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NONERGODIC BEHAVIOUR IN THE TRANSVERSE ISING MODEL

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INTRODUCTION

The Hamiltonian of an Ising model with a transverse field is usually written in the form

$$H = -\Omega \sum_i S_i^x - \frac{1}{2} \sum_{ij} J_{ij} S_i^z S_j^z , \qquad (1)$$

where S_i^{α} is the operator of spin $S = 1/2$. The interaction $J_{ij} > 0$ $(i \neq j)$ leads to an ordering of spin z-components if the transverse field is small enough, $\Omega < \Omega_c \approx (1/2) J_0 = 1/2 \sum_j J_{ij}$ [1]. Unlike the conventional Ising model (i.e., $\Omega = 0$), model (1) has a proper dynamics, i.e., spin operators in the Heisenberg representation depend on the time: $S_i^{\alpha}(t) = \exp(iHt) S_i^{\alpha} \exp(-iHt)$. For this reason model (1) is certainly useful for studying the time dependence of correlation functions in systems with the simplest interactions of an Ising type.

An important problem in studying the dynamics is the investigation of the behaviour of time correlation functions at large times, $t \to \infty$. In real physical systems that are ergodic, fluctuation correlations are damped with time, and the time correlation function when $t \to \infty$ is factorized into a product of independent averages. As Kubo [2] has noted, a model consideration may break the property of ergodicity so that the limiting value of a correlation function will be nonzero:

$$L_{iK}^{\alpha\beta} = \lim_{t \to \infty} \langle \delta S_i^{\alpha}(t) \delta S_K^{\beta} \rangle \neq 0, \qquad (2)$$

where $\delta S_i^{\alpha} = S_i^{\alpha} - \langle S_i^{\alpha} \rangle$ and the brackets mean statistical averaging over an equilibrium state. The parameter of nonergodicity (2) is connected with the difference of static isothermal χ^T and isolated, χ^K, susceptibilities (see ref. [2]):

$$L_{AB} = \beta(\chi_{AB}^T - \chi_{AB}^K), \quad \beta = 1/T, \qquad (2a)$$

where A and B are arbitrary dynamic operators.

The study of model (1) has revealed that it possesses the property of being nonergodic in the paraphase, i.e., at $T_c \leq T < \infty$, where T_c is the temperature of phase transition into a state with $\langle S_i^z \rangle \neq 0$. In ref. [3] it has been found that in the random-phase approximation $L_q^{xx} \neq 0$ for any wave vectors q.

In ref. [4] it has been shown that this inequality can be strictly proved for the case $q = 0$. However, in a general case when $q \neq 0$, it is not clear whether the nonergodicity is the model or approximation property. On the other hand our recent studies [5] of the phonon model with anharmonicity of fourth order in the mode-coupling approximation have demonstrated that the system does become nonergodic only in a phase-transition region at some temperature $T_f > T_c$. Since model (1) corresponds to the phonon model in a strong-anharmonic limit, one may expect it will also be nonergodic. Thus the problem of nonergodicity of model (1) requires a more careful consideration.

In this paper, we studied the nonergodic behaviour of model (1) in the paraphase when $\Omega < \Omega_c$. Using the Green-function projection method [6], we calculated the isothermal relaxation funcion in the mode-coupling approximation, obtained a closed set of equations for nonergodicity parameters (2) and analysed their temperature behaviour versus the transverse field Ω.

1. EQUATIONS FOR RELAXATION FUNCTIONS

Let us consider the isothermal relaxation function for model (2)

$$\Phi_{iK}^{\alpha\beta}(t) \equiv (\delta S_i^\alpha(t) \mid \delta S_K^\beta) = \int_0^\beta d\tau < \delta S_i^\alpha(t - i\tau)\, \delta S_K^\beta > , \qquad (3)$$

where the angular brackets denote the average over a canonical ensemble, and $\alpha = x, y, z$. Let us introduce a space-time Fourier transformation for function (3) according to the definition:

$$\Phi_{iK}^{\alpha\beta}(z) = ((\delta S_i^\alpha \mid \delta S_K^\beta)) = \pm i \int_{-\infty}^{\infty} \theta(\tau - t) e^{izt} \Phi_{iK}^{\alpha\beta}(t) = \frac{1}{N}\sum_q e^{i\bar{q}(\bar{R}_i - \bar{R}_K)} \Phi_{\bar{q}}^{\alpha\beta}(z), \qquad (4)$$

where the coordinates $\bar{R}_i$ determine points of a three-dimensional lattice.

Using the projection method proposed in [6] for Green functions we obtain in the second order the following exact representation for Fourier components of function (4):

$$\Phi_{\bar{q}}^{\alpha\beta}(z) = \frac{-\chi_{\bar{q}}^{\alpha\beta}}{z - a_{\bar{q}}^{\alpha\beta}/\chi_{\bar{q}}^{\alpha\beta} - \dfrac{\Delta_{\bar{q}}^{\alpha\beta}/\chi_{\bar{q}}^{\alpha\beta}}{z - b_{\bar{q}}^{\alpha\beta}/\Delta_{\bar{q}}^{\alpha\beta} + a_{\bar{q}}^{\alpha\beta}/\chi_{\bar{q}}^{\alpha\beta} + M_{\bar{q}}(z)/\Delta_{\bar{q}}^{\alpha\beta}}}, \qquad (5)$$

where, analogously to (4) spatial Fourier components of the isothermal susceptibility

$$\chi_{ik}^{\alpha\beta} = \Phi_{ik}^{\alpha\beta}(t = 0), \qquad (6)$$

the relaxational kernel

$$M_{ik}^{\alpha\beta}(z) = ((\ddot{S}_i^\alpha \mid \ddot{S}_k^\beta)) \qquad (7)$$

and equilibrium correlation functions

$$a_{ik}^{\alpha\beta} = (i S_i^\alpha \mid S_k^\beta), \qquad (8)$$

$$\Delta_{ik}^{\alpha\beta} = (\dot{S}_i^\alpha \mid \dot{S}_k^\beta)_1, \qquad (9)$$

$$b_{ik}^{\alpha\beta} = (i \ddot{S}_i^\alpha \mid \dot{S}_k^\beta)_1 \qquad (10)$$

are introduced.

