Decay of the metastable phase in $d=1$ and $d=2$ Ising models

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(Received 8 April 1999)

We calculate perturbatively the tunneling decay rate Γ of the metastable phase in the quantum $d=1$ Ising model in a skew magnetic field near the coexistence line $0<h_x<1$, $h_z\to -0$ at $T=0$. It is shown that Γ oscillates in the magnetic field h_z due to discreteness of the excitation energy spectrum. After mapping of the obtained results onto the extreme anisotropic $d=2$ Ising model at $T<T_c$, we verify in the latter model the droplet theory predictions for the free energy analytically continued to the metastable phase. We also find evidence for the discrete-lattice corrections in this metastable phase free energy. [S0163-1829(99)04341-6]

It is widely accepted (Refs. 1 and 2, for review, see Ref. 3) that for all $T<T_c$, the free energy $F(H)$ of the two-dimensional Ising model analytically continued from the positive real axis $H>0$ into the complex H plane, has a branch cut singularity at the origin. Near the cut drawn along the negative real axis $H<0$, the imaginary part of the free energy is believed to have the following form:[4]

$$\operatorname{Im} F(e^{\pm i\pi}|H|)=\pm B|H|\exp(-A/|H|) \tag{1}$$

for small $|H|$. This expression extrapolates to the Ising model the results obtained by Langer[5] and Günther *et al.*[6] in the droplet field theory analysis of the coarse-grained Ginzburg-Landau model. In the droplet theory, the free energy continued to the cut $H<0$ is interpreted as the free energy of the metastable state $F_{ms}(H)\equiv F(e^{i\pi}|H|)$. Langer conjectured[5] that $\operatorname{Im} F_{ms}(H)$ may be identified (up to a dynamical factor) with the metastable phase decay rate provided by the thermally activated nucleation.

The phenomenological droplet theory prediction for the amplitude A in Eq. (1) is[3,4,7]

$$A=\frac{\beta\hat{\Sigma}^2}{8M}, \tag{2}$$

where M is the spontaneous magnetization, and $\hat{\Sigma}^2$ denotes the square of surface free energy of the equilibrium-shaped droplet divided by its area. Both $\hat{\Sigma}^2$ and M relate to the equilibrium zero-field state, and are known exactly. The quantity $\hat{\Sigma}^2$ can be calculated by use of the Wulff's construction from the exact anisotropic surface tension, as it was shown by Zia and Avron,[9] and M was obtained by Yang.[10] The linear dependence on $|H|$ prefactor in Eq. (1) arises in the continuum droplet field theory[6] from the contribution of the surface excitations (Goldstone modes) of the critical droplet.

Equations (1) and (2) were confirmed by Günther, Rikvold, and Novotny[7] in numerical constrained transfer-matrix calculations (see also Ref. 8), and by Harris in numerical analysis of certain power series.[4] However, no analytic microscopic evaluation of Eqs. (1) and (2) for the $d=2$ Ising model did exist. The purpose of the present paper is to perform analytic verification of Eqs. (1) and (2) for the $d=2$ Ising model in the extreme anisotropic limit.

We start from the anisotropic Ising model on the square lattice. It is characterized by the nearest-neighbor in-row and in-column coupling constants $J_1>0$, $J_2>0$, the magnetic field H, and the inverse temperature $\beta=1/(k_BT)$. The extreme anisotropic limit of the model is defined as follows:[11]

$$\tau\equiv\exp(-2\beta J_2)\to 0, \tag{3}$$

$$J_1=\frac{\tau}{\beta h_x}\to 0,\quad H=h_zJ_1\to 0,$$

with constant h_x and h_z. The transfer matrix of the $d=2$ Ising model in this limit can be written up to a nonsignificant numerical factor as $\exp(-\beta J_1\mathcal{H})$, where $\mathcal{H}$ denotes the quantum spin-1/2 Hamiltonian of the Ising chain in a skewed magnetic field:

$$\mathcal{H}=-\sum_{n=1}^{N}(\sigma_n^z\sigma_{n+1}^z+h_x\sigma_n^x+h_z\sigma_n^z). \tag{4}$$

