Relaxation dynamics of the Ising model in the cluster approximation

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The cluster approximation, well known in phase-transition statistics, is used to investigate the relaxation properties of the Ising model. The basic properties of the dynamic generalization of the cluster model are illustrated by the example of a simple two-particle cluster. Expressions are obtained for the relaxation time τ of the average spin $\langle \sigma^z \rangle$ above and below the phase transition point T_c for different Ising lattices. It is noted that the function $\tau^{-1}(\epsilon)$, where $\epsilon = (T - T_c)/T_c$ is not linear. A comparison is made with numerical results for a plane square lattice.

1. INTRODUCTION

The Ising model, which is a lattice of dipoles each of which can assume only two positions, is a unique example of a system exhibiting a nontrivial second-order phase transition and capable of exact solution in the two-dimensional case. [1] This model is especially effective in the investigation of real systems such as binary alloys, ferroelectric and antiferroelectric materials, and certain ferromagnetic materials. The simplest method for the theoretical description of such systems is the molecular field approximation (MFA). [2] However, MFA is found to be unsatisfactory when the crystal contains strong short-period correlations. These correlations are taken into account in the cluster approximation (CA), [2] which gives good agreement with experiment in relation to the thermodynamics of transitions in different materials. [3,4] Although statistical studies of order-disorder-type transitions have led to a degree of understanding of the microscopic picture, the nonequilibrium relaxation properties have not been extensively investigated.

The simplest model describing the dynamic behavior of cooperative systems in the critical region is the so-called dynamic Ising model (DIM), proposed by Glauber. [5] It admits of an exact solution in zero magnetic field H in the one-dimensional case ($d = 1$), since DIM with $d = 1$ is equivalent to the equilibrium MFA with $d = 2$. [6]

Studies of the nonequilibrium relaxation properties described by DIM began only recently. Most attention has been paid to problems such as the properties of the model in the MFA approximation, [7] numerical calculations by the Monte Carlo method, [8-11] high-temperature and $(4 - d)$ expansions, [12,13] possible generalizations of DIM with $d = 1$ to the case where $H \neq 0$, [14] and so on. [15-17] Attempts to take into account nearest-neighbor correlations were reduced to the combinatorial method, [18] which is very laborious and difficult to generalize further.

In this paper, we shall consider in detail the DIM solution with $d = 1, 2, 3$ and the cluster approximation which, in the static case, is more accurate than MFA. This approach will enable us not only to improve the agreement with computer calculations of the relaxation time τ of the order parameter, but will lead to a qualitatively new result as compared with MFA, namely, a departure from linearity of the function $\tau^{-1}(\epsilon)$, where $\epsilon = (T - T_c)/T_c$ and T_c is the transition point. The basic properties of the dynamic generalization of the cluster method will be given in Sec. 2 in the case of a simple Ising lattice. In Sec. 3, we shall obtain expressions for the relaxation time τ by analyzing different lattices in the two-particle cluster approximation.

2. DYNAMIC GENERALIZATION OF THE CLUSTER METHOD IN THE ISING MODEL

Consider a lattice ($d = 1, 2, 3$) of N particles with spin $\sigma_i^z = \sigma_i = \pm 1$. If we introduce the distribution function $P(\sigma_1, \ldots, \sigma_i, \ldots, \sigma_N; t)$, we can write down the equation of motion in the form [7]

$$\frac{d}{dt} P(\sigma_1, \ldots, \sigma_N; t) = -\sum_i w_i(\sigma_i) P(\sigma_1, \ldots, \sigma_N; t)$$
$$+ \sum_i w_i(-\sigma_i) P(\sigma_1, \ldots, -\sigma_i, \ldots, \sigma_N; t), \quad (1)$$

where $w_i(\pm \sigma_i)$ is the probability that the spin i will turn over from $\pm \sigma_i$ to $\mp \sigma_i$, the other spins remaining fixed. In its physical properties, Eq. (1) is analogous to the usual Fokker-Planck equation for stochastic Markov processes. [19] However, the transition probability matrix is no longer symmetric, in contrast to the latter processes. [19] Owing to the interaction of the system with the thermostat introduced into it [5] (for example, vibrational degrees of freedom, and so on), the reorientation of spins occurs with a change in the total energy of the lattice and the probabilities of forward and reverse transitions are no longer equal.

