Microscopic observations on a kinetic Ising model[a)]

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We comment on the practical realization and physical relevance of a *kinetic* Ising model which has played an important role during the last decade as a guide for real experiments and for the development of theory. We stress the possibility of performing *microscopic* observations during the computer evolution of the model system. This is illustrated by discussing the observed behavior of some general concepts of physics such as energy, specific heat, and metastable states.

I. INTRODUCTION

The simulation of the behavior of a model system on a computer has become a widely used tool when analyzing physical processes. This is particularly true within the realm of phase transitions and other cooperative phenomena where a model with relative mathematical simplicity may capture the details (dimensionality, symmetries, etc.) which are essential to the behavior of a real system. The model can thus provide a simple and economical test of theory: any theory claiming to describe a given process in real physical systems should also be able to describe in a quantitative way what happens in a well-constructed model system. It then follows that the computer simulation of the behavior of a model system may represent in some cases an actual alternative to real experiments with the extra advantage that one may suppress any competitive effects which would obscure the process of interest in a real system. Even more important, the model, because of its flexibility, can be used very often to identify the important physical steps in the process which need to be built into a good theory.

There is a large number of examples in the recent literature about the efficient use of computer simulations as an aid or as an alternative to real experiments.[1] The computer analysis of *Ising-like* models,[2–4] for instance, has proved very useful to our understanding of a great variety of phenomena, in part because it allows the neglect when necessary of gravity or hydrodynamic effects, lattice strains, gradients and many other difficulties (like a precise control of temperature or other external parameters) which frequently beset experimentalists. This results in a drastic simplification of the observed phenomena, and sometimes it leads to the development of theory.

One of the most exciting facts about computer simulations, intimately related with the above features, is the possibility of performing direct *microscopic* observations on the behavior of a model system. These, which are impossible or very difficult in practice when dealing with a real system, may generally allow an easier understanding of the meaning and properties of familiar physical concepts. This paper tries to illustrate that fact with special reference to the concepts of energy, specific heat and metastable states. To this end we performed a series of Monte Carlo (MC) simulations of the kinetics of the simplest "ferromagnetic" Ising model with a conserved order parameter, a situation which is physically relevant to the study of binary alloys segregrating into two phases after quenching, to the condensation phenomena in a suddenly cooled vapor, etc. Our simulations here refer to quenches into states at the coexistence curve or very close to it in the two-phase region of the phase diagram so that it was possible to follow the evolution until the system had practically reached equilibrium or a quasistationary state. This is a rare situation in practice for a "large" Ising model with conserved order parameter because the evolution is drastically slowed down when phase separation sets in due to the necessary diffusion of the order-parameter magnitude throughout the lattice. In this way, we are able to analyze with detail the nature and properties of the equilibrium state as compared to that of other stationary or quasistationary conditions. The equilibrium energy is computed and compared with series expansions. We also study the fluctuations of the energy with time which, in the equilibrium state, are simply related to the specific heat. This allows one to determine whether the model has reached the actual equilibrium state. It also allows one to reveal the existence of metastable states in the Ising model with short-ranged interactions and to describe their nature from a microscopic point of view.

We also discuss the practical realization of the simulations reported here (so that they can be reproduced in a classroom experiment showing explicitly the meaning of some general physical concepts) and would be willing to supply any interested reader with a sample FORTRAN code producing energy values and actual configurations during the temporal evolution of a two-dimensional Ising model using a personal computer. The code refers to the two-dimensional model because it is simpler and needs less computational time for a given size (due to periodic boundary conditions, etc.) and also because the exact solution is known in that case[4] so that one may compare and evaluate the validity of the Monte Carlo result, study the influence of finite size effects, etc.

II. THE MODEL SYSTEM

A. Ising Hamiltonian

The familiar Ising problem[2] considers a regular lattice with *spin variables* n_i capable of two values, $+1$ ("spin up") and -1 ("spin down"), attached to the vertices $\mathbf{r}_i$ ($i=1,2,\cdots,N$) of the lattice. This gives 2^N possible configurations $\{n_i\}$ which are assumed to have configurational (interaction) energies

$$H\{n_i\} = -J\sum_{ij}{}' n_i n_j - h\sum_i n_i, \quad J>0. \tag{1}$$

The first sum here is over nearest-neighbor sites, J represents the strength of the corresponding interaction and h is an *external field* coupled to the variables. The model is then appropriate for simulating the equilibrium properties of

some hypothetical, oversimplified ferromagnetic materials.

According to standard statistical mechanics,[4] one may obtain the equilibrium properties of the system by calculating the partition function:

$$Z = \mathrm{Tr}\exp(-\beta H), \tag{2}$$

where $\beta = 1/k_B T$ is the usual inverse temperature. Thermal averages of any quantity $b(\{n_i\})$ are then given by

$$\langle b \rangle = \frac{1}{Z}\mathrm{Tr}[b(\{n_i\})\exp(-\beta H)]. \tag{3}$$

Most equilibrium properties are nowadays very well known from exact computations or approximate methods.[4]

The Hamiltonian (1) may also constitute a model for a gas, e.g., to describe condensation phenomena.[3] To this end $n_i = \pm 1$ is interpreted as the lattice site i being occupied or unoccupied by a particle, respectively, $(h = 0)$. It can also model the equilibrium properties of some binary (AB) alloys such as Al–Zn which present equilibrium states of phase segregration.[3,5] In this case the N lattice sites are assumed to be occupied by either an A particle $(n_i = +1)$ or a B particle $(n_i = -1)$.