Here $\sigma^{x,z}$ are the Pauli matrices, N is the number of sites in the chain, cyclic boundary conditions are supposed. The free energy F per the lattice site of the two-dimensional Ising model is proportional in limit (3) to the ground-state energy $E(h_x,h_z)$ of the quantum Hamiltonian (4):

$$F=J_1\lim_{N\to\infty}\left[\frac{E(h_x,h_z)}{N}\right]. \tag{5}$$

Our strategy contains two steps. (i) We calculate perturbatively the tunneling decay rate (proportional to the imaginary part of the energy) of the metastable state in model (4) at zero temperature. (ii) By use of mapping Eq. (5) we obtain then the imaginary part of the metastable free energy $F_{ms}(H)$ at $T<T_c$ for the $d=2$ Ising model in limit (3).

It should be noted, that models like Eq. (4) have been widely used to describe dynamical properties observed in real quasi-one-dimensional Ising ferromagnets.[12,13] So, the problem outlined in step (i) is by itself of considerable physical interest.

In the small field limit $h_x\ll 1$, $h_z\ll 1$ model (4) was studied by Fogedby.[14] In the free-fermion point $h_z=0$ Hamiltonian (4) reduces to the form[15]

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$$\mathcal{H}_0 \equiv \mathcal{H}|_{h_z=0} = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} \omega(\theta) \psi^\dagger(\theta) \psi(\theta) + \text{const}, \quad (6)$$

where θ is the quasimomentum, fermionic operators $\psi^\dagger(\theta)$, $\psi(\theta)$ satisfy the canonical anticommutational relations

$$\{\psi(\theta), \psi(\theta')\} = \{\psi^\dagger(\theta), \psi^\dagger(\theta')\} = 0,$$

$$\{\psi^\dagger(\theta), \psi(\theta')\} = 2\pi\delta(\theta - \theta'),$$

and

$$\omega(\theta) = 2\left[(1-h_x)^2 + 4h_x \sin^2\frac{\theta}{2}\right]^{1/2}.$$

At zero temperature, there is a phase transition point $h_x = 1$, which divides ordered $(0 < h_x < 1)$ and disordered $(h_x > 1)$ phases. Two ferromagnetic ground states $|0_+\rangle$ and $|0_-\rangle$ coexist in the interval $0 < h_x < 1$. They are distinguished by the sign of the spontaneous magnetization $\langle 0_\pm | \sigma_n^z | 0_\pm \rangle = \pm M$, where $M = (1-h_x^2)^{1/8}$.

A small negative longitudinal magnetic field $h_z < 0$ removes the ground-state degeneration. The following fermionic representation for the Hamiltonian (4) is valid in the thermodynamic limit $N \to \infty$,

$$\mathcal{H} = \mathcal{H}_0 + V + \text{const}, \quad (7)$$

where $\mathcal{H}_0$ denotes the free-fermionic Hamiltonian (6), V is given by

$$V = |h_z| M \sum_{n \in Z} :\exp\left(\frac{\varrho_n}{2}\right):, \quad (8)$$

$$\frac{\varrho_n}{2} = -\sum_{j<n} \psi_j^{(+)} \psi_j^{(-)},$$

$$\psi_j^{(+)} = i \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} \frac{\exp(ij\theta)}{\sqrt{\omega(\theta)}} [\psi(\theta) + \psi^\dagger(-\theta)],$$

$$\psi_j^{(-)} = i \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} \exp(ij\theta) \sqrt{\omega(\theta)} [-\psi(\theta) + \psi^\dagger(-\theta)],$$

and $\psi(\theta)|0_+\rangle = 0$ for all θ. We have used the conventional notation $:\cdots:$ for the normal ordering with respect to the fermionic operators $\psi(\theta), \psi^\dagger(\theta)$. Representation (7), (8) can be obtained from Eq. (4) by applying the Jordan-Wigner[16] and duality[11] transformations. In performing the normal ordering of fermionic operators in Eq. (8) we followed Jimbo *et al.*[17]