The lower indices of the brackets denote projections according to the rules

$$((A_i^\alpha \mid B_k^\beta))_2 = ((A_i^\alpha \mid B_k^\beta))_1 - ((A_i^\alpha \mid \dot{S}_\ell^\beta))_1 [((\dot{S}^\alpha \mid \dot{S}^\beta))_1]^{-1}_{\ell m} ((\dot{S}_m^\alpha \mid B_k^\beta))_1 \qquad (11)$$

$$((A_i^\alpha \mid B_k^\beta))_1^{\alpha\beta} = ((A_i^\alpha \mid B_k^\beta)) - ((A_i^\alpha \mid \delta S_\ell^\beta)) [((\delta S^\alpha \mid \delta S^\beta))]^{-1}_{\ell m} ((\delta S_m^\alpha \mid B_k^\beta)) \qquad (12)$$

and an analogous rule (12) for $(A^\alpha \mid B^\beta)_1$. Here and in the following summation over repeated lattice indices is assumed.

Let us remark that the correlation functions in (6), (8-10) are connected with the frequency moments of the spectrum $\Phi''(\omega)$ of the relaxation function $\Phi(\omega \pm i0) = \Phi'(\omega) \pm i\Phi''(\omega)$ by the general relation

$$(i^m \frac{d^m}{dt_1^m} \delta S_i^\alpha(t_1) \mid (-i)^n \frac{d^n}{dt_2^n} \delta S_k^\beta(t_2))_{t_1 = t_2} = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega^{m+n} \mathrm{Im}\, \Phi_{ik}^{\alpha\beta}(\omega). \qquad (13)$$

Furthermore, the relaxation function is related to the isolated or Kubo dynamical susceptibility $\chi^K(z)$ by the relation

$$z\Phi_{ik}^{\alpha\beta}(z) = [\chi_{ik}^{\alpha\beta}(z)]^K - \chi_{ik}^{\alpha\beta}, \qquad (14)$$

where $\chi_{ik}^{\alpha\beta}$ is the isothermal static susceptibility (6).

Let us now consider equation (5). From the equation of motion $\dot{S}_i^\alpha = i[H, S_i^\alpha]$ we obtain with the definition $\hat{H}_i^\alpha = \sum_\ell J_{i\ell} S_\ell^\alpha$:

$$\dot{S}_i^x = \hat{H}_i^z S_i^y, \quad \dot{S}_i^y = \Omega S_i^z - \hat{H}_i^z S_i^x, \quad \dot{S}_i^z = -\Omega S_i^y, \qquad (15a-c)$$

$$\ddot{S}_i^x = \Omega \hat{H}_i^z S_i^z - (\hat{H}_i^z)^2 S_i^x - \Omega \hat{H}_i^y S_i^y, \qquad (16a)$$

$$\ddot{S}_i^y = -\Omega^2 S_i^y - (H_i^z)^2 S_i^y + \Omega \hat{H}_i^y S_i^x, \tag{16b}$$

$$\ddot{S}_i^z = -\Omega^2 S_i^z + \Omega \hat{H}_i^z S_i^x, \tag{16c}$$

which represent generalized currents $\dot{S}_i^\alpha$ and forces $\ddot{S}_i^\alpha$ of our problem.

At first let us note some useful strong relations which may be obtained from $\langle \dot{S}_i^\alpha \rangle = 0$, $\langle \ddot{S}_i^\alpha \rangle = 0$ and from the simple connection (15c) between the spin components S^y and S^z. In the paraphase the thermodynamical average of (15) and (16) yields

$$\langle \hat{H}_i^z S_i^y \rangle = 0, \quad \langle \hat{H}_i^z S_i^x \rangle = 0, \quad \langle S_i^y \rangle = 0,$$
$$\Omega \langle \hat{H}_i^z S_i^z \rangle = \langle \hat{H}_i^z \hat{H}_i^z S_i^x \rangle + \Omega \langle \hat{H}_i^y S_i^y \rangle . \tag{17a-d}$$

Employing the identities

$$((i\dot{A} \mid B)) = (A \mid B) + z((A \mid B)), \tag{18a}$$

$$((\dot{A} \mid \dot{B})) = (i\dot{A} \mid B) + z(A \mid B) + z^2((A \mid B)), \tag{18b}$$

$$(i\dot{A} \mid B) = \langle [A, B] \rangle , \tag{18c}$$

and taking into account (15c), we find

$$\Phi^{y\alpha} = (i/\Omega)(\chi^{z\alpha} + z\Phi^{z\alpha}), \quad \Phi^{\alpha y} = (-i/\Omega)(\chi^{\alpha z} + z\Phi^{\alpha z}), \; \alpha = x, z \tag{19}$$

$$\Phi^{yy} = (z/\Omega^2)(\chi^{zz} + z\Phi^{zz}) \tag{20}$$

as well as

$$\chi_{ik}^{yy} = (\Omega/S)\,\delta_{ik}, \quad S \equiv \langle S_i^x \rangle , \tag{21}$$

$$\chi_{ik}^{y\alpha} = \chi_{ik}^{\alpha y} = 0, \quad \alpha = x, z. \tag{22}$$

This means that all relaxation functions involving the spin component S^y may be expressed by the other relaxation functions $\Phi^{\alpha\beta}$ with $\alpha, \beta = x, z$, and therefore, they contain no additional information about the dynamics of the system. In the following we concentrate on the calculation of the relaxation functions Φ^{xx} and Φ^{zz}.

