Journal of Statistical Physics, Vol. 66, Nos. 5/6, 1992

Molecular Dynamics Calculation for the Modified *xy* Model

Peter Litz,[1,2] Stefan Langenbach,[1,3] and Alfred Hüller[1]

Received September 17, 1991; final October 28, 1991

In order to demonstrate the effectiveness of molecular dynamics (MD) for the determination of the density of states of a system that suffers an abrupt change of state, we have performed extensive calculations for the modified rotor model, defined by the interaction potential $V(\varphi) = 2J\{1 - [\cos(\varphi/2)]^{p^2}\}$ between neighboring rotors. Our results for 2-dimensional $L \times L$ lattices with $L = 8$, 16, 32, and 64 demonstrate clearly that the transition is continuous for $p^2 \leqslant 24$, but suggest a first-order transition for $p^2 \geqslant 28$.

KEY WORDS: Modified *xy* model; first order-transitions; molecular dynamics calculations.

In spite of the pronounced signature of a discontinuous phase transition in the form of a latent heat, it is extremely difficult to distinguish a discontinuous transition from a continuous one on the basis of numerical data.(1)

Because the discrimination between continuous and discontinuous transitions is of prime importance not only in statistical mechanics, but also in high-energy physics,(2) a considerable effort is going into the determination of the density of states $\Omega(\varepsilon)$ by means of the histogram MC method.(3,4)

We have undertaken extensive MD calculations and it turned out that $\Omega(\varepsilon)$ [or equivalently the microcanonically defined temperature $T_m(\varepsilon)$] can be extracted quite easily and with good accuracy from these data. We shall try to extrapolate $T_m(\varepsilon)$ to an infinite number of particles. For the case studied below, T_m is not a single-valued function of ε ($\varepsilon = E/N$ is the energy per particle). Figure 1a shows examples of the inverse function $\varepsilon(T_m)$,

---

[1] Institut für Theoretische Physik I, Universität Erlangen, W-8520 Erlangen, Germany.

[2] Present address: Siemens AG, Munich, Germany.

[3] Present address: Neugebauer Software, Nuremberg, Germany.