B. Kinetics of the model

A model based on the Hamiltonian (1) has proved very useful[5] when studying the processes of phase segregation (*nucleation*, *spinodal decomposition*, *coarsening*, etc.) which occur in many alloys following an instantaneous cooling from the melt into the miscibility gap. Since there is no time during the quench for any process of spatial segregation to take place the system finds itself, immediately after the quench, in a homogeneous nonequilibrium state. The system then evolves toward the equilibrium state at the final temperature. This is characterized by the coexistence of two phases with different compositions: an A-rich phase which may present itself as a collection of clusters or droplets made of the minority A-particles with some "impurities" (B-particles) and a B-rich (or A-poor) background.

The model as defined in Sec. II A, however, does not have any dynamics of its own. Of course, one may think of kinetic energy terms to be added to the Hamiltonian (1). These would also depend on $\{n_i\}$ and thus provide a time evolution of the configuration, but they are mostly unknown or too complicated to be considered explicitly.

Instead one may realize that an alloy system after the quench is usually in a solid phase which makes atomic migration difficult. The thermal vibrations of the lattice or phonons, nevertheless, can supply the energy necessary for an evolution of the configurational part of the system. Since the $\{n_i\}$ evolve on a much slower time scale than the lattice vibrations do, one may treat the latter as a heat bath. This, in equilibrium at the temperature T to which the system was quenched, induces random exchanges between neighboring atoms which drive $\{n_i\}$ toward equilibrium at the temperature T.

The isomorphism suggested in Sec. II A between magnets, lattice gases and binary alloys[4] cannot be maintained in principle when considering kinetic models. One should notice for instance that the existence of a phonon heat bath, which is distinct to lowest order from the spatial composition of the system, makes the binary alloy problem in some ways conceptually simpler than the condensation of liquid droplets in a supersaturated vapor where the thermal motion of the atoms cannot be separated from changes in the spatial density.

In order to include the above facts explicitly into a kinetic model, one considers a Gibbs ensemble of the systems so far described and denotes $P(x)$ the fraction of systems with the configuration $x \equiv \{n_i\}$. Then, when the ensemble is in equilibrium at temperature T one has

$$P_{\mathrm{eq}}(x) = Z^{-1}\exp[-\beta H(x)], \quad h = 0. \tag{4}$$

Since memory effects are only important on the time scale of the lattice vibrations, one may ignore them as far as the evolution of the $\{n_i\}$ is concerned. This is then described[6] in terms of a Markovian master equation (or rate equation),

$$\frac{dP(x,t)}{dt} = -P(x,t)\sum_{x'} W(x\to x') + \sum_{x'} W(x'\to x)P(x',t). \tag{5}$$

Here $W(x\to x')$ gives the probability that the system makes a transition from a (microscopic) state x to a new state x'. The transitions considered in practice permit only the *interchange* of some n_i with a neighboring n_j. This ensures that the "magnetization" $\bar{n}$ and the density ρ (fraction of the minority A particles), where

$$\bar{n} = N^{-1}\left|\sum_i n_i\right| = |2\rho - 1| \tag{6}$$

stay constant during the evolution (note that this condition would not be appropriate for a magnet).

The determination of the transition probabilities $W(x\to x')$ from basic principles is in general a difficult matter. It is clear that the condition of detailed balance,

$$W(x\to x')\exp[-\beta H(x)] = (Wx'\to x)\exp[-\beta H(x')] \tag{7}$$

is sufficient, although not necessary, to ensure that the equilibrium distribution (4) is a stationary solution of the master equation (5). Of course, condition (7) does not specify $W(x\to x')$ uniquely but, assuming that this should only depend on δH, the increase of energy brought about by the proposed interchange, (7) leads to

$$W(x\to x') = \alpha\exp(-\beta\delta H/2)f(\delta H), \tag{8a}$$

where f is an even function. We shall consider here the choice

$$f(\delta H) = [2\cosh(\beta\delta H/2)]^{-1}. \tag{8b}$$

The coefficient α^{-1}, assumed to be independent of x and x', is taken to determine the unit of time and treated as a temperature-independent quantity. In comparisons with experiments on real materials, α will certainly need to be taken material and temperature dependent since the strength of the phonon heat bath decreases with temperature.[7]

III. DETAILS OF THE SIMULATION

To carry out the computer simulation one chooses a given lattice and a system size N and, using Monte Carlo methods,[1] explicitly performs the Markov process described by Eqs. (5) and (8).

The size N is dictated by a competition between the desire to make the system as large as possible, so that it imitates a macroscopic system, and practical computational considerations. The actual computer experiments we refer to in this paper correspond to a simple cubic lattice with

$N = 27\,000$ or $125\,000$ sites. In addition, periodic (*toroidal*) boundary conditions are used in order to avoid edge effects due to free surfaces. Nevertheless, one has to worry about possible finite size effects.[1,5,13]

When dealing with one-phase equilibrium states, finite size effects become important if the linear dimension of the system has the same order of magnitude as the correlation length for fluctuations. This, however, is not so dramatic in computer simulations because one has to avoid then in practice a temperature region of a few per cent around the critical point T_c where "critical slowing down" effects would make necessary very large amounts of computing time. When studying the kinetics of phase separation, finite size problems may occur even far from T_c due to the interface between the two phases. The relative magnitude of this contribution to the energy of the final state is of the same order as the inverse linear dimension d, $N^{-1/d}$, of the system. Although the coefficient of the $N^{-1/d}$ term can be quite large, one may correct the results from these interface effects; see Refs. 1 and 9 for more details.