The principle of detailed balancing [7] shows that, in (1),

$$w_i(\sigma_i) P_0(\sigma_1, \ldots, \sigma_N) = w_i(-\sigma_i) P_0(\sigma_1, \ldots, -\sigma_i, \ldots, \sigma_N), \quad (2)$$

where P_0 is the distribution function in the state of equilibrium, given by

$$P_0 = Z^{-1} \exp(-\beta \mathcal{H}), \quad Z = \mathrm{Sp} \exp(-\beta \mathcal{H}), \quad \beta = 1/T. \quad (3)$$

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If we write the energy of the spin system in the form

$$\mathcal{H}=-\sum_{i\neq j}J_{ij}\sigma_i\sigma_j-\mu H\sum_i\sigma_i \qquad (4)$$

where H is the magnetic field, we find from (2) and (3) that the transition probability $w_i(\sigma_i)$ is given by

$$w_i(\sigma_i)=\frac{1}{2\tau_0}(1-\sigma_i\,\mathrm{th}\,(\beta E_i)),$$
$$E_i=\mu H+\sum_j J_{ij}\sigma_j. \qquad (5)$$

The quantity τ_0 in (5) can be interpreted physically as the relaxation time associated with the interaction of the spin system with the thermostat. Clearly, τ_0 is a very slow function of temperature, so that we shall henceforth, assume that it is a constant and set it equal to unity for simplicity. We now introduce the average

$$g_h(t)=\langle A\rangle=\sum_{(\sigma)}A(\sigma_h)P(\sigma_1,\ldots,\sigma_N;t), \qquad (6)$$

so that, using (1), (5), and (6), we obtain the following equation of motion:

$$\frac{d}{dt}\Big\langle\prod_{i=1}^N\sigma_i\Big\rangle=-\sum_{j=1}^N\Big[\Big\langle\prod_{i=1}^N\sigma_i\Big\rangle-\Big\langle\Big(\prod_{i\neq j}\sigma_i\Big)\mathrm{th}(\beta E_j)\Big\rangle\Big]. \qquad (7)$$

We must now consider this equation in the cluster approximation. Let us take the simplest two-particle cluster with the Hamiltonian[2]

$$\mathcal{H}_2=-J\sigma_1\sigma_2-\varphi(1-1/n)(\sigma_1+\sigma_2), \qquad (8)$$

where φ is the field due to the $n-1$ external spins which, in equilibrium, is determined from the self-consistency condition[2]: the average spin calculated with the Hamiltonian $\mathcal{H}_2$ is equal to the average spin determined with the molecular-field Hamiltonian

$$\mathcal{H}_1=-\sigma_1\varphi. \qquad (9)$$

Using (7)–(9), we can write the equations for the mean spin $\langle\sigma^2\rangle=g_1(t)$ in the form

$$(10a)$$
$$-\dot{g}_1=(1-a_1)g_1-a_2,$$
$$-\dot{g}_1=g_1-\mathrm{th}\,(\varphi\beta), \qquad (10b)$$

where $\dot{g}=dg(t)/dt$, a_i are given by

$$a_1=(1-\mathrm{th}^2\,(\beta\varphi m))\gamma Y^{-1},$$
$$a_2=\mathrm{th}\,(\beta\varphi m)(1-\gamma^2)Y^{-1}, \qquad (11)$$
$$Y=1-\gamma^2\,\mathrm{th}^2\,(\beta\varphi m),$$

and $m=1-1/n$, $\gamma=\tanh(\beta J)$. We note that (10) and (11) lead to the usual thermodynamic relations[2] [$K=\exp(-2\beta J)$, $\alpha=2/n$]

$$\mathrm{sh}\,(\beta[\varphi_0(1-\alpha)])=K\,\mathrm{sh}\,(\beta\varphi_0), \qquad (12)$$
$$g_1{}^0=\langle\sigma^2\rangle_0=\mathrm{th}\,(\beta\varphi_0),\quad T_c=2J/\ln\,(1-\alpha)^{-1}.$$