0022-4715/92/0300-1659$06.50/0

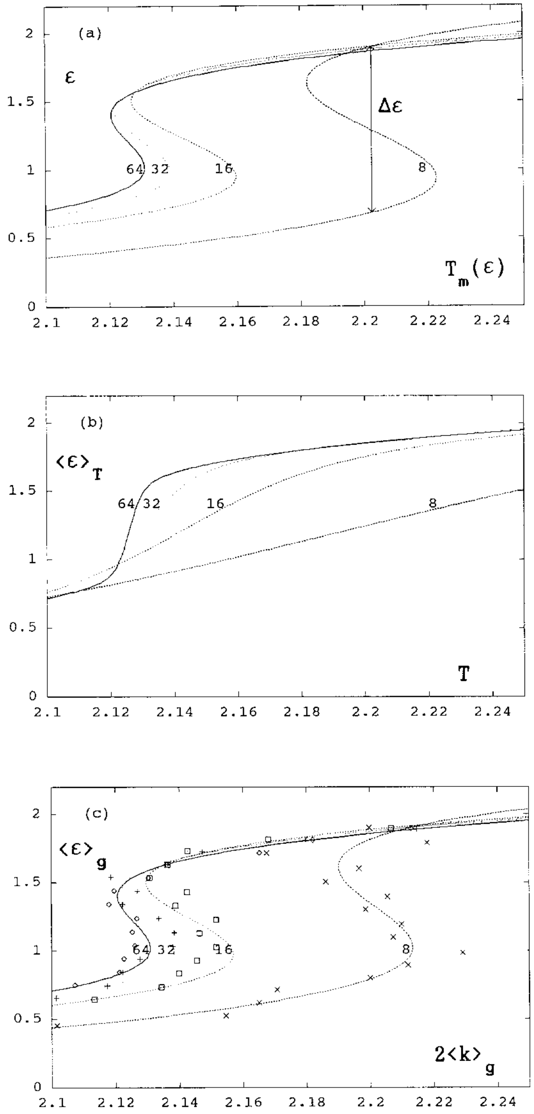

Fig. 1. (a) The microcanonical temperature $T(\varepsilon)$ as a function of the energy per particle for $p^2 = 32$ and the four lattice sizes $L = 8$, 16, 32, and 64 ($N = L \times L$). Equation (3) has been used to derive $T(\varepsilon)$ from the entropy $s_N(\varepsilon)$ which is obtained from our MD calculations. (b) The canonical mean value $\langle\varepsilon\rangle_T$ as a function of the bath temperature is calculated from the same expressions for the entropy using the partition function of Eq. (4). (c) Data points of the present MD calculation for $p^2 = 32$ and $L = 8$ (×), 16 (□), 32 (+), and 64 (◇). Also shown are the best fits of the mean kinetic energy as a function of the total energy g using $s_N(\varepsilon)$ from Eq. (8).

whose S shape becomes less pronounced as N increases. The question is whether $\varepsilon(T_m)$ develops into a step (first-order transition) or something else for $N \to \infty$.

As the object for our study we have chosen the modified xy model or planar rotor model on a 2-dimensional square lattice, defined by the Hamiltonian(5)

$$H = E = \sum_{\langle i,j \rangle} V(\varphi_i - \varphi_j) \tag{1}$$

where

$$V(\varphi) = 2J\{1 - [\cos(\varphi/2)]^{p^2}\} \tag{2}$$

The summation runs over nearest neighbor bonds with periodic boundary conditions. We put $J = 1$ and $k_B = 1$; then all energies and temperatures are measured in units of J.

This model, with an infinitely degenerate ground state, is interesting because of the absence of long-range order(6) for all temperatures $T > 0$ despite the occurrence of a phase transition(7) at a finite T_0. The transition separates the low-temperature phase with an algebraic decay of the correlations from the high-temperature phase where the correlations decay exponentially with distance. The most common form of $V(\varphi)$ with $p^2 = 1$ produces a continuous transition with rather unusual critical exponents.

There has been a controversy about the order of the phase transition for larger values of p^2. An early MC calculation(5) suggested that the transition is first order for $p^2 = 50$ and $p^2 = 100$; another MC study(8) as well as the construction of the corresponding Villain model(9) propose that the transition is a first-order one for $p^2 > 9$; whereas other MC calculations(10) and Migdal–Kadanoff (MK) renormalization(11) indicate that the transition is continuous even for $p^2 = 50$. In a more recent MK study(12) a discontinuity is found for $p^2 \geqslant 50$.

In this paper we report on a molecular dynamics (MD) study of the modified xy model as defined by (1) and (2) for several values of p^2 and four different lattice sizes. MD is very well suited for finding $s_N(\varepsilon)$, the entropy per particle, of a system of $N = L \times L$ rotors. Later we will extract $s_N(\varepsilon)$ from our numerical data, but for the moment let us assume that the expressions for $s_N(\varepsilon)$ which will result from our MD calculations are exact. Let us anticipate these results and use them as a basis for a standard canonical analysis.

From $s_N(\varepsilon)$ we find the microcanonical temperature $T_m = 1/\beta_m$ using the definition

$$\beta_m(\varepsilon) = ds_N(\varepsilon)/d\varepsilon \tag{3}$$

$T_m(\varepsilon)$ is plotted in Fig. 1a for $p^2 = 32$ and four lattice sizes as a function of ε with the T_m and the ε axes interchanged. The interest in the system lies in the S shape of the plot, which in the limit of infinite particle number may approach a finite step (discontinuous transition with latent heat), an infinite slope (second-order transition), or a finite slope (a transition with no singularity in the specific heat).