A further effect related to the finite size of the system is the statistical inaccuracy; e.g., one expects statistical fluctuations in the energy of the system whose relative order of magnitude is $N^{-1/2}$, so that very small values of N should be avoided.

A series of Monte Carlo computations on the present model system[5,7,15] seem to indicate that one obtains in practice reasonably accurate estimates of the thermal equilibrium properties of infinite systems with the sizes we are considering here; e.g., the relative accuracy is known to be better than 1% in the case of the energy. We shall come again to this point later on.

The first step in the simulation is to generate a starting configuration x_0 of the system. If the initial temperature is very high ($T_i \to \infty$), as in the cases considered here, one selects a specified number ρN of randomly chosen sites to be occupied by A particles and the rest by B particles. This will approximately simulate a state with uniform composition and no correlation between particles at different positions. To consider a finite initial temperature T_i, one would have to let the system evolve from the random starting configuration until "thermal equilibrium" is reached at the temperature T_i. This previous evolution can be performed using the ordinary, faster *Glauber dynamics*[8] where the dynamical process is a succession of *spin flips* (instead of *spin interchanges*).

The configuration at T_i is then used as a starting configuration for the *Kawasaki dynamics* described in Sec. II B. This starts selecting at random a pair of nearest-neighbor particles to be considered for an interchange. The energy change (i.e., number of unlike nearest-neighbor pairs) which would cause that interchange is calculated. This change depends only on the configuration of the ten sites surrounding the selected pair. Then one computes the transition probability W from Eq. (8) with $\alpha^{-1} = 1$, and W is compared to a random fraction R ("pseudorandom number") that is chosen each time with uniform probability over the interval (0,1). If $W \geqslant R$ the interchange is performed, otherwise the old configuration is retained and the process (*try*) is repeated by selecting a new pair of nearest neighbor particles. In this way a stochastic evolution is simulated in which the number of tries per lattice site is the natural unit of time.

Note that a very large sequence of random numbers R is needed here, namely to generate the initial configuration x_0, to pick the atoms to be considered in each time step and to decide whether or not they have to be interchanged. Typically, the period of the required (pseudo-)random number generator is larger than 10^8, a condition which is not fulfilled by some standard algorithms in most computers. This point should be carefully checked before performing a simulation and, when necessary, an appropriate random number generator has to be incorporated into the main program; see, for instance, Refs. 1 and 21 for more specific details.

As the system approaches the equilibrium state, it becomes more unlikely that a pair of nearest neighbors selected at random will be different, that is, more tries are necessary in order to perform an interchange. Thus, after a relatively rapid early evolution it is necessary to use a large amount of computer time, especially at low temperatures, to proceed further in the simulation. This problem can be largely avoided when studying long time effects by selecting only neighboring sites with different particles and by making an *a priori* classification of the particles according to their probability of interchange; the time variable is then computed in a stochastic way.[10]

IV. ENERGY

The configurational energy of the system, Eq. (1) with $h = 0$, can also be written as

$$H = -J(N_{AA} + N_{BB} - N_{AB}), \tag{9}$$

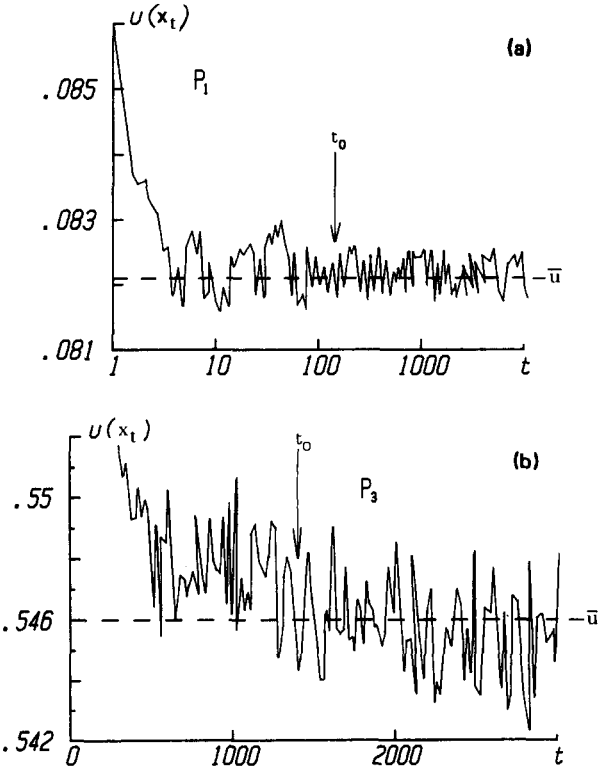

Fig. 1. Time evolution of a "microscopic" measure of the configurational energy of the system, $u(x_t)$ as defined in Sec. IV, in the case of the system relaxation at (a) P_1 ($\rho = 0.015$, $T = 0.6\ T_c$) and (b) P_3 ($\rho = 0.125$, $T = 0.9\ T_c$) both on the coexistence line. The approximate time t_0 at which $u(x_t)$ shows Gaussian fluctuations around the stationary value $\bar{u}$ increases with temperature (note, however, a different time scale in the graphs). Moreover, the fluctuations are not yet stabilized during the experiment at P_3; see Fig. 2.

where N_{AA}, N_{BB}, and N_{AB} represent, respectively, the number of nearest-neighbor pairs *A–A*, *B–B*, and *A–B* in the system. These satisfy

$$N_{AA} + N_{BB} + N_{AB} = \frac{q}{2} N, \tag{10}$$

where q is the lattice coordination number; $q = 6$ in the case considered here. It then follows from Eq. (9):

$$H = JN(2u - 3), \tag{11}$$

so that $u \equiv N_{AB}/N$, the number of *A–B* bonds per lattice site, is a natural measure of the system energy and will hereafter be called energy.