The zero index on g_i and φ indicates the state of equilibrium. Equations (10) and (11) form a closed system

defining the quantity $g_1(t)$. The solution is difficult for arbitrary n but, in the two-dimensional case, when $n=2$, Eq. (10a) can be reduced to the form

$$-\dot{g}_1=2K\,\frac{g_1[\mathrm{ch}\,(\beta\varphi)+K]-\mathrm{sh}\,(\beta\varphi)}{1+2K\,\mathrm{ch}\,(\beta\varphi)+K^2}. \qquad (13)$$

and, if we eliminate φ with the aid of (10b) from (13), we obtain

$$-\dot{g}_1=\frac{2K^2}{1+K^2}\,g_1. \qquad (14)$$

This equation is identical with the result given by Glauber,[5] i.e., as in the $d=1$ statistics,[2] the cluster approximation gives an exact result. It follows from (14) that, in the average-spin approximation, the relaxation time τ is given by[5]

$$\tau=(1+K^2)/2K^2=(1-\gamma')^{-1},\quad\gamma'=\mathrm{th}\,(2\beta J). \qquad (15)$$

Let us now consider the case of arbitrary n. We shall suppose that the deviations from the position of equilibrium are small ($\nu\ll1$):

$$g_1(t)=g_1{}^0+\nu g_1(t),$$
$$\varphi(t)=\varphi_0+\nu\varphi(t), \qquad (16)$$

and $\tanh[\beta\nu\varphi(t)]\sim\beta\nu\varphi(t)$. If we linearize (10), we obtain the following expressions ($\beta\varphi-\varphi$):

$$-\dot{g}_1=\frac{1-\gamma}{1-\gamma^2\alpha_0{}^2}\{g_1(1+\gamma\alpha_0{}^2)-\varphi m[(1+\gamma)(1+2\alpha_0{}^2)-g_1{}^0\alpha_0(3+\gamma\alpha_0{}^2+2\gamma)]\}, \qquad (17a)$$

$$-\dot{g}_1=g_1+\varphi(g_1{}^0\,\mathrm{th}\,(\beta\varphi_0)-1), \qquad (17b)$$

where $\alpha_0=\tanh(\beta m\varphi_0)$. Eliminating φ from (17a) with the aid of (17b), and taking into account the self-consistency conditions (12), we obtain the equation analogous to (14) with the relaxation time τ given by

$$\tau^{-1}=\frac{2KP_1}{R}\Big\{\frac{P_1+P_2\alpha_0{}^2}{P_1}-m(\alpha_0{}^2-1)P_2M[2mKM+R(1-(g_1{}^0)^2)]^{-1}\Big\}, \qquad (18a)$$

$$\varphi_0=\frac{1}{2}\ln\frac{1+g_1{}^0}{1-g_1{}^0}. \qquad (18b)$$

where, for simplicity, we have substituted

$$1\pm K=P_{1,2},\quad R=P_1{}^2-\alpha_0{}^2P_2{}^2,$$
$$M=2(1+2\alpha_0{}^2)-g_1{}^0\alpha_0(5+\alpha_0{}^2)-Kg_1{}^0\alpha_0(1-\alpha_0{}^2).$$

Equation (18) is valid both above and below T_c. Thus, for $T>T_c$, where $g_1^0=\varphi_0=0$, Eq. (18) simplifies and assumes the form

$$\tau^{-1}=\frac{2K(P_1-2m)}{P_1{}^2-4mK}. \qquad (19)$$

To investigate the $T<T_c$ region, we must substitute in (18) the equilibrium values g_1^0, found from the free energy F with the Hamiltonian (8):

$$\beta F=-\frac{n}{2}\ln[2\,\mathrm{ch}\,(2\beta\varphi_0 m)+2K]+(n-1)\ln[2\,\mathrm{ch}\,(\beta\varphi_c)], \qquad (20)$$
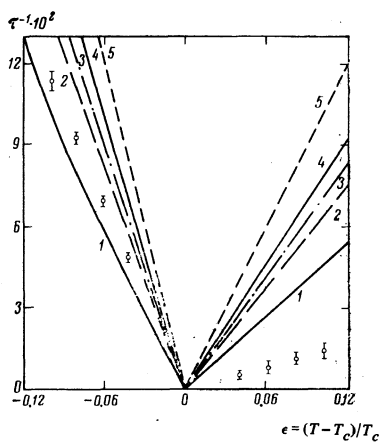
where φ_0 is calculated from (18b).