Due to the symmetry of the Hamiltonian with respect to the unitary transformation of the coordinate system $y \to -y$, $z \to -z$ (x unchanged) all equilibrium correlation functions involving products of an odd number or spin components S^y or S^z are equal to zero in the paraphase. Taking this into account, it is easy to show that the odd frequency moments of the spectrum $(\dot{S}_i^\alpha \mid \delta S_k^\beta)_c$ and $(\ddot{S}_i^\alpha \mid \dot{S}_k^\beta)$ vanish for $\alpha, \beta = x, z$, and the continued fraction expansion (5) simplifies to

$$\Phi_q^{\alpha\beta}(z) = - \cfrac{\chi_q^{\alpha\beta}}{z - \cfrac{\Delta_q^{\alpha\beta}/\chi_q^{\alpha\beta}}{z + M_q^{\alpha\beta}(z)/\Delta_q^{\alpha\beta}}} \qquad \alpha, \beta = x, z. \tag{23}$$

The correlation functions $\Delta_{ik}^{\alpha\beta}$ in (23) are given by

$$\Delta_{ik}^{xx} = \langle \hat{H}_i^z S_i^z \rangle \delta_{ik} - J_{ik} \langle S_k^y S_i^y \rangle =$$
$$= (\Omega^{-1} \langle \hat{H}_i^z \hat{H}_i^z S_i^x \rangle + \langle \hat{H}_i^y S_i^y \rangle \delta_{ik} - J_{ik} \langle S_k^y S_i^y \rangle , \tag{24}$$

$$\Delta_{ik}^{zz} = \Omega S \delta_{ik}, \qquad \Delta_{ik}^{xz} = \Delta_{ik}^{zx} = 0, \tag{25}$$

where the second equation in (24), which is more suitable for further approximations, has been obtained from (17d). In the theory established in the following the susceptibilities $\chi^{\alpha\beta}$ and the equilibrium correlation functions appearing in (24), (25) are considered as given input quantities playing the role of initail conditions.

2. MODE-COUPLING APPROXIMATION

Let us now turn to the calculation of the relaxation kernel $M^{\alpha\beta}(z)$ in the mode-coupling approximation. From (7), (11), (12) we find explicitly (suppressing site indices)

$$M^{\alpha\beta} = ((\ddot{S}^\alpha \mid \ddot{S}^\beta))_1 - ((\ddot{S}^\alpha \mid \dot{S}^\beta))_1 [((\dot{S}^\alpha \mid \dot{S}^\beta))_1]^{-1} ((\dot{S}^\alpha \mid \ddot{S}^\beta))_1 . \tag{26}$$

Now one can insert expressions (15) and (16) for the currents $\dot{S}^\alpha$ and forces $\ddot{S}^\alpha$ into (26), and then the higher-order force-force, force-current, force-spin, and current-spin correlation functions may be factorized. This has been done in our previous work [7]. Another possibility that we will use in the given paper is to eliminate at first the current from (26) employing the identities (18a), (18b) and $(\dot{S}^\alpha \mid \delta S^\beta) = 0$ (for $\alpha, \beta = x, z$), which yields

$$M^{\alpha\beta} = ((\ddot{S}^\alpha \mid \ddot{S}^\beta))_1 + [(\ddot{S}^\alpha \mid \delta S^\beta)(\chi^{\alpha\beta})^{-1} - ((\ddot{S}^\alpha \mid \delta S^\beta))(\Phi^{\alpha\beta})^{-1}]$$
$$[(\chi^{\alpha\beta})^{-1} + (\Phi^{\alpha\beta})^{-1}][(\chi^{\alpha\beta})^{-1}(\delta S^\alpha \mid \ddot{S}^\beta) - (\Phi^{\alpha\beta})^{-1}((\delta S^\alpha \mid \ddot{S}^\beta))] \tag{27}$$

and after that we have only to factorize higher-order force-force and force-spin correlation functions in (27). To illustrate the procedure, let us start with the simple case of calculation of the relaxation kernel M^{zz}:

$$M_{ik}^{zz} = \Omega^2((-\Omega S_i^z + \hat{H}_i^z S_i^x | -\Omega S_k^z + \hat{H}_k^z S_k^x))_2^{zz} = \Omega^2 J_{i\ell} J_{km}((S_\ell^z \delta S_i^x | S_m^z \delta S_k^x))_2^{zz}. \tag{28}$$

As it is easy to see from (27), the terms $\sim S_i^z$ are projected out of (28). Expression (28) contains only one type of higher-order correlation function of an even number of spin fluctuations, the factorization of which yields with (17b)

$$\langle \delta S_\ell^z(t-i\tau)\delta S_i^x(t-i\tau)\delta S_m^z \delta S_k^x\rangle \approx \langle \delta S_\ell^z(t-i\tau)\delta S_m^z\rangle\langle \delta S_i^x(t-i\tau)\delta S_k^x\rangle + \langle \delta S_\ell^z(t-i\tau)\delta S_k^x\rangle\langle \delta S_i^x(t-i\tau)\delta S_m^z\rangle. \tag{29}$$