For a random starting configuration ($T_i = \infty$) one has approximately in our finite system

$$u_0(T) \equiv u_{eq}(T_i = \infty) \simeq q(1-\rho)\rho. \tag{12}$$

Here ρ is the density of the minority species, say *A* [see Eq. (6)].

The change of $u_t(T)$ with time during the system evolution gives some idea about the rate of the phase segregration processes in the system. We thus recorded $u(x_t)$, the number of *A–B* bonds in the configuration x_t obtained by the procedure in Sec. III at the time step t. This presents the typical relaxation shown by Fig. 1. That is, the *microscopic* measure of the energy $u(x_t)$, shows up a fluctuating behavior rarely observed in a real experiment. These fluctuations are not a consequence of "experimental errors" but the expected canonical fluctuations in a system where the temperature is fixed by means of an efficient contact with a heat bath, the phonon heat bath described in Sec. II B which is incorporated into the model system through the use of the transition probabilities (8).

The temporal evolution of the energy can be compared directly with some theoretical predictions.[5] To this end, however, $u(x_t)$ is not in principle the relevant quantity because it represents the value of the energy in only one member of the hypothetical ensemble. Instead one is interested in the expected value of the energy at time t as defined by

$$u_t = \sum_x P(x,t)u(x). \tag{13}$$

This is obtained in practice by taking the average over the ensemble with the initial state x_0 distributed according to the probability $P(x_0,0)$. That is, one has to take the average of $u(x_t)$ over "many" independent evolutions of the model system. One expects, however, that for functions which are extensive, like the energy, the number of independent runs needed should decrease with increasing system size because it then decreases the probability that a starting configuration not be a "typical" one: for a macroscopic size system almost every run should produce the same results. We have confirmed *a posteriori* that eight runs when $N = 27\,000$ or one run when $N = 125\,000$ are a good approximation to "many runs" in the above sense.

One should also notice that $u(x_t)$ was only recorded in practice at suitable time steps. Typically we let the system undergo 50 000 or 150 000 actual exchanges (depending on the value of the system size N) between two successive measurements because of economic reasons and also in order to avoid correlations.

V. SPECIFIC HEAT

The energy fluctuations in Fig. 1 contain indeed very useful physical information about the system. We shall give two examples of this fact. Namely they can be used as a criterion to decide whether or not the system has reached its equilibrium state, and they are very closely related to the value of the specific heat, an important property of the equilibrium state.

The observation of the graphs in Fig. 1 seems in principle to suggest that every system considered here is in equilibri-

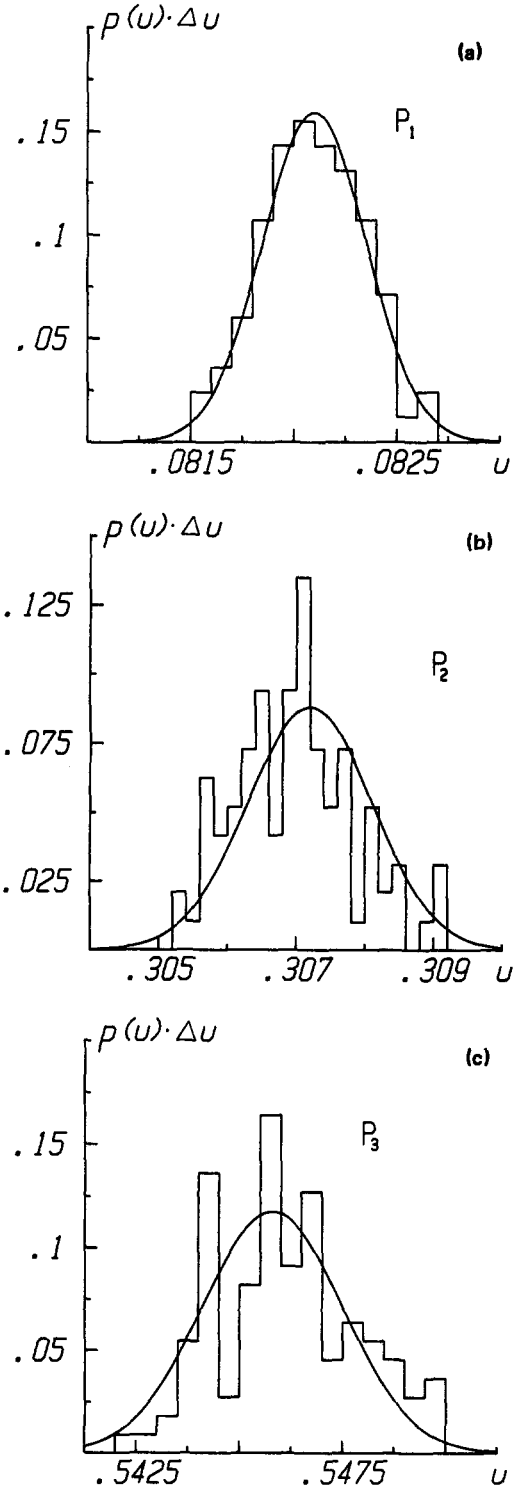

Fig. 2. Histograms corresponding to the experimental energy distribution $p(u)$ obtained from the stationary part of the system evolution at (a) P_1 ($\rho = 0.015$, $T = 0.6\ T_c$), (b) P_2 ($\rho = 0.061$, $T = 0.8\ T_c$), and (c) P_3 ($\rho = 0.125$, $T = 0.9\ T_c$). The solid curve is the Gaussian Eq. (15) corresponding to the mean and deviation measured experimentally.

