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Analytic Verification of the Droplet Picture in the Two-Dimensional Ising Model

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It is widely accepted that the free energy $F(H)$ of the two-dimensional Ising model in the ferromagnetic phase $T<T_c$ has an essential branch cut singularity at the origin $H=0$. The phenomenological droplet theory predicts that near the cut drawn along the negative real axis $H<0$, the imaginary part of the free energy per lattice site has the form $\operatorname{Im} F[\exp(\pm i\pi)\,|H|]=\pm B\,|H|\exp(-A/|H|)$ for small $|H|$. We verify this prediction in analytical perturbative transfer matrix calculations for the square lattice Ising model for all temperatures $0<T<T_c$ and arbitrary anisotropy ratio J_1/J_2. We obtain an expression for the constant A which coincides exactly with the prediction of the droplet theory. For the amplitude B we obtain $B=\pi M/18$, where M is the equilibrium spontaneous magnetization. In addition we find discrete-lattice corrections to the above mentioned phenomenological formula for Im F, which oscillate in H^{-1}.

KEY WORDS: Ising model; droplet singularity; metastable state; false vacuum decay.

1. INTRODUCTION

It is well known,[(1–3)] that in the ferromagnetic phase $0<T<T_c$ the free energy of the two-dimensional Ising model as the function of the magnetic field H has a so-called droplet singularity at the origin $H=0$. This singularity prevents analytical continuation of the free energy from positive to negative values of H along the real H-axis. The phenomenological droplet (nucleation) theory[(4–6)] claims, however, that the free energy can be continued from positive to negative magnetic fields along a circle going around the origin in the complex H-plane (see Fig. 1). According to this theory, the free energy per lattice site $F(H)$ continued in such a way gains on the

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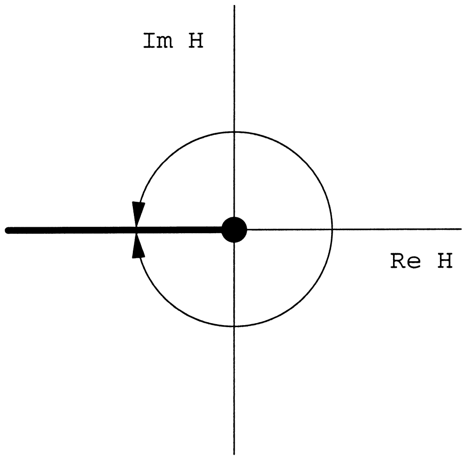

Fig. 1. Free energy continuation paths from the positive real axis $H > 0$ to the cut going along the negative real axis $H < 0$.

negative real axis $H < 0$ a nonzero imaginary part, which is expected to have the form

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

for small $|H|$. The sign of this imaginary part depends on the side, from which one approaches to the negative real axis $H < 0$. Expression (1) extrapolates to the ferromagnetic Ising model the results obtained in the semiclassical nucleation field theory analysis of the coarse-grained Ginzburg–Landau model.[7–12] In the nucleation 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,[7] that Im $F_{ms}(H)$ may be identified (up to a dynamical factor) with the metastable phase decay rate provided by the thermally activated nucleation of the critical droplet.

The phenomenological droplet theory prediction for the amplitude A in (1) is[13]

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

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 linear depending on $|H|$ prefactor in (1) arises in the continuum droplet field theory[7–9] from the contribution of the surface excitations of the critical droplet. Voloshin claimed[18] that, if fluctuations are continuum and isotropic, the prefactor in (1) becomes universal. Extrapolation of the Voloshin's continuum droplet field theory result to the $d=2$ Ising model leads to the following prediction for the amplitude B:

$$B \mapsto B_V = \frac{M}{2\pi}. \tag{3}$$

In the continuum field theory, the imaginary part of the free energy appears in the functional integral calculations. In the alternative approach to the droplet singularity problem, one deals with eigenvalues of the Ising model transfer-matrix. Numerical transfer-matrix calculations initiated by Privman and Schulman[19] and continued by Günther, Rikvold and Novotny[16,17] confirm Eqs. (1) and (2). These equations were confirmed also by Lowe and Wallace,[14] and by Harris[15] in numerical analysis of the small-H power expansion for the magnetization $M(H)$. Recently analytic transfer-matrix derivation of Eqs. (1), (2) for the $d=2$ Ising model has been done[20] in the extreme anisotropic limit.