Correlation function of an odd number of spin fluctuations are neglected. The pair correlation functions can be expressed by the fluctuation dissipation theorem in terms of the spectrum of the relaxation function, e.g.,

$$\langle S_\ell^z(t) S_m^z\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} e^{-i\omega t}\, \omega\, n(\omega)\, e^{\beta\omega}\, \mathrm{Im}\, \Phi_{\ell m}^{zz}(\omega), \tag{30}$$

where $n(\omega) = (e^{\beta\omega} - 1)^{-1}$. Within this approximation scheme, the calculation of the current relaxation kernel is straightforward, and the final result reads

$$M_{ik}^{zz}(z) = \Omega^2 J_{i\ell} J_{km} \mathfrak{M}[\Phi_{\ell m}^{zz}\Phi_{ik}^{xx} + \Phi_{\ell k}^{zx}\Phi_{im}^{xz}], \tag{31}$$

where for abbreviation of further formulae the symbolic notation

$$\mathfrak{M}[\Phi^{\alpha_1\beta_1}\Phi^{\alpha_2\beta_2}\ldots\Phi^{\alpha_n\beta_n}] \equiv$$

$$\equiv \frac{1}{\pi^n}\int_{-\infty}^{\infty} \frac{d\omega_1 \ldots d\omega_n}{\omega_1 + \ldots + \omega_2 - z}\; \frac{\omega_1 n(\omega_1)\ldots\omega_n n(\omega_n)}{(\omega_1+\omega_2+\ldots\omega_n)\, n(\omega_1+\ldots\omega_n)} \times \tag{32}$$

$$\times\ \mathrm{Im}\,\Phi^{\alpha_1\beta_1}(\omega_1)\ldots\mathrm{Im}\,\Phi^{\alpha_n\beta_n}(\omega_n).$$

has been introduced. Thus, according to (31) the kernel M^{zz} is given by the relaxation functions Φ^{xx}, Φ^{zz}, Φ^{xz} and Φ^{zx}, which reflects the coupling of the spin component S^z to the component S^x. In the classic limit the nondiagonal relaxation functions Φ^{xz}, Φ^{zx} vanish since, e.g., $\Phi^{zx} \sim \chi^{zx} = T\langle S^z \delta S^x\rangle$ and the correlation function $\langle S^z\delta S^x\rangle$ is zero due to the symmetry of the Hamiltonian (cf. discussion above (23)).

Analogous calculation of the relaxation kernel M^{xx} is straightforward but lengthy, and we quote only the final result

$$M_{ij}^{xx} = ((\ddot{S}_i^x|\ddot{S}_j^x))_2 =$$

$$= ((\Omega\hat{H}_i^z S_i^z - \hat{H}_i^z\hat{H}_i^z S_i^x - \Omega\hat{H}_i^y S_i^y | \Omega\hat{H}_j^z S_j^z - \hat{H}_j^z\hat{H}_j^z S_j^x - \Omega\hat{H}_j^y S_j^y))_2 \approx$$

$$\approx \mathfrak{M}\{\Omega^2[\Phi_{ij}^{zz}((\delta\hat{H}_i^z|\delta\hat{H}_j^z)) + ((\delta S_i^z|\delta\hat{H}_j^z))((\delta\hat{H}_i^z|\delta S_j^z)) +$$

$$+ \Phi_{ij}^{yy}((\delta\hat{H}_i^y|\delta\hat{H}_j^y)) + ((\delta S_i^y|\delta\hat{H}_j^y))((\delta\hat{H}_i^y|\delta S_j^y))] + 2((\delta\hat{H}_i^z|\delta\hat{H}_j^z)) \times$$

$$\times[((\delta\hat{H}_i^z|\delta\hat{H}_j^z))(S^2 + \Phi_{ij}^{xx}) + 2((\delta S_i^x|\delta\hat{H}_j^z))((\delta\hat{H}_i^z|\delta S_j^x)) - \tag{33}$$

$$- 2\Omega S((\delta\hat{H}_i^z|\delta\hat{H}_j^z))[((\delta S_i^z|\delta\hat{H}_j^z)) + ((\delta\hat{H}_i^z|\delta S_j^z))] +$$

$$+ 2\Omega S[((\delta\hat{H}_i^z|\delta S_j^y)) + ((\delta S_i^y|\delta\hat{H}_j^z))((\delta\hat{H}_i^y|\delta\hat{H}_j^z))] -$$

$$- \Omega^2[((\delta\hat{H}_i^z|\delta\hat{H}_j^y))\Phi_{ij}^{zy} + ((\delta S_i^z|\delta\hat{H}_j^y))((\delta\hat{H}_i^z|\delta S_j^y)) +$$

$$+ \Phi_{ij}^{yz}((\delta\hat{H}_i^y|\delta\hat{H}_j^z]] + ((\delta S_i^y|\delta\hat{H}_j^z))((\delta\hat{H}_i^y|\delta S_j^z))]\},$$

where $\delta\hat{H}_i^\alpha = \sum_\ell J_{i\ell}\,\delta S_\ell^\alpha$.

Let us note that the relatively simple form of M^{zz} (31) and M^{xx} (33) is due to the fact that all higher-order correlation functions appearing in the second term of the rhs of (27) depend on an odd number of spin fluctuations, and therefore, this term vanishes owing to the applied factorization approximation. On the contrary, starting from (26) and inserting $\dot{S}_i^\alpha$ (15) and $\ddot{S}_i^\alpha$ (16) into (26) as was done in /7/, we obtain within the same factorization approximation, a nonvanishing contribution from the second term of the rhs of (26). For a special example discussed below the difference between both procedures has been found to be small. In general, the procedure, when only force-force and force-spin correlation functions are factorized, might be expected to be better than the additional factorization of force-current and current-spin correlation functions.