The nonlinear interaction term V in Eq. (7) prevents the exact integrability of the model. So, the natural way to study model (7) for small $|h_z| \neq 0$ is to use a certain perturbation expansion. It is clear, however, that the straightforward perturbation theory with the zero-order Hamiltonian $\mathcal{H}_0$ and perturbation V is useless in the considered problem. This is due to the fact that the term V contains the long-range interaction V_0 between fermions, which is given by

$$V_0 \equiv V|_{\omega(\theta)\to 1} = |h_z| M \sum_{n \in Z} :\exp\left(-2\sum_{j<n} b_j^\dagger b_j\right):, \quad (9)$$

where

$$b_j = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} \psi(\theta) \exp(ij\theta),$$

$$b_j^\dagger = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} \psi^\dagger(\theta) \exp(-ij\theta).$$

Operator V_0 is diagonal in the coordinate representation:

$$V_0 b_{j_{2n}}^\dagger b_{j_{2n-1}}^\dagger \cdots b_{j_1}^\dagger |0_+\rangle = -h_z M\left[N - 2\sum_{l=1}^{n} (j_{2l} - j_{2l-1})\right] b_{j_{2n}}^\dagger b_{j_{2n-1}}^\dagger \cdots b_{j_1}^\dagger |0_+\rangle, \quad (10)$$

where $j_l < j_{l+1}$. Since interaction (10) depends linearly on the distance between fermions, it changes the structure of the energy spectrum of model (7) at arbitrary small longitudinal magnetic field $h_z \neq 0$. So, to describe decay of the metastable vacuum, one should include the long-range interaction V_0 into the zero-order Hamiltonian. This phenomenon is well known in the Stark effect.[18] To describe ionization of an atom by the uniform electric field $\mathbf{E}$, one needs to consider the corresponding electrostatic energy $e\mathbf{E}\mathbf{r}$ in a nonperturbative way.

Accordingly, we subdivide the Hamiltonian (7) into the zero-order and interaction parts, as follows:

$$\mathcal{H} = \tilde{\mathcal{H}}_0 + \tilde{V}, \quad (11)$$

where

$$\tilde{\mathcal{H}}_0 \equiv \mathcal{H}_0 + V_0 + \text{const}, \quad (12)$$

$$\tilde{V} \equiv V - V_0. \quad (13)$$

The numerical constant in Eq. (12) is chosen to provide $\tilde{\mathcal{H}}_0 |0_+\rangle = 0$. Since the new zero-order Hamiltonian $\tilde{\mathcal{H}}_0$ conserves the number of fermions, its eigenstates can be classified by the fermion number. It is clear from Eq. (10), that fermions created by operators $b_n^\dagger$ are just the domain walls dividing the chain into oppositely magnetized domains.

One can easily verify in the small h_x limit, that the metastable vacuum $|0_+\rangle$ decays preferably into a one-domain state. We suppose, that this is true also in the general case $0 < h_x < 1$. So, below we shall contract the space of considered states to the two-fermion (i.e., one-domain) sector.

Let $|\phi_l\rangle$ be the translation invariant two-fermion eigenstate of the Hamiltonian $\tilde{\mathcal{H}}_0$. In the coordinate representation, the zero-order eigenvalue problem $\tilde{\mathcal{H}}_0 |\phi_l\rangle = E_l |\phi\rangle$ takes the form

$$\sum_{n' \in Z} K_{nn'} \phi_l(n') - M|n h_z| \phi_l(n) = \frac{E_l}{2} \phi_l(n),$$

where

$$K_{nn'} = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} \omega(\theta) \exp[i(n-n')\theta],$$

$$\phi_l(n)=\langle 0_+|b_0 b_n|\phi_l\rangle, \quad \phi_l(-n)=-\phi_l(n).$$

If the energy E_l is small enough, $E_l<\varepsilon$, where $\varepsilon\ll\omega(0)$, the wave function $\phi_l(n)$ is mainly concentrated far from the origin in the classically available region $|n|>\omega(0)/(|h_z|M)$. Therefore, we can apply the ''strong-coupling approximation''[19] to represent the wave function in the form

$$\phi_l(n)\cong\varphi_l(n)-\varphi_l(-n), \tag{14}$$

where the function $\varphi_l(n)$ solves the equation

$$\sum_{n'\in Z} K_{nn'}\varphi_l(n')-|h_z|Mn\varphi_l(n)=\frac{E_l}{2}\varphi_l(n).$$