In this paper we generalize the transfer matrix approach developed in paper[20] and verify analytically the droplet theory predictions (1), (2) for the square lattice Ising model for all temperatures $0<T<T_c$ and arbitrary anisotropy ratio J_1/J_2. We obtain an expression for the constant A which coincides exactly with the prediction of the droplet theory. For the amplitude B we find $B=\pi M/18$, which is very close to Voloshin's result (3): $B/B_V=\pi^2/9\approx 1.0966$. We suppose, that this small discrepancy results from approximations used in our calculations. Obtained values for the amplitude B are compared with those extracted numerically from the known coefficients of the expansion of the magnetization in powers of H by means of dispersion relations.[14, 21]

We find also the discrete-lattice corrections to the phenomenological formula (1), which oscillate in H^{-1}. The period of oscillations agrees well with that observed by Günther *et al.*[17] in numerical constrained transfer matrix calculations.

2. TRANSFER MATRIX AND HAMILTONIAN

The nearest neighbor Ising model on the square lattice in the magnetic field H is defined by the energy

$$\mathscr{E} = -\sum_{n=1}^{\mathscr{N}} \sum_{m=1}^{\mathscr{M}} (J_1\sigma_{m,n}\sigma_{m+1,n} + J_2\sigma_{m,n}\sigma_{m,n+1} + H\sigma_{m,n}) \tag{4}$$

where $\sigma_{m,n} = \pm 1$, the first/second index of $\sigma_{m,n}$ specifies the row/column of the lattice, $\mathscr{M}$ and $\mathscr{N}$ denote the number of rows and columns in the lattice, respectively. Periodic boundary conditions are implied.

The row to row transfer matrix may be defined as $\hat{T} = e^U \hat{T}_2 \hat{T}_1$, where

$$\hat{T}_1 = [2\sinh(2K_1)]^{\mathscr{N}/2} \exp\left(K_1^* \sum_{n=1}^{\mathscr{N}} \sigma_n^1\right), \qquad \hat{T}_2 = \exp\left(K_2 \sum_{n=1}^{\mathscr{N}} \sigma_n^3 \sigma_{n+1}^3\right),$$
$$U = h \sum_{n=1}^{\mathscr{N}} \sigma_n^3. \tag{5}$$

Here we have used the standard notations

$$K_1 = \beta J_1, \qquad K_2 = \beta J_2, \qquad h = \beta H, \qquad 2K_1^* = -\ln(\tanh K_1),$$

β is the inverse temperature, σ_n^α ($\alpha = 1, 2, 3$) are the Pauli matrices relating to the cite n in the row.

The transfer matrix may be chosen in the symmetric form

$$\hat{T}_S = [\hat{T}_S^{(0)}]^{1/2}\, e^U [\hat{T}_S^{(0)}]^{1/2},$$

where $\hat{T}_S^{(0)}$ is the symmetric transfer matrix of the Ising model in zero magnetic field:

$$\hat{T}_S^{(0)} = \hat{T}_2^{1/2} \hat{T}_1 \hat{T}_2^{1/2}.$$

As it was shown by Schultz, Mattis and Lieb,[22] the latter becomes diagonal in fermionic variables:

$$\hat{T}_S^{(0)} = C \exp(-\mathscr{H}^{(0)}),$$
$$\mathscr{H}^{(0)} = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi}\, \omega(\theta)\, \psi^\dagger(\theta)\, \psi(\theta), \tag{6}$$

where $\mathscr{H}^{(0)}$ is the zero-field Hamiltonian, θ is the quasi-momentum, C is an insufficient numerical factor. Fermionic operators $\psi^\dagger(\theta)$, $\psi(\theta)$ satisfying the canonical anticommutational relations

$$\{\psi(\theta), \psi(\theta')\} = \{\psi^\dagger(\theta), \psi^\dagger(\theta')\} = 0, \qquad \{\psi^\dagger(\theta), \psi(\theta')\} = 2\pi\delta(\theta - \theta')$$

can be expressed in terms of the initial Pauli matrices by use of the Jordan–Wigner and duality transformation (see Appendix). The fermionic spectrum $\omega(\theta)$ is given by

$$\exp\omega(\theta) = \cosh 2K_1^* \cosh 2K_2 - \cos\theta \sinh 2K_1^* \sinh 2K_2 + [(\cosh 2K_1^* \cosh 2K_2 - \cos\theta \sinh 2K_1^* \sinh 2K_2)^2 - 1]^{1/2}. \tag{7}$$