um during the latest part of the computer experiment, say for $t > t_0$ where a first approximation to t_0 can be obtained by direct inspection of the data. This is the conclusion when one realizes that $u(x_t)$ fluctuates for $t > t_0$ around a constant value $u_{eq}(T)$. This, however, is not a sufficient condition for equilibrium.

The equilibrium energy fluctuations in the canonical ensemble are characterized by a Gaussian distribution,

$$p(H) \alpha \exp[-(H - \langle H \rangle)^2/2k_B T^2 C_v], \quad (14)$$

where $p(H)dH$ represents the probability that the system energy is within the interval $(H, H + dH)$, and the mean square fluctuation is related to the specific heat at constant volume C_v by the familiar *Einstein's formula.*[11] Using again u as a variable it follows that

$$p(u) \alpha \exp[-2J^2N^2(u - \langle u \rangle)^2/k_B T^2 C_N] \quad (15)$$

and

$$C_N = 4J^2N^2(\langle u^2 \rangle - \langle u \rangle^2)/k_B T^2, \quad (16)$$

where $\langle u \rangle = u_{eq}(T)$, in the case of our model system.

In Fig. 2 we present histograms where $p(u)\,\Delta u$ is plotted versus u in the case of three quenches to the final temperatures $T \simeq 0.6\,T_c\,(P_1)$, $0.8\,T_c\,(P_2)$ and $0.9\,T_c\,(P_3)$ along the coexistence line (i.e., for zero magnetic field in the language appropriate to the magnet). When making those graphs only values of $u(x_t)$ for $t > t_0$ were included; t_0 was then adjusted in order to obtain the best fit of the data to the expected Gaussian. In addition we tried to include only noncorrelated $u(x_t)$ values; that is, values of $u(x_t)$ well separated in time. Fig. 2(a) shows up indeed a very reasonable Gaussian distribution at $T \simeq 0.6\,T_c$, thus indicating that the model system is in equilibrium for $t > t_0$ in this case. The histograms in Figs. 2(b) and 2(c), however, clearly depart from a Gaussian distribution. This fact should be interpreted as a strong evidence that the system at $T > 0.6\,T_c$, during the evolution $t > t_0$, presents an "untypical" flexibility to modify its energy as a response to small changes in temperature. That is, the model system has not yet completely reached its real equilibrium state. This situation is more evident in the case $T \simeq 0.9\,T_c$ [Fig. 2(c)] than at $T \simeq 0.8\,T_c$ [Fig. 2(b)]. This seems to indicate that the evolution is slower in terms of "real" time, the higher the temperature for $T < T_c$. It also supports the overall conclusion that, while the energy stabilizes relatively early during the relaxation, the fluctuations take a much longer time to reach typical equilibrium values. That is, the mean value of the energy has a shorter relaxation time than its fluctuations. This fact may be observed (indirectly) sometimes when trying to measure quantities such as the specific heat in real materials.

Other pieces of information can be obtained from the energy distributions in Fig. 2, namely the mean values $u = u_{eq}(T)$. These can be compared with the results from series expansions. The comparison is made in Fig. 3 where we present the equilibrium values of the energy (computed by the above method) at P_1, P_2, P_3, and also at P_4 ($T \simeq 1.1\,T_c, \rho = 0.5$) and P_5 ($T \simeq 1.5, \rho = 0.5$) (i.e., both are also at "zero magnetic field") together with the energy-temperature profile for different system sizes N.[12] There is very good agreement with the results from series expansions and also our results for the equilibrium value of the energy when $N = 27\,000$ or $125\,000$ do not differ appreciably from the corresponding ones for the infinite system.

A stringent test of the above conclusions may be ob-

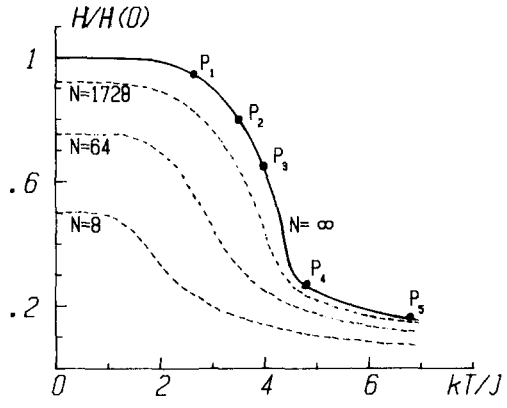

Fig. 3. The experimental equilibrium energy $H/H(T = 0\ \mathrm{K})$ computed by averaging $u(x_t)$ for $t > t_0$ (see Fig. 1) at P_1, P_2, P_3, P_4 ($\rho = 0.5$, $T = 1.1\,T_c$), and P_5 ($\rho = 0.5$, $T = 1.5\,T_c$) is compared here with the expected value for different system sizes N.[12,13] The agreement between the values for $N = 27\,000$ or $125\,000$ with the curve for $N = \infty$ is excellent.

tained from the analysis of the specific heat at constant volume. The values obtained during the simulation of Eq. (16) are compared in Fig. 4 with the results from series expansions and with results for "small" systems.[12] It follows again from Fig. 4 that only the simulation at P_1 ($T \simeq 0.6\,T_c$) has reached the real equilibrium state of the system. Notice that the departure of C_N from the results for the infinite system in Fig. 4 cannot be interpreted as a consequence of the finite size of our model because this would produce the opposite effect to the one shown by Fig. 4.