FIG. 1. Reciprocal of relaxation time as a function of reduced temperature: 1—$n=4$; 2—$n=6$; 3—$n=8$; 4—$n=12$; 5—molecular-field approximation; points correspond to a numerical result $(n=4)$.[8-13]

The expressions given by (18)–(20) solve the problem, since they give the relaxation time τ in terms of the interaction constant J and the type of lattice n.

3. CONSEQUENCES OF THE ABOVE RESULTS

Equations (18)–(20) can be used to investigate the relaxation time for different Ising lattices, and to compare these results with numerical computations.[8-13] The dependence of τ^{-1} on ε is shown in Fig. 1 for the following Ising lattices: $n=4$ (curve 1, square lattice), $n=6$ (curve 2, simple cubic lattice), $n=8$ (curve 3, body-centered cubic lattice), and $n=12$ (curve 4, body-centered cubic lattice). For comparison, the figure also shows the MFA data (curve 5) and the numerical results reported by different authors[8-13] for the $n=4$ case. It is clear from the figure that the cluster approximation is in better agreement with the numerical results than the molecular-field approximation. Moreover, as in statistics (see, for example, the specific heat data[2]), the cluster approximation provides a better description of the region above T_c than that below T_c. We note also that there is a deviation Δ from the linear law $\tau^{-1}(\varepsilon)$ in this model, which is particularly appreciable for $T < T_c$. Thus, for $T < T_c$ ($n=4$) and $\varepsilon \sim 0.07$, this deviation is $\Delta \sim 2\%$ and, for $\varepsilon \sim 0.14$, the deviation is $\Delta \sim 14\%$. For $T > T_c$, these deviations are much smaller and, for $\varepsilon \sim 0.14$ ($n=4$), amount to only about 1%. This is easily understood if we write

$$\tau^{-1} = A(T)(T - T_c),\tag{21}$$

where, according to (18), the coefficient A is a function of temperature. Moreover, as $|\varepsilon|$ increases, this dependence becomes sharper. Although the above analysis is valid for values of ε for which $\Delta g/g_1 \ll 1$ (16), one hopes that the proposed model provides a correct qualitative description of the behavior of τ. It is, therefore, interesting to compare the experimental results for $\tau^{-1}(\varepsilon)$ with the expressions given by (18)–(20). In many crystals, for example, NH_4Cl,[20] DKDP,[21] and for some alums,[22] an analogous deviation from linearity

has been observed for both $T < T_c$ and $T > T_c$. In MaSeD,[22] for example, the deviation for $T > T_c$, $\varepsilon \sim 0.06$ is $\Delta \sim 15\%$. It does not seem possible to describe this behavior of τ in the molecular-field approximation or the various "oscillator" models.[23]

We conclude with a methodological remark in relation to the possibility of several relaxation times in a system.[2] If we extend the cluster in the model (8) up to the k-particle system, the set of closed equations given by (10a) will consist of $k-1$ equations in the quantities $\langle\sigma_1\rangle(t)$, $\langle\sigma_1\sigma_2\rangle(t)$, $\langle\sigma_1\rangle, \ldots, \langle\sigma_{k-1}\rangle(t)$, where each average has its own effective relaxation time τ_k. The dispersion of permittivity $\varepsilon(\omega)$[2] can then be represented by

$$\varepsilon(\omega) = \sum_{n=1}^{k-1} \frac{\varepsilon_n(0)}{1 + i\omega\tau_n},\tag{22}$$

where ε_n and τ_n are functions of J and T. The increase in the size of the cluster in the model described by (8) may lead not only to a slow increase in inaccuracy but, occasionally, even to its deterioration.[2] In some systems, on the other hand, especially in real systems, an increase in size is necessary for the adequate description of order phenomena. This analysis is, therefore, more conveniently carried out for particular crystals such as DKDP, NH_4X, and so on, for which a model has been chosen and correctly reflects the thermodynamic properties. Moreover, the three-dimensional cluster will probably also increase the accuracy of the analysis in a similar way to what happens as a result of transition from $d=2$ to $d=3$ statistics. Studies of this kind, based on the above methods, will be carried out in future.