Operator U defined by (5) also can be represented in the thermodynamic limit $\mathcal{N} \to \infty$ in the fermionic variables:

$$U = hM \sum_{n\in\mathbb{Z}} :\exp\frac{\rho_n}{2}:, \tag{8}$$

where

$$\frac{\rho_n}{2} = -\sum_{j<n} \psi_j^{(+)}\psi_j^{(-)}, \tag{9}$$

$$\psi_j^{(+)} = i\int_{-\pi}^{\pi} \frac{d\theta}{2\pi}\frac{\exp(ij\theta)}{\epsilon(\theta)}[\psi(\theta)+\psi^\dagger(-\theta)], \tag{10}$$

$$\psi_j^{(-)} = i\int_{-\pi}^{\pi} \frac{d\theta}{2\pi}\exp(ij\theta)\,\epsilon(\theta)[-\psi(\theta)+\psi^\dagger(-\theta)], \tag{11}$$

$$\epsilon(\theta) = \left(\frac{z_1+z_1^{-1}-2\cos\theta}{z_2+z_2^{-1}-2\cos\theta}\right)^{1/4},$$

$$z_1 = \tanh K_1^*/\tanh K_2, \qquad z_2 = \tanh K_1^* \tanh K_2, \tag{12}$$

and M is the zero-field magnetization. In the ferromagnetic phase $M = [1-k^2]^{1/8}$, and $k<1$, where $k = (\sinh 2K_1 \sinh 2K_2)^{-1}$. We have used in (8) the conventional notation $:\cdots:$ for the normal ordering with respect to the fermionic operators $\psi(\theta)$, $\psi^\dagger(\theta)$. Derivation of Eqs. (8)–(11) is described in the Appendix, in the main points of which we follow Jimbo *et al.*[23]

At zero magnetic field, the Hamiltonian $\mathscr{H}^{(0)}$ of the Ising model is given by (6). Two ferromagnetic ground states $|0_+\rangle$ and $|0_-\rangle$ coexist in the ferromagnetic phase $k<1$. They are distinguished by the sign of the spontaneous magnetization $\langle 0_\pm|\,\sigma_n^z\,|0_\pm\rangle = \pm M$. The state $|0_+\rangle$ characterized by the positive magnetization $+M$ is the ferromagnetic vacuum of $\psi(\theta)$-operators: $\psi(\theta)\,|0_+\rangle = 0$ for all θ.

A small magnetic field $h\neq 0$ changes the Hamiltonian $\mathscr{H}^{(0)}$ to

$$\mathscr{H}(h) = -\ln(e^{-\mathscr{H}^{(0)}/2}e^U e^{-\mathscr{H}^{(0)}/2}), \qquad \mathscr{H}(0) = \mathscr{H}^{(0)}. \tag{13}$$

It can be expanded in powers[2] of h:

$$\mathscr{H}(h) = \sum_{j=0}^{\infty} \mathscr{H}^{(j)}, \tag{14}$$

where $\mathscr{H}^{(j)} \sim h^j$.

3. MODIFIED PERTURBATION THEORY

Let us consider the eigenvalue problem

$$\mathscr{H}(h) \, |\phi_+(h)\rangle = E(h) \, |\phi_+(h)\rangle, \tag{15}$$

where $|\phi_+(0)\rangle = |0_+\rangle$.

If $h > 0$, the eigenvector $|\phi_+(h)\rangle$ is the ground state of the Hamiltonian (13), and the corresponding energy $E(h)$ is directly related with the Ising model free energy per lattice cite $F(h, \beta)$:

$$F(h, \beta) = F(0, \beta) + \frac{E(h)}{\beta \mathscr{N}}. \tag{16}$$

The energy can be expanded in the formal power series

$$E(h) = \sum_{j=1}^{\infty} h^j C_j,$$

which coefficients C_j can be, in principal, determined from the standard Rayleigh–Schrödinger perturbation theory.

However, if the magnetic field is small and negative $h < 0$, the state $|\phi_+(h)\rangle$ (with positive magnetization almost equal to M) must be identified with the metastable (false) vacuum. It decays due to the quantum tunneling, and the decay rate[3] Γ is proportional to the imaginary part of the energy $E(h)$ continued to negative magnetic fields:[24, 25]

$$\Gamma = -2 \, \mathrm{Im} \, E(h). \tag{17}$$

[2] In the extreme anisotropic limit[20] the Hamiltonian expansion (14) containes only two terms: $\mathscr{H}(h) = \mathscr{H}^{(0)} + \mathscr{H}^{(1)}$, where $\mathscr{H}^{(1)} = -U$.

[3] Strictly speaking, the term "decay rate" here relates to the quantum-mechanical model with Hamiltonian (14), but not to the initial two-dimensional Ising model (4). The nucleation rate in the latter model contains also the so-called kinetic prefactor, which depends on the detailed non-equilibrium dynamics.[13]

It turns out, however, that Γ can not be determined from the straightforward perturbation theory with the zero-order Hamiltonian $\mathscr{H}^{(0)}$. This is due to the fact that the term $\mathscr{H}^{(1)}$ in the expansion (14) contains the long-range interaction $(-U_0)$ between fermions, which is given by

$$-U_0 \equiv -U|_{\epsilon(\theta)\to 1} = |h|\, M \sum_{n\in\mathbb{Z}} :\exp\left(-2\sum_{j<n} b_j^\dagger b_j\right):. \tag{18}$$

Here

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

are the operators which create/annihilate a fermion at the cite j. Interaction (18) increases linearly with the distance between fermions,[20] and therefore changes the structure of the Hamiltonian spectrum. So, to describe decay of metastable vacuum $|\phi_+(h)\rangle$, one should include the long-range interaction (18) into the zero-order Hamiltonian.