Equations (23), (31)-(33) together with the strong relations (19), (20) represent a closed set of integral equations for a self-consistent calculation of the relaxation functions $\Phi^{\alpha\beta}$. Integrations have to be performed both over the frequency and wave vector and the integrals may be calculated only with a great numerical effort. To simplify further calculations, we neglect the dispersion of the relaxation kernels (31) and (34), i.e., we use the local approximation: $M_{ik}^{\alpha\beta} = M_{ii}^{\alpha\beta}\,\delta_{ik}$. Furthermore all spin correlation functions appearing in these kernels are also approximated by their local values, i.e. for example $\langle S_i^z(t) S_\ell^z\rangle \approx \langle S_i^z(t) S_i^z\rangle\,\delta_{i\ell}$. Within this approximation we get from (31) and (33)

$$M^{zz}_{ii}(z) = \Omega^2 J_2^2 \mathfrak{M}[\Phi^{zz}_{ii}\Phi^{xx}_{ii}], \quad J_2^2 \equiv \sum_{\ell} J^2_{i\ell} \tag{34}$$

$$M^{xx}_{ii}(z) = J_2^2 \mathfrak{M}[\Omega^2\{(\Phi^{zz}_{ii})^2 + (\Phi^{yy}_{ii})^2 - (\Phi^{zy}_{ii})^2 - (\Phi^{yz}_{ii})^2\} + 2J_2^2(\Phi^{zz}_{ii})^2(S^2 + \Phi^{xx}_{ii})]. \tag{35}$$

The solution of the obtained set of equations e.g. by iteration remains a still difficult due to the necessity to calculate the remaining frequency integrals. An analytical calculation is possible in the classic limit.

3. NONERGODIC BEHAVIOUR OF THE MODEL

The set of equations obtained in the previous section allows us to investigate the nonergodic behaviour of the model if we take into account the connection of nonergodicity parameters (2) with isothermal relaxation functions:

$$L^{\alpha\beta}_{ij} = T \lim_{z\to io} [-z\Phi^{\alpha\beta}_{ij}(z)]. \tag{36}$$

Then, using eq.(23), we obtain for the spatial Fourier representation of nonergodicity parameters the following equation:

$$L^{\alpha\beta}_{\bar q} = T\chi^{\alpha\beta}_{\bar q}[1 + (\Delta^{\alpha\beta}_{\bar q})^2/\chi^{\alpha\beta}_{\bar q}\, m^{\alpha\beta}_{\bar q}]^{-1}, \tag{37}$$

where

$$m^{\alpha\beta}_{\bar q} = \lim_{z\to io}[-zM^{\alpha\beta}_{\bar q}(z)]$$

represents the power of the nonergodicity pole of the kernel $M(z)$. From (30) one can see that the existence of a constant $L \neq 0$ requires a singularity $\sim\delta(\omega)$ in the spectrum $\Phi''(\omega)$, i.e.,

$$\mathrm{Im}\,\Phi^{\alpha\beta}_{ik}(\omega) = \pi\beta L^{\alpha\beta}_{ik}\,\delta(\omega) + \text{reg. terms} \tag{38}$$

The power $m^{\alpha\beta}_q$ of the pole of the relaxation kernel $M^{\alpha\beta}_q(z)$ is obtained by insertion of (38) into the mode-coupling approximation of $M^{\alpha\beta}_q(z)$. Taking into account the definition (32), we find generally

$$\lim_{z\to io}\{-z\,\mathfrak{M}[\Phi^{\alpha_1\beta_1}\Phi^{\alpha_2\beta_2}\ldots\Phi^{\alpha_n\beta_n}]\} = \beta L^{\alpha_1\beta_1}L^{\alpha_2\beta_2}\ldots L^{\alpha_n\beta_n}. \tag{39}$$

By using (39) one gets from (34) and (35)

$$m^{zz}_{ii} = \beta\Omega^2 J_2^2 L^{xx}L^{zz}, \tag{40}$$

$$m^{xx}_{ii} = \beta J_2^4 (L^{zz})^2[\Omega^2/J_2^2 + 2(S^2 + L^{xx})], \tag{41}$$

where $L^{xx} = L^{xx}_{ii}$ and $L^{zz} \equiv L^{zz}_{ii}$. In (41) we have further considered the strong relations (19), (20) that yield $L^{yz} = L^{zy} = L^{yy} = 0$.

A remaining crucial point is the calculation of thermodynamic equilibrium functions χ and Δ. In the framework of the present paper we adopt results of the random-phase approximation derived in a previous work [3]. Here we briefly list the quantities of interest

$$S = (1/2)\tanh(\Omega/2T), \tag{42}$$

$$\chi^{xx}_{\bar q} = (1/T)(1/4 - S^2), \tag{43}$$

$$\chi^{zz}_{\bar q} = 1/(\Omega/S - J_{\bar q}), \quad J_{\bar q} \equiv (1/N)\sum_{ij} e^{i\bar q(\bar R_i - \bar R_j)} J_{ij}. \tag{44}$$