Once $s_N(\varepsilon)$ is known, canonical averages are calculated from the partition function

$$Z_N(\beta) = \int d\varepsilon \exp\{N[s_N(\varepsilon) - \beta\varepsilon]\} \tag{4}$$

where $T = 1/\beta$ is the bath temperature. From Eq. (4) we calculate $\langle\varepsilon\rangle_T = -N^{-1}\, d\ln Z_N/d\beta$ and $c_N(T) = d\langle\varepsilon\rangle_T/dT$, the specific heat per particle. The mean energy $\langle\varepsilon\rangle_T$ is shown as a function of T in Fig. 1b. The large value of the slope for $2.1 < T < 2.2$ gives rise to a peak of the specific heat $c_N(T)$ per particle whose maximum value increases sharply with N. In a conventional MC calculation, $\langle\varepsilon\rangle_T$ or $c_N(T)$ is calculated directly. As $s_N(\varepsilon)$ depends only little on N (see Fig. 1a), the sharp increase of $c_N(T)$ is almost entirely due to the factor N which multiplies $s_N(\varepsilon)$ in the exponent of (4). This strong N dependence has to be sorted out from the weak one of $s_N(\varepsilon)$, which in the end determines if the transition is continuous or discontinuous.

For the purpose of a MD calculation we have to introduce a dynamics for the system. This is very naturally achieved by adding a kinetic energy term to the Hamiltonian (1):

$$G = \sum_i l_i^2/2 + \sum_{\langle i,j\rangle} V(\varphi_i - \varphi_j) \tag{5}$$

where l_i is the angular momentum conjugate to the angle φ_i and the moment of inertia is unity. The dynamical equations obeyed by the system are Hamilton's equations following from (5),

$$\dot{\varphi}_i = \partial G/\partial l_i \qquad \text{and} \qquad \dot{l}_i = -\partial G/\partial \varphi_i \tag{6}$$

The total energy $G = K + E$ (kinetic + potential) is a constant of the motion; thus the system moves on a constant-energy surface. For low temperatures the system behaves like a harmonic solid with Hamilton's equations being nearly linear. For high temperatures the system approaches the limit of free rotors with linear equations of motion once again. Around the phase transition temperature the dynamics is governed by the strongly anharmonic part of the potential. The equations of motion are highly nonlinear. The point representing the system in phase space moves in an essentially chaotic way over the constant-energy surface and it may therefore rightfully be assumed that time averages provide very good approximations to ensemble averages.

We have implemented the equations of motion (6) on the distributed array processor ICL-DAP2 of the Institute for Mathematical Machines and Data Processing at the University of Erlangen. The problem is very well adapted to this type of parallel computer, with 1024 processors arranged in a quadratic 32×32 grid with nearest neighbor interactions and periodic boundary conditions implemented. The equations of motion have been integrated using an algorithm correct in three orders of the time step.

Constant-energy simulations were performed over 200,000 time steps of a duration Δt between 0.015 and 0.040 (depending on the kinetic energy). The first one in a series of runs was started with all rotors pointing in one direction (all $\varphi_i = 0$), i.e., $\varepsilon = 0$. The momenta were chosen randomly with a Gaussian distribution of zero mean and a width such that the energy per particle was $g = 0.4$. The second and all subsequent runs were started in the configuration of the angles taken from the last time step of the previous run with a new Gaussian velocity distribution such that the total energy was at the desired level. In this manner the energy was discontinuously increased to values well beyond the phase transition. The first 80,000 time steps were discarded to allow for equilibration, then time averages were performed with samplings every 5 time steps.

During the runs at constant total energy ($G = Ng$) the kinetic energy k per particle has been monitored and (time) averages $\langle k \rangle_g$ have been formed. The data points of $\langle \varepsilon \rangle_g = g - \langle k \rangle_g$ falling into the window of Fig. 1c are plotted there against $2\langle k \rangle_g$ for $p^2 = 32$ and $N = 64$, 256, 1024, and 4096. On the other hand, knowing the density of states $\Omega_k(k) \propto k^{(N-2)/2}$ in momentum space, we may generate $\langle k \rangle_g$ from $s_N(\varepsilon)$:

$$\langle k \rangle_g = \int d\varepsilon\, (g-\varepsilon)^{N/2} \exp\{N s_N(\varepsilon)\} \Big/ \int d\varepsilon\, (g-\varepsilon)^{(N-2)/2} \exp\{N s_N(\varepsilon)\} \qquad (7)$$

We have used the following expression for the unknown entropy:

$$\begin{aligned} s_N(\varepsilon) = {} & A_1(\varepsilon - A_3) + A_2(\varepsilon - A_3)^2 + A_4(\varepsilon - A_3)^4 \\ & - A_5 \exp\{(\varepsilon - A_6)/A_7\} - A_8 \exp\{-(\varepsilon - A_9)/A_{10}\} \end{aligned} \qquad (8)$$

with ten adjustable parameters A_i, for a least squares fit of $\langle k \rangle_g$ as a function of g. The lines in Fig. 1c show the results of such a procedure for $p^2 = 32$. The plots in Figs. 1a and 1b were generated from the functions $s_N(\varepsilon)$ as obtained from these fits.

