for a MCS (we shall set both $a$ and $\tau$ to unity hereafter), and $\varepsilon$ is the energy transmitted along one nearest-neighbor bond when a single spin attempts a flip: It has the value $\pm 2J$ for a successful flip, but is otherwise zero. The factor of 4 arises because each site adjoins two bonds in the $x$ direction, and each bond is affected twice during a pass through the lattice. As $T \rightarrow \infty$, flips are always successful, and $\langle \varepsilon^2\rangle$ is $4J^2$, giving

$$\kappa = \frac{16J^2}{T^2} .$$

Corrections to this expression come about because even at high $T$, some demons do not have sufficient energy to allow spins to flip. An expansion to lowest order in $1/T$ gives

$$\kappa = \frac{16J^2}{T^2}\left[1 - \frac{3J}{2T} + \cdots \right] .$$

This expression is plotted in Fig. 2; it agrees well with the high-temperature data. Note that the conductivity actually vanishes as $T \rightarrow \infty$. This is because there is a limited capacity for a spin to "hold heat" in the Ising model; the maximum energy per spin is $2J$.

At low temperatures, transport is limited by microscopic activated processes. It is natural to expect that the major temperature dependence of any transport coefficient is given by $e^{-A/T}$, where $A$ is a microscopic activation energy. We can straightforwardly calculate $A$ because, when almost all spins are aligned, the probability that a given spin will flip is proportional to either the probability that it is a minority spin, or the probability that a demon has sufficient energy for the flip of a spin aligned with its neighbors. Both these possibilities carry factors $e^{-8J/T}$ and we find that the conductivity is given by

$$\kappa = \frac{32J^2}{T^2} e^{-8J/T} ,$$

for $T \rightarrow 0$. That is, the activation energy at low temperatures is $8J$. This gives the other solid line plotted on the Fig. 2. The fact that it fits the data close to $T_c$ is only fortuitous; its relation to the low-temperature data is discussed below. First, however, we discuss the errors in the computation of $\kappa$.

Since $\kappa$ is obtained from numerical differentiation, its errors are largely due to the errors in the measurement of temperature. The theory of thermodynamic fluctuations[9] gives

$$\langle(\Delta T)^2\rangle = \frac{T^2}{C_v},$$

where $C_v$ is the heat capacity. At high temperatures, the heat capacity is $C_v \approx 4J^2N/T^2$. Thus, given these fluctuations in $T$, we expect that the errors in $\beta$ will be independent of temperature, at high temperatures, and of order $1/(2J\sqrt{L})$ where $L$ is the number of spins per row. Indeed, the value $0.05/J$ is roughly $\sqrt{10^5}$ times the error bars shown in Fig. 1; recall that the data is averaged over $10^4$ MCS's in each of 10 independent runs. This implies that our configurations have reached local thermal equilibrium. Note that the temperature difference across the sample is substantially greater than the magnitude of the fluctuations. We found this to be the most efficient way to generate data over a wide range of temperatures. Smaller temperature differences required more MCS per run for comparable accuracy.

Thermodynamic fluctuations in the temperature also play an important role at temperatures below $T_c$. This can be seen from Fig. 3, which is a representative configuration obtained during one of these runs. It is evident that the local fluctuations in the magnetization are on the scale of the correlation length,[10] shown in the right margin of Fig. 3, corresponding to the local temperature. This is again consistent with local thermodynamic equilibrium, so that temperature fluctuations will be given by

$$\langle(\Delta T)^2\rangle = \frac{T^4}{4J^2N}e^{8J/T},$$

where we have used the form of the heat capacity for $T \rightarrow 0$. For $L = 96$, these fluctuations are exceedingly large for $T \approx 0.7T_c$, so that accurate measurements of the temperature gradient are difficult (see Fig. 2). Indeed, we show no estimates for $\kappa$ below $0.9T_c$ since we can extract no reliable values from the noise.

The expressions we have given above for the conductivity are the first terms in the high- and low-temperature series expansions. For other temperatures, in particular

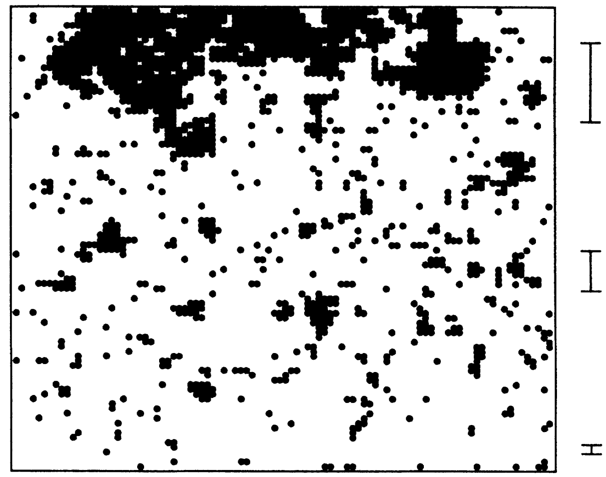


FIG. 3. Typical configuration for a system at low temperature whose boundaries are kept at $T \approx 0.99T_c$ and $T \approx 0.7T_c$. In the right-hand margin the "error bars" show the value of the thermal correlation length for the temperature of a particular row.

for the critical region $T \approx T_c$, the calculation of the conductivity requires a detailed analysis of fluctuations in the energy density and its associated currents. It should also be noted that our method of obtaining $\kappa$ from temperature gradients is subject to large finite-size effects in the critical regime. Thus we have obtained no data in this narrow region. Of course, the conductivity will vanish at $T_c$ due to critical slowing down: there is an exact result for $z$, the exponent for critical slowing down, in model $C$.[7]

In conclusion, we have demonstrated the value of a new technique for the Monte Carlo simulation of systems which are not in thermal equilibrium. We have obtained the thermal conductivity of a two-dimensional kinetic Ising model, and given explanations of the form of its temperature dependence. In the future we shall study the effect of thermal fields in other nonequilibrium phenomena, such as pattern formation during dendritic growth.

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