Analogously as in m^{xx}_{ik}, the spin correlation functions appearing in Δ^{xx}_{ik} are approximated by their diagonal parts, which results in

$$\Delta^{xx}_{\bar q} = SJ_2^2/4\Omega. \tag{45}$$

Inserting equations (40)-(45) into (37) (neglecting the dispersion of $m^{\alpha\beta}_{\bar q}$), we finally get the following set of equations for the local nonergodicity constants $L = L_{ii} = (1/N)\sum_{\bar q} L_{\bar q}$

$$L^{xx} = \frac{1/4 - S^2}{1 + (TS/4\Omega)^2/(1/4 - S^2)(L^{zz})^2(\Omega^2/J_2^2 + 2S^2 2L^{xx})}, \tag{46}$$

$$L^{zz} = (T/J_o N)\sum_{\bar q}[(\Delta_o + 1 - J_{\bar q}/J_o)^{-1} - (\Delta_1 + 1 - J_{\bar q}/J_o)^{-1}] \simeq (T/J_o)[F(\Delta_o) - F(\Delta_1)], \quad J_o \equiv \sum_j J_{ij} = J_{\bar q = o} \tag{47}$$

with

$$\Delta_o = \Omega/SJ_o - 1$$

$$\Delta_1 = \Delta_o + L^{xx}L^{zz}J_2^2/S^2TJ_o,$$

and for the calculation of the q-integrals in (42) a simple cubic lattice (lattice constant a) and nearest neighbour interactions are assumed, i.e., $J_{\bar q} = (J_o/3)\sum_{\alpha}\cos(q_\alpha a)$. The q-integrals are as usual approximated by

$$\frac{1}{N}\sum_{q}\frac{1}{\Delta + 1 - J_q/J_o} \approx 2[\Delta + 1 - \sqrt{(\Delta + 1)^2 - 1}\,] \equiv F(\Delta),$$

defining the function $F(\Delta)$.

Let us now turn to analysing the set of equations (46), (47). There exists always a trivial solution $L^{xx} = L^{zz} = 0$. In the high-temperature limit the nontrivial solutions are governed by

$$L^{xx} = (1/4)[1 + 1/64(L^{zz})^2(\Omega^2/J_2^2 + 2L^{xx})]^{-1}, \qquad (48)$$

$$L^{zz} = (1/4)(1 - \Omega^2/J_2^2 L^{xx}). \qquad (49)$$

Numerical calculation shows that for small values of $\Omega < \Omega_c^o$ two nontrivial solutions with positive L^{xx} and L^{zz} exist. This means that in this region the system behaves like in the limit of the conventional Ising model $\Omega \to 0$. Since for that Ising model the magnetization is a constant of motion, we have $L^{zz} = 1/4$ and from (48) we find $L^{xx} = 1/8$. The dependence of L^{xx} on Ω as $T = \infty$ is shown in Fig. 1. As one can see, there are two solutions, coinciding when $\Omega = \Omega_c^o$ and disappearing when $\Omega > \Omega_c^o$. Thus, at $\Omega > \Omega_c^o$ the set of equations has no solutions and the model is ergodic. However, at $\Omega < \Omega_c^o$ it is nonergodic like the usual Ising model.

Consider finite temperatures. In Fig. 2 the result is shown of a numerical solution of eqs. (46), (47) by iteration. As one can see, the solutions L^{xx} and L^{zz} appear discontinuously at a temperature $T_f > T_c$ when $\Omega < \Omega_c$. Note that a phase transition temperature T_c is determined by the divergence of the isothermal susceptibility $\chi^{zz}_{q=o}$ (44). The dependence of T_c and T_f on the magnitude of transverse field Ω is shown in Fig. 3. At $\Omega \doteq \Omega_c^o \approx 0.05\,J_o$ the temperature T_f tends to infinity, and for $\Omega \gtrsim 0.3\,J_o$,

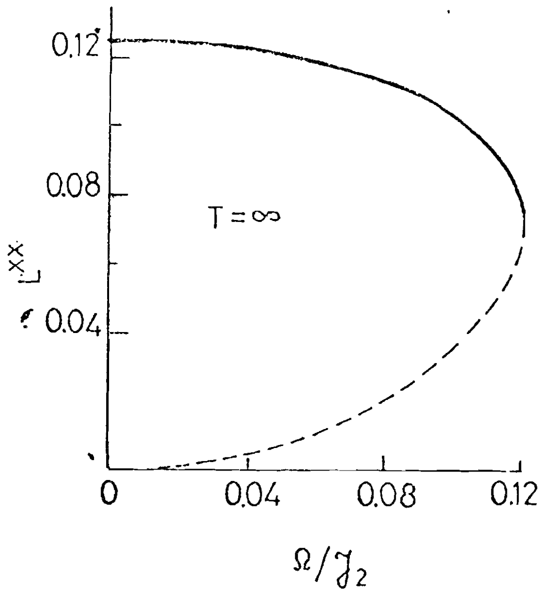

Fig. 1. Dependence of the nonergodicity parameter L^{xx} on the magnitude of the transverse field for $T = \infty$.