In the thermodynamic limit, Figs. 1a–c become identical, but it is

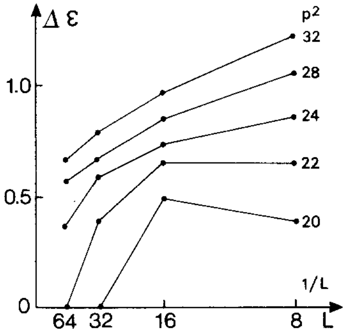

Fig. 2. Plot of $\Delta(\varepsilon)$ as defined in Fig. 1a for several values of p^2 and four lattice sizes. Clearly, the data do not extrapolate to a finite jump for $p^2 < 24$, but it is our opinion that they do for $p^2 \geqslant 28$.

evident that $\varepsilon(T_m)$ and $\langle \varepsilon \rangle_g$ approach each other much faster than $\varepsilon(T_m)$ and $\langle \varepsilon \rangle_T$ (which suffers from a trivial N dependence). Consequently, a MD calculation provides a much better access to the density of states than a canonical approach. Even in a histogram MC calculation it is difficult to obtain good statistics for the region of low density of states between the maxima of probability density. This is not the case in MD, where the (constant) energy can be chosen right in the middle of the step between low- and high-temperature phase.

The step height $\Delta\varepsilon$ [halfway between the extrema of $T_m(\varepsilon)$ as indicated by the arrow in Fig. 1a for $N = 64$] has been carried over into Fig. 2 for $p^2 = 20$, 22, 24, 28, and 32 and the four lattice sizes. It is clearly seen that for $p^2 \leqslant 24$ there remains no step in $\varepsilon(T_m)$ as $N \to \infty$. We believe that the data extrapolate to a finite step for $p^2 \geqslant 28$. It is, however, true that an extrapolation of numerical data to infinite lattice size cannot substitute for a mathematical proof. The data in Fig. 2 seem to be of adequate accuracy, but calculations for larger lattice sizes would be desirable in order to make the extrapolation more convincing.

ACKNOWLEDGMENTS

One of us (A.H.) would like to thank K. Broderix, N. Heldt, and G. Voll for helpful discussions. We are indebted to the members of the Institute for Mathematical Machines and Data Processing (IMMD VII) at the University at Erlangen for their technical assistance and the opportunity to use the DAP computer.

REFERENCES

1. K. Binder, in *The Monte Carlo Method in Condensed Matter Physics* (Springer-Verlag, Berlin, 1991).
2. M. Fukugita, M. Okawa, and A. Ukawa, *Phys. Rev. Lett.* **63**:1768 (1989).
3. A. M. Ferrenberg and R. H. Swendsen, *Phys. Rev. Lett.* **61**:2635 (1988).
4. J. Lee and J. M. Kosterlitz, *Phys. Rev. Lett.* **65**:137 (1990).
5. E. Domany, M. Schick, and R. H. Swendsen, *Phys. Rev. Lett.* **52**:1535 (1984).
6. N. D. Mermin and H. Wagner, *Phys. Rev. Lett.* **17**:1133 (1966).
7. J. M. Kosterlitz and D. J. Thouless, *J. Phys. C* **6**:1181 (1973).
8. J. E. Van Himbergen, *Phys. Rev. Lett.* **53**:5 (1984).
9. J. E. Van Himbergen, *Phys. Rev. B* **29**:6387 (1984).
10. J. E. Van Himbergen, *Solid State Commun.* **55**:289 (1985).
11. H. J. F. Knops, *Phys. Rev. B* **30**:470 (1984).
12. T. Garel, J. C. Niel, and H. Orland, *Europhys. Lett.* **11**:349 (1990).

Communicated by D. Stauffer