After the Fourier transform, we obtain

$$\varphi_l(n)=\int_{-\pi}^{\pi}\frac{d\theta}{2\pi}\varphi_l(\theta)\exp(in\theta),$$

where

$$\varphi_l(\theta)=C\exp\left\{-\frac{i}{2|h_z|M}[f(\theta)-E_l\theta]\right\}, \tag{15}$$

$$C=(2|h_z|MN)^{-1/2},$$

$$f(\theta)=2\int_0^{\theta}d\alpha\,\omega(\alpha).$$

The 2π-periodicity condition for the function $\varphi_l(\theta)$ determines the energy levels E_l:

$$E_l=\frac{f(\pi)}{\pi}-2|h_z|Ml. \tag{16}$$

The normalization constant C in Eq. (15) is chosen to yield

$$\langle\phi_l|\phi_{l'}\rangle=\frac{\delta_{ll'}}{\Delta E},$$

where $\Delta E=2|h_z|M$ is the interlevel distance.

To determine the decay rate Γ of the metastable vacuum we use the following natural, though nonrigorous, procedure. In the second-order correction $E_{ms}^{(2)}$ to the metastable vacuum energy we shift the excitation energy levels downwards into the complex E plane:

$$E_{ms}^{(2)}=-\Delta E\sum_l\frac{|\langle 0_+|\tilde V|\phi_l\rangle|^2}{E_l-i\gamma}. \tag{17}$$

The width γ describes phenomenologically the decay rate of one-domain states $|\phi_l\rangle$. Decay of these states can be caused both by term (13) and by other interactions not included into the Hamiltonian (4). As the result, the metastable vacuum energy gains the imaginary part

$$\mathrm{Im}\ E_{ms}\cong-\pi g(h_z)|\langle 0_+|\tilde V|\phi_l\rangle|^2_{E_l=0}, \tag{18}$$

where

$$g(h_z)=\mathrm{Im}\cot\left[\frac{f(\pi)-i\pi\gamma}{2|h_z|M}\right].$$

In deriving Eq. (18) we have extracted from the sum the slowly depending on l factor $|\langle 0_+|\tilde V|\phi_l\rangle|^2$ in the right-hand side of Eq. (17).

The metastable vacuum relaxation rate Γ is determined then in the usual way,

$$\Gamma=-2\ \mathrm{Im}\ E_{ms}. \tag{19}$$

It is evident from Eqs. (18) and (19) that Γ oscillates in h_z^{-1} with the period $2\pi M/f(\pi)$. These oscillations become considerable in the case of the resonant tunneling $\gamma\lesssim\Delta E$. In the opposite limit $\gamma\gg\Delta E$ oscillations in h_z^{-1} vanish and relations (18) and (19) transform to Fermi's golden rule,[18,20]

$$\Gamma=2\pi|\langle 0_+|\tilde V|\phi_l\rangle|^2_{E_l=0}. \tag{20}$$

In the limit $h_z\to-0$ the matrix element of the interaction operator can be asymptotically written as

$$\langle 0_+|\tilde V|\phi_l\rangle\cong i|h_z|MN\int_{-\pi}^{\pi}\frac{d\theta}{2\pi}\varphi_l(\theta)\frac{d\ln[\omega(\theta)]}{d\theta}$$

$$\cong\frac{1}{3\sqrt{2}}(|h_z|MN)^{1/2}\exp\left\{-\frac{|f(\theta_0)|}{2|h_z|M}\right\}, \tag{21}$$

where $\theta_0=i|\ln h_x|$ is the imaginary zero of the function $\omega(\theta)$, $\omega(\theta_0)=0$. Substitution of Eq. (21) into Eq. (18) yields finally

$$\mathrm{Im}\ E_{ms}=-\frac{\pi}{18}N|h_z|Mg(h_z)\exp\left\{-\frac{|f(\theta_0)|}{|h_z|M}\right\}. \tag{22}$$

Perhaps, described by Eqs. (19) and (22) oscillations in h_z of the metastable state decay rate could be observed (indeed, in somewhat modified form) in real quasi-one-dimensional Ising ferromagnets at very low temperatures.