VI. METASTABLE STATES

Metastable states are often observed in nature as supercooled or supersaturated states. They naturally emerge

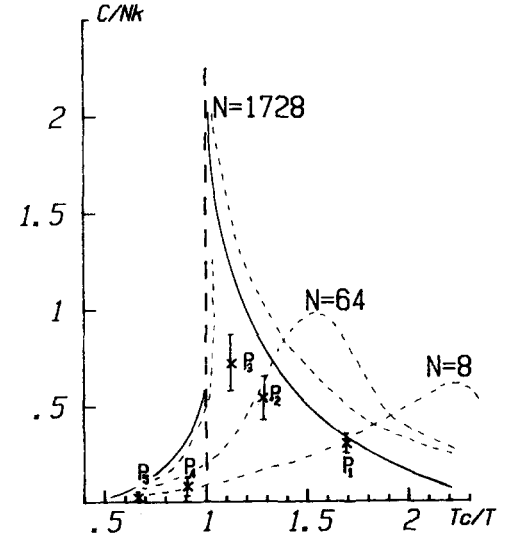

Fig. 4. The experimental value for the specific heat at $P_1 - P_5$, computed from energy fluctuations as shown by Eq. (16), is compared here with the expected value for $N = \infty$. The discrepancies are interpreted as due to the fact that the system at $P_2 - P_5$ is not yet in equilibrium in spite of the evidence shown in Fig. 3. Some curves for small N (Ref. 12) are also included to show that the discrepancies cannot be a consequence of small size effects.

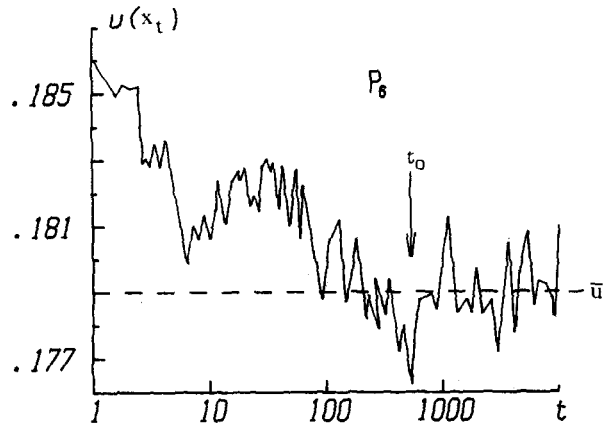

Fig. 5. Same as Fig. 1 in the case of the phase point P_6 ($\rho = 0.035$, $T = 6\ T_c$) which is a candidate for metastability.

within the context of mean field theory.[4] Real experiments and such a thermodynamic (and usually unrealistic) description gives, however, rather poor information about their microscopic or dynamical properties.

Penrose and Lebowitz[14] have listed three properties characterizing metastable states: (i) only one thermodynamic phase is present, and usual thermodynamics applies to it; (ii) an isolated system that starts in this state is likely to take a very long time (say years) to get out; and (iii) escape from the metastable state is an irreversible process. Computer experiments may in principle provide a microscopic view of these and other properties of metastable states.

Following the description by Penrose and Lebowitz,[14] metastable states can arise when some thermodynamic parameter of the system (such as T or h) is changed from a value for which the stable equilibrium state has a single thermodynamic phase, to one for which it would consist of more than one phase or, as in hysteresis, a single but different phase. Thus we have quenched our system to $T = 0.6$ T_c and $\rho = 0.035 (P_6)$. The saturation density at that temperature is $\rho_s \simeq 0.015$ (corresponding to P_1) so that P_6 is inside but very close to the coexistence line for the model

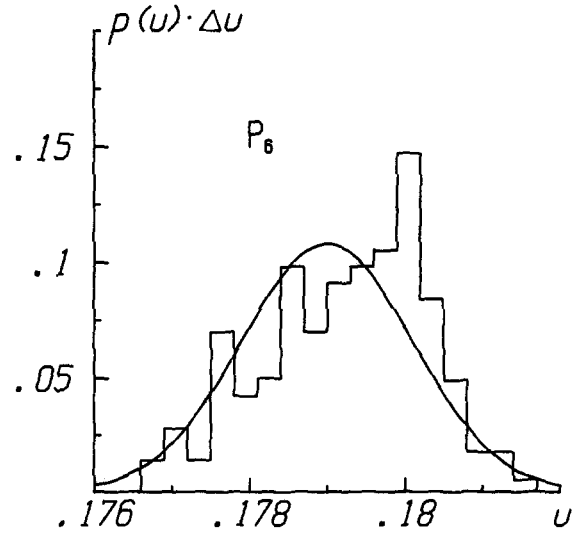

Fig. 6. Same as Fig. 2 in the case of P_6.

and thus a candidate for metastability. As a matter of fact, it seems that the (gradual) separation between metastable and unstable states at that temperature is around $\rho = 0.045$[15,16] (a sharp distinction only seems to occur for long range interactions[17]). The behavior at P_6 can also be compared with that at P_7 ($T \simeq 0.6\ T_c$, $\rho = 0.05$) where a clear phase transition was observed before $t \simeq 3000$ (in a run which lasted up to $t \simeq 14\,000$).[7]

We observed at P_6 that the system had not made indeed the appropriate phase transition up to $t = 16\,300$. Instead it went over continuously into a one-phase state which clearly appears to be stationary in time, during the time range 5000–16 300, in the same manner as a stable equilibrium state such as the one at P_1. That is, only small, A-rich clusters (*vapor phase* in the lattice gas language) are present in our final state at P_6 while much larger (by a factor of 10) clusters (*liquid droplets*) were observed at P_7.