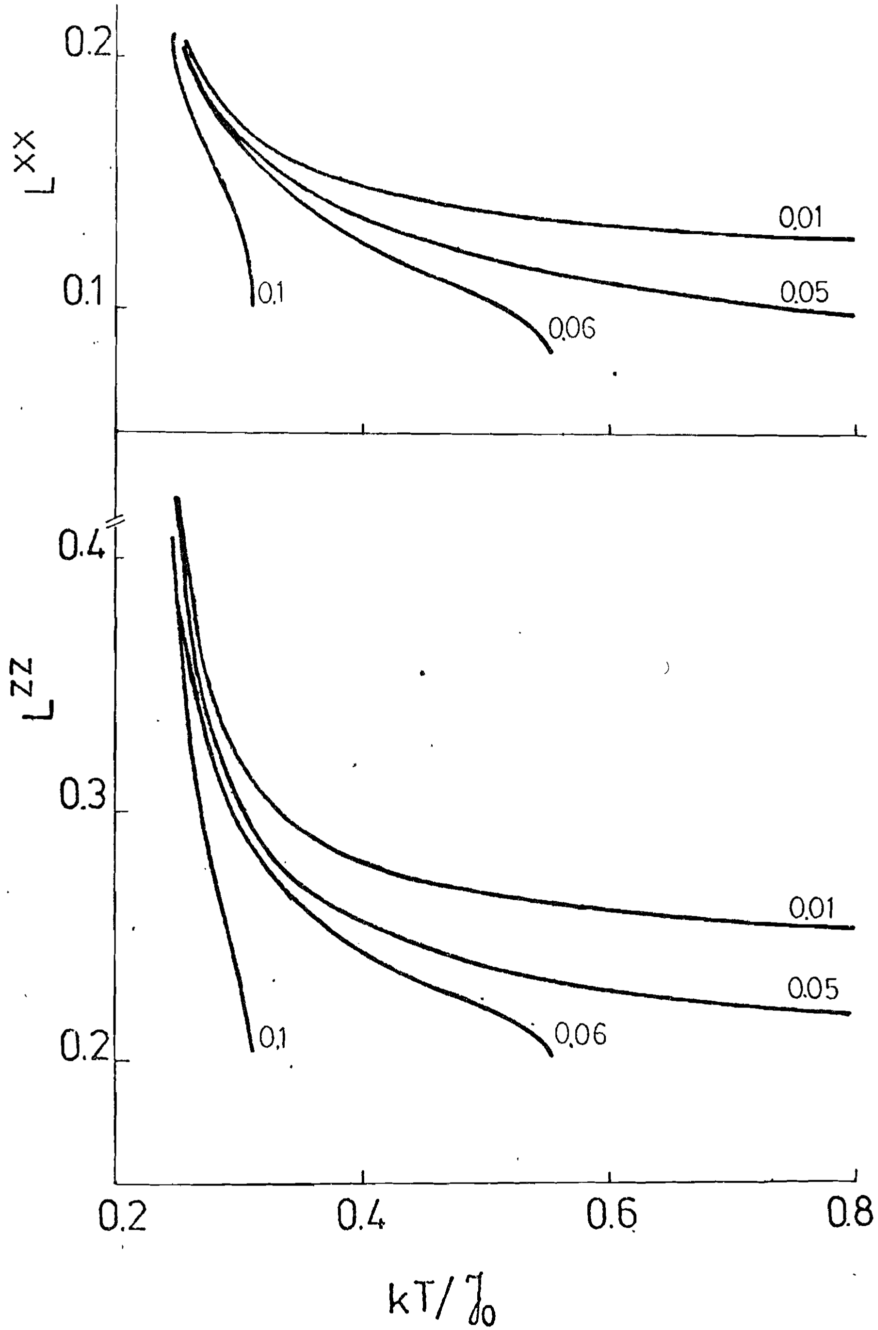

Fig. 2. Temperature dependence of the nonergodicity parameters L^{xx} and L^{zz} for various values of the transverse field Ω/J_o.

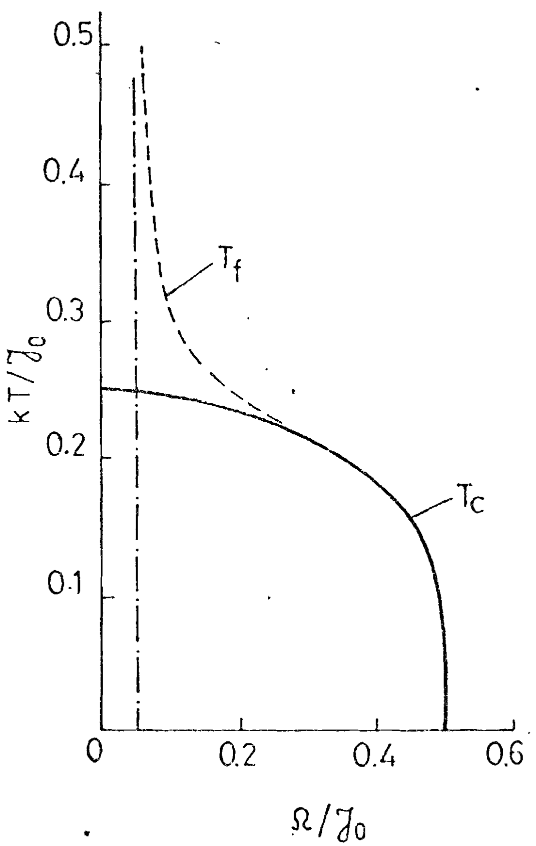

Fig. 3. Dependence of the phase-transition temperature T_c and the temperature of onset of the nonergodic behaviour T_f on the transverse field.

within a numerical error lower than one percent, it coincides with T_c. All calculations were performed for a simple cubic lattice with nearest neighbour interactions where $J_2^2 = J_0^2/6$.

Thus, the nonergodic behaviour for local longitudinal and transverse correlation functions arises in the phase transition region at temperatures $T_c < T < T_f$ and values of the transverse field $\Omega_c^0 < \Omega < \Omega_c$. The temperature region of nonergodicity increases when Ω decreases, and at $\Omega < \Omega_c^0$ the model is nonergodic at any temperatures.

Note that at $T = T_f$ two solutions of eqs. (46) and (47) can appear, where $L_1(T_f) = L_2(T_f)$ and $L_1(T) < L_2(T)$ at $T < T_f$. However, we were able to obtain the lower solution only in a special case of $T = \infty$ (see Fig.1). At finite temperatures it is not stable with respect to iteration, which agrees with results of the general investigation of this problem in paper [8].