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Deformation of electron-hole drops in a magnetic field

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The stationary shape of an electron-hole drops (EHD) in a constant magnetic field is calculated in the hydrodynamic approximation with allowance for the recombination magnetization and the surface tension.

It was previously shown[1] that in electron-hole drops (EHD) application of an external magnetic field should produce circular currents that lead to recombination magnetization of the drops. This phenomenon was used in a number of papers[2-4] to explain the magnetostriction of the EHD. It was assumed in these papers that the drops are ellipsoids of revolution. In the present paper the drop shape is determined by solving a differential equation obtained from the EHD equilibrium conditions.

Consider an EHD in a magnetic field under conditions of stationary photoexcitation. The carrier recombination in the drop leads to the appearance of electron and hole fluxes from the surface to the interior of the EHD. We assume that the carrier densities n vary little inside the drops. In this case the carrier fluxes are given by

$$\text{div } \mathbf{v} = -1/\tau. \tag{1}$$

Here $\mathbf{v}$ is the velocity of the carrier flux and τ is the EHD lifetime. The solution of (1) in a cylindrical coordinate frame $(\rho, \varphi, z \parallel \mathbf{H})$ is

$$v_\rho = -\frac{B\rho}{\tau}, \quad v_z = -\frac{(1-2B)z}{\tau}, \quad v_\varphi = 0, \tag{2}$$

where B is a constant that specifies the distribution of the fluxes in the drop.

The distribution of the pressure p in the EHD is described by the equation[5]

$$\text{grad } p = [\mathbf{j} \times \mathbf{H}]/c. \tag{3}$$

Here $j = \sigma \mathbf{v} \times \mathbf{H}/c$ is the current density, σ is the conductivity, and c is the speed of light. From (3), with account taken of (2), we obtain the following expression for the pressure:

$$p = p(0) + \frac{4\alpha\varepsilon}{a} u^2, \quad u = \frac{\rho}{a}, \tag{4}$$

where $p(0)$ is the pressure on the z axis, $\varepsilon = a^3 \sigma B H^2 / 8\alpha c^2 \tau$ is a dimensionless parameter, α is the surface-tension coefficient, and a is the value of ρ on the EHD equator.

At equilibrium, the pressure p at each point of the EHD drop should equal $-2\alpha k$ (k is the average curvature of the surface). For the curve $z = af(u)$, rotation around the z-axis of which describes the surface of the drop, this condition can be written in the form

$$f''(1+f'^2)^{-3/2} + f' u^{-1} (1+f'^2)^{-1/2} + ap/\alpha = 0. \tag{5}$$

The solution of (5) with allowance for the boundary conditions $f'(0) = 0$ on the poles of the EHD and $f(1) = 0$ and $f'(1) = -\infty$ on the equator, can be represented in the form

$$f(u) = \int_1^u \frac{K\,dt}{(1-K^2)^{1/2}},$$

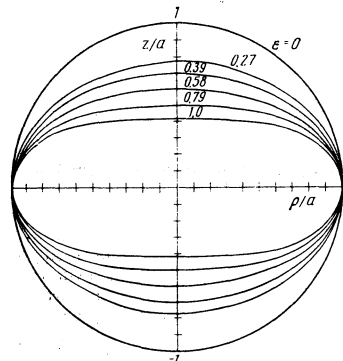$$K(t) = -\frac{a}{\alpha t} \int_0^t p(u)\, u\, du. \tag{6}$$

FIG. 1. Shape of the intersection of the EHD with the plane passing through the z axis, as calculated from formulas (6) for different values of ε.

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