A distinguishing feature of a metastable state[14] is that,

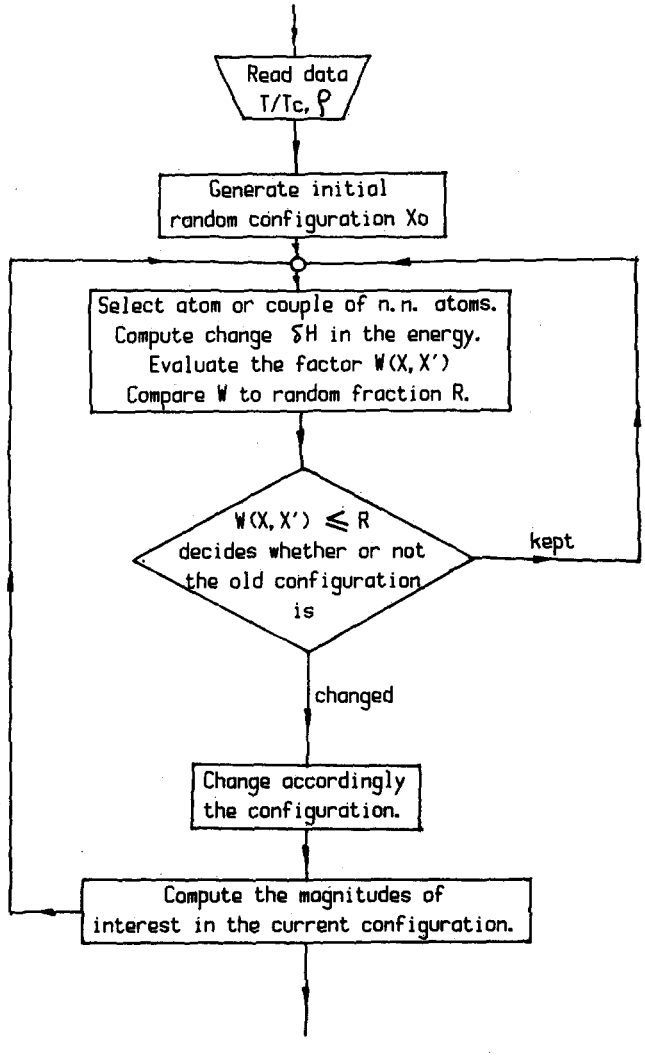

Fig. 7. Flow diagram of the main program. The basic iterative step of the program generates a new configuration x' from the previous one x by choosing randomly an atom and flipping it (*Glauber dynamics*) or by choosing a couple of nearest neighbor atoms which are then interchanged (*Kawasaki dynamics*) according to a prescribed criterion. This compels the system to evolve toward the canonical equilibrium state at the temperature of quenching. See Sec. II and III and Refs. 1 and 21 for more explicit details. When performing the simulation in a personal computer this basic step, including the random number generator algorithm, should be written in machine language; see Sec. III and Ref. 20.

Table I. The experimental equilibrium energy and its fluctuations as measured by Eq. (16) for three phase points at $T = 0.6\,T_c$. P_1 is on the coexistence line, P_7 is in the two-phase region, and P_6 (inside coexistence as well) is a clear candidate for metastability. Note that the values for P_6 do not follow the trend suggested by P_1 and P_7. We have also included for comparison the approximate values expected[18] for the true two-phase equilibrium at P_6 and P_7; it is clear that the system at P_6 is still far from real equilibrium, i.e., it is a metastable state.

				Two-phase equilibrium	
	ρ	$\bar{u}_{\text{exp}}$	$C_{\text{exp}}/N_B k_B$	$\bar{u}$ appr.	$C_{\text{appr.}}/N_B k_B$
P_1	1.456%	0.0821 ± 0.0001	0.303 ± 0.03	...	...
P_6	3.5%	0.179 ± 0.001	2.47 ± 0.2	0.14	1.75
P_7	5%	0.1565 ± 0.0002	1.56 ± 0.2	0.16	1.54

eventually, either through some external disturbance or a spontaneous fluctuation which nucleates the missing phase in some small part of the system, the system begins an irreversible process which leads it inexorably to the corresponding stable equilibrium state. This ultimate part of the evolution was never observed during our experiment at P_6. From a simple point of view this is just a consequence of having such a small number of A particles at P_6 that a large enough fluctuation (nucleus) leading the system out of the metastable state is highly improbable. More quantitative statements are also possible; see, for instance, Ref. 15.

Interestingly enough, a closer inspection of the evolution at P_6 shows up some features which are characteristics of a true equilibrium state and others which are not. We show in Figs. 5 and 6 the evolution of $u(x_t)$ and the energy distribution $p(u)$ obtained from the stationary part of the evolution, respectively. This is very similar to the situation depicted in Figs. 1 and 2 for P_1 although the fluctuations and deviations from a Gaussian distribution are now more important. Table I compares the values measured by us for $\langle u \rangle$ and C_N, as defined in Eq. (16), at P_1, P_6, and P_7. One realizes there that the values at the metastable state P_6 are indeed much higher than the ones corresponding to a true two-phase equilibrium state at the same temperature and composition.