Now let us map obtained results to the $d=2$ Ising model. Applying Eq. (5) to Eq. (22) we obtain

$$\mathrm{Im}\ F_{ms}=B|H|\tilde g(H)\exp(-A/|H|), \tag{23}$$

where

$$\tilde g(H)=\mathrm{Im}\cot\left\{\frac{J_1[f(\pi)-i\pi\gamma]}{2|H|M}\right\}, \tag{24}$$

$$A=\frac{J_1}{M}|f(-i\ln h_x)|, \tag{25}$$

$$B=\frac{\pi}{18}M, \tag{26}$$

and $H\to-0$. These expressions should be compared with the droplet theory predictions (1) and (2).

First, let us verify, that expressions (2) and (25) for the amplitude A are equivalent. To do this, we need to determine the quantity $\hat\Sigma^2$ in limit (3).

The droplet equilibrium shape in the $d=2$ Ising model is described by the equation[9]

$$a_1\cosh(\beta\lambda x_1)+a_2\cosh(\beta\lambda x_2)=1, \tag{27}$$

where x_1, x_2 denote Descartes coordinates of a point on the droplet boundary, the scale parameter λ determines the droplet size, and

$$a_1 = \frac{\tanh(2\beta J_2)}{\cosh(2\beta J_1)}, \quad a_2 = \frac{\tanh(2\beta J_1)}{\cosh(2\beta J_2)}.$$

In the extreme anisotropic limit

$$a_1 \cong 1 - 2\tau^2(1 + h_x^{-2}), \quad a_2 \cong 4\tau^2/h_x$$

and Eq. (27) simplifies to

$$x_1 = \pm \frac{J_1}{\lambda}\omega(i\beta\lambda x_2).$$

Integrating in x_2 this equation we obtain the area of the equilibrium-shaped droplet $S(\lambda) = W/\lambda^2$, where

$$W = \frac{2J_1}{\beta}|f(-i \ln h_x)|.$$

It follows from Wulff's theorem[9] that the surface energy $\Sigma(\lambda)$ also can be expressed in W: $\Sigma(\lambda) = 2W/\lambda$. Therefore, $\hat{\Sigma}^2 = 4W$, and

$$A = \frac{\beta\hat{\Sigma}^2}{8M} = \frac{J_1}{M}|f(-i \ln h_x)|$$

in exact agreement with Eq. (25).

Further, expression (23) differs from Eq. (1) by the oscillating factor $\tilde{g}(H)$. We interpret this factor as the correction coursed by the discrete-lattice effects. Those may be significant at low temperatures in the presence of strong anisotropy.[21] The following observation supports such an interpretation.

At low temperatures ($h_x \to 0$), the factor $\tilde{g}(H)$ can be written as

$$\tilde{g}(H) = \operatorname{Im} \cot\left\{\pi 2x_1(H) - \frac{i\pi\gamma J_1}{2|H|M}\right\}, \tag{28}$$

where $2x_1(H) = 2J_1/(M|H|)$ is the continuum nucleation theory value of the critical droplet diameter in the x_1 direction. Maximum points in Eq. (28) just correspond to discrete values of this diameter.

The oscillatory factor $\tilde{g}(H)$ contains parameter γ, which remains undetermined in the present incomplete theory. One would expect, however, that in the critical region ($h_x \to 1$) parameter γ is large enough, so that $\tilde{g}(H) \cong 1$, and oscillations in Eq. (23) vanish. Really, in this limit spectrum (16) becomes continuous, and Γ can be obtained directly from Eq. (20) without referring to Eqs. (17) and (18).

In the critical region expression (26) for the ampiltude B in Eq. (23) agrees with our previous result.[22]

This work was supported by the Fund of Fundamental Investigations of Republic of Belarus.

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