4. DISCUSSION

Having calculated the local nonergodicity parameters (2) $L_{ii}^{aa} = (1/N)\sum_{\bar{q}} L_{\bar{q}}^{aa}$ $(a = x, z)$ for the Ising model with a transverse field (1) we arrive at the following conclusions: i) There exists a lower critical value of the transverse field $\Omega_c^0 \approx 0.05 J_0$ such that for $\Omega < \Omega_c^0$ the model correlation functions are nonergodic ($L_{ii}^{aa} \neq 0$) at any temperatures in the paraphase ($T_c < T < \infty$), like in the standard Ising model ($\Omega = 0$ is to be put in (1)); ii) For $\Omega_c^0 < \Omega < \Omega_c$ ($\approx 0.5 J_0$) the nonergodicity constants L_{ii}^{aa}

are discontinuous at a temperature $T = T_f > T_c$; iii) The temperature interval of nonergodicity $T_f - T_c \to 0$ when $\Omega \to \Omega_c$. Consequently, a large enough value of the transverse field Ω results in the ergodic behaviour of correlation functions in the model (1), i.e., $L_{ii}^{aa} = 0$ in (2).

These results were established by calculating the isothermal relaxation function (3) in the mode-coupling approximation (29) as well as static susceptibilities and equilibrium correlation functions (23) in the random-phase approximation. The latter approximation does not correctly take into account the longitudinal spin fluctuations as $T \to T_c$ (see, e.g.,[3]). As a result, when $\Omega \to 0$, a wrong asymptotic follows for the constant L_{ii}^{zz}:

$$L^{zz} = \frac{T}{N}\sum_{\bar{q}} \chi_{\bar{q}}^{zz} = \frac{T}{J_0} F\left(\frac{4T}{J_0} - 1\right) \geq \frac{1}{4},$$

since the general relation (2) gives $L_{ii}^{zz} \leq \langle(\delta S_i^z)^2\rangle \leq 1/4$. Note, however, that breaking of the sum role for the longitudinal susceptibility in the random-phase approximation as well as violation of the dynamical scaling in the mode-coupling approximation occur only in a critical region, when $T \to T_c$, whereas the nonergodic behaviour we have obtained sets in outside the critical region and is not directly related to critical singularities at the phase transition in model (1). Therefore, we suppose that the accepted approximations being appropriately amended would only produce quantitative corrections to Ω_c^0 and T_f, with no change in the qualitative pattern of the nonergodicity origin in model (1).

Of certain interest would be the comparison of the obtained results with rigorous calculations of the static susceptibility for exactly solvable models. In ref. [9] the isothermal susceptibility $\chi_{\bar{q}=0}^{xx}$ has been computed for some two-dimensional lattices, and in ref. [10] the corresponding expressions have been derived for the isolated susceptibility. Comparison of these susceptibilities shows that for a honeycombed lattice their difference equals zero, and $L_{\bar{q}=0}^{xx} = 0$, whereas for a square lattice it is nonzero, and $L_{\bar{q}=0}^{xx} \neq 0$, which testifies the dependence of nonergodicity of the system on the topology of a lattice. However, these results, like the ones of ref.[4] for $L_{\bar{q}=0}^{xx}$, are not sufficient for their comparison with our computations of local constants $L = (1/N)\sum_{\bar{q}} L_{\bar{q}}$ since $L_{\bar{q}=0}$ gives a negligible contribution (about $1/N$ to L).

It is also interesting to note that the results found in this paper are in qualitative agreement with the results of studies of the nonergodic behaviour in ref.[5] for the ϕ^4 model which like model (1), belongs to the Ising class of universality. This model of a structural phase transition displays the nonergodic behaviour for a strong enough anharmonicity, when it, like model (1), describes an order-disorder transition. And the temperature behaviour of the nonergodicity local parameter is in it of the same shape as shown in Fig. 2. As has been established in ref./5/, the nonergodic behaviour originates from the localization of order parameter fluctuations, and therefore, like in the ϕ^4 model, the nonergodic behaviour in model (1) can be related to the clusters of short range order arising above the phase transition temperature.

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Неэргодическое поведение в модели Изинга с поперечным полем

В приближении взаимодействующих мод исследовано неэргодическое поведение модели Изинга с поперечным полем относительно временных корреляционных функций продольных и поперечных компонент спина. Показано, что имеется нижнее критическое значение величины поперечного поля $\Omega = \Omega_c^0$, такое, что при $\Omega < \Omega_c^0$ система неэргодична при любых температурах подобно обычной модели Изинга. При $\Omega_c^0 < \Omega < \Omega_c$ /Ω_c - верхнее критическое значение, при котором исчезает фазовый переход в модели/ неэргодическое поведение появляется при температуре $T_f > T_c$ - температуры фазового перехода. Разность $T_f - T_c \to 0$ при $\Omega \to \Omega_c$ и $T_f - T_c \to \infty$ при $\Omega \to \Omega_c^0$.

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Nonergodic Behaviour in the Transverse Ising Model

The mode-coupling approximation is applied to study the nonergodic behaviour of an Ising model with a transverse field in terms of time correlation functions of spin longitudinal and transverse components. A lower critical value is found for the transverse field $\Omega = \Omega_c^0$ such that for $\Omega < \Omega_c^0$ the system is nonergodic at any temperatures, like the conventional Ising model. When $\Omega_c^0 < \Omega < \Omega_c$ (Ω_c is an upper critical value at which there is no phase transition in the model), the system gets nonergodic at a temperature T_f larger than the phase transition temperature T_c. The difference $T_f - T_c \to 0$, when $\Omega \to \Omega_c$, and $T_f \to T_c \to \infty$, when $\Omega \to \Omega_c^0$.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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