VIII. CONCLUSION

The similarity between the results obtained from lattice models and those observed experimentally led, during the last few decades, to the now common belief that these models, in the beginning regarded as mathematical curiosities, actually capture many of the essential physical features of equilibrium cooperative phenomena. In fact, the Ising model is now recognized to have certain relevance for many phase transitions in nature.

The physical relevance of Ising-like models in the study of nonequilibrium phenomena is in principle less clear cut. The necessary assumptions about the transition probabilities make the situation more artificial.

The model we have described, however, shows an undeniable physical relevance in relation to the kinetics of phase segregation in quenched real materials. As a matter of fact, a series of computer simulations[5,7,15] based on that model have played an important role during the last decade as a guide for real experiments and for the development of theory. One may mention, for instance, that those computations were able to identify and/or reproduce the shape and dynamical scaling properties of the structure function as measured by means of small angle scattering of x rays, light or neutrons in many alloys, liquid and glassy mixtures, protein solutions, etc. over a broad range of temperatures and compositions.[7,19] Those computations also reproduce cluster or droplet distributions closely related to the ones observed by using electron or field ion microscopy in real mixtures.[5,15]

We have also described in this paper new computer experiments on the same model system in order to illustrate the *microscopic* nature of the relaxation toward equilibrium. Namely we have focused our attention on the behavior of the energy and its fluctuations, and on the possibility of measuring the system equilibrium energy and specific heat. It then becomes clear that the system stabilizes relatively early with respect to the value of the energy while its fluctuations (specific heat) may yet be far from the corresponding equilibrium value. It also becomes clear that a size $N = 27\,000$ may mean "large enough" for many purposes. One of the computer experiments was performed on a phase point showing metastability. We obtained in this case anomalous "equilibrium" values, as expected. The metastability was associated with a very low probability that the system evolves toward full phase segregation given that it contains less A particles than necessary for a thermal fluctuation to produce a nucleus of the new phase.

Finally, we also find interesting to mention that ordinary personal computers may in principle be used[20] to perform computer simulations such as the ones described in this paper (Fig. 7); those simulations can thus serve as a convenient and economic tool when teaching basic physical concepts. Following a suggestion from the editor, we are willing to supply with copies of a program for the two-dimensional Ising model upon request; this can be used for a classroom experiment with any IBM PC compatible personal computer.

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A basic acoustic diffraction experiment for demonstrating the geometrical theory of diffraction

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An apparatus is described in which acoustic diffractions are generated. Such diffractions are recorded in the field when seismic data is collected over a geological area that has many faults and truncated geological structures. The design of the experiment is considered from the point of view of theoretical feasibility and practical implementation. A computer-controlled transceiver is guided on a traverse perpendicular to a model of a rigid half-plane. At each transceiver location an acoustic pulse is emitted, and the scattered acoustic pulse is recorded. Results of this experiment are presented and analyzed from the perspective of Keller's geometric theory of diffraction. The predicted asymmetry of the diffraction hyperbola is observed in the model data collected.

I. INTRODUCTION

In this paper we describe an experiment which we use to demonstrate pulsed acoustical diffraction and reflection from a rigid half-plane. This experiment offers an excellent demonstration of Young's[1] observation that diffracting edges appear luminous for light sources. Therefore, he inferred that a wave arises from the edge of the diffracting object. As we will demonstrate below, an analogous phenomenon exists for acoustic waves. Furthermore, this experiment is able to simulate the type of data collection which is used in the seismological exploration for hydrocarbons. The type of reflection-diffraction data presented forthwith is an idealization of seismic field data collection. (See Appendix.)

For this experiment, we are dealing only with acoustic rather than elastic waves. In the exploration for oil using seismic methods, the acoustic model for wave propagation is normally assumed. The seismic source and receiver are replaced by an acoustic transceiver. The truncated geological bed is idealized by an aluminum plate, which serves as the rigid half-plane. The acoustic diffractions generated in this experiment are often seen in field seismic data. Therefore, the experiment is extremely useful in developing an understanding of the basic seismic diffraction phenomenon. In addition, it can be directly related to the extension of geometrical optics, the geometrical theory of diffraction as proposed by Keller.[2] Keller's extension of geometrical optics puts on a firm footing the intuitive observations proposed by Young. Since Keller's initial development of the geometrical theory of diffraction, many extensions have been proposed which again serve to support the theory of Young. Thus, this experiment offers an excellent opportunity for students to correlate diffraction theory as outlined in the geometrical theory of diffraction, with the experimental data collected.

II. BASIC THEORY

Before building the experimental appartus, we embarked on a feasibility study, which necessitated the analysis of the relative strengths of the reflected and diffracted pulses. We used as a model the theory of Bowman, Senior, and Uslenghi,[3] for an acoustical point source situated over a rigid half-plane. (See Fig. 1 for a description of the geometry and algebraic nomenclature.) This proceeds as follows.

Assume a sinusoidal time dependence $e^{-i\omega t}$ for the velocity potential V of a point source given by:

$$V_i = e^{ikR}/R, \tag{1}$$

where

$$R = \sqrt{(x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2}$$

and V_i represents the incident field.

Then it can be shown that the contour integral represen-