Accordingly, we subdivide the Hamiltonian (14) into the zero-order $\mathscr{H}_0$ and interaction V parts, as follows:

$$\mathscr{H}(h) = \mathscr{H}_0 + V, \tag{19}$$

where

$$\mathscr{H}_0 \equiv \mathscr{H}^{(0)} - U_0 - \mathscr{N}\, |h|\, M, \tag{20}$$

$$V \equiv \mathscr{H}^{(1)} + U_0 + \mathscr{N}\, |h|\, M + \sum_{j=2}^{\infty} \mathscr{H}^{(j)}. \tag{21}$$

The numerical constant $\mathscr{N}\, |h|\, M$ in (20) is chosen to provide $\mathscr{H}_0\, |0_+\rangle = 0$.

3.1. Zero Order Spectrum

Consider the zero-order eigenvalue problem

$$\mathscr{H}_0\, |\phi_l\rangle = E_l\, |\phi_l\rangle. \tag{22}$$

First note, that eigenstates $|\phi_l\rangle$ can be classified by the fermion number, since the modified zero-order Hamiltonian (20) conserves the number of fermions. As in paper,[20] we shall consider only two-fermion (i.e., one-domain) states in (22). Physically, this means that we neglect interaction between nucleating droplets of the stable phase.

In the coordinate representation Eq. (22) takes the form

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

where

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

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

If the energy E_l is small enough $E_l \ll \omega(0)$, the wavefunction $\phi_l(n)$ is mainly concentrated far from the origin in the classically available region $|n| > \omega(0)/(|h|\,M)$. Therefore, we can apply the "strong coupling approximation"(26) to represent the wavefunction in the form

$$\phi_l(n) \simeq \varphi_l(n) - \varphi_l(-n), \tag{23}$$

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

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

After the Fourier transform, we obtain

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

where

$$\varphi_l(\theta) = C\,\exp\left\{-\frac{i}{2\,|h|\,M}\,[f(\theta) - E_l\theta]\right\},$$
$$C = (2\,|h|\,M\mathcal{N})^{-1/2}, \tag{24}$$
$$f(\theta) = 2\int_0^{\theta} \mathrm{d}\chi\,\omega(\chi).$$

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

$$E_l = \frac{f(\pi)}{\pi} - 2\,|h|\,Ml. \tag{25}$$

The normalization constant C in (24) is chosen to yield

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

where $\Delta E = 2\,|h|\,M$ is the interlevel distance. The energy spectrum (25) of the Hamiltonian (20) is discrete in an arbitrary small magnetic field h. This result has a clear physical interpretation.

At $h = 0$, $T > 0$, the Hamiltonian eigenstates $|\phi\rangle$ in the two-fermion sector are comprised of two uncoupled domain walls moving along the spin chain. If the total quasi-momentum in such a state is zero, the domain walls are descried by two plain waves with quasi-momenta θ and $-\theta$ and with the total energy $2\omega(\theta)$. At $h = 0, T > 0$ these states form a continuous band $\omega(0) < \omega(\theta) < \omega(\pi)$.

If a nonzero magnetic field is applied, it induces a linear potential $2hMn$ acting on the domain wall positioned near the site n. This linear potential provides localization of both domain walls forming the eigenstate in the two-fermion sector. The domain wall localization is analogous to the localization of an electrons in a single isolated zone by a linear electric field.[26] The localized domain wall can be thought of as moving back and forth near its localization point. During this motion the domain wall quasi-momentum θ varies between $-\pi$ and π. Correspondingly, the energy of a two-fermion eigenstate now takes the form (25), which can be written as:

$$E_l = 2\langle \omega(\theta) \rangle - 2\,|h|\,Ml. \tag{26}$$

where l is the distance between the two localized domain walls, $\langle \cdots \rangle$ denotes averaging over θ, $-\pi < \theta < \pi$. Thus, an arbitrary small magnetic field h provides localization of domain walls in the discrete spin chain leading to the discreteness of the energy spectrum in the two-fermion sector.

3.2. Decay Rate

The first-order correction to the false vacuum energy is trivial: $E^{(1)} = \langle 0_+ |\, V\, | 0_+ \rangle = \mathcal{N}\,|h|\,M$, the second-order correction is given by

$$E^{(2)} = -\Delta E \sum_l \frac{|\langle \phi_l |\, V\, | 0_+ \rangle|^2}{E_l}. \tag{27}$$

To determine the decay rate of the false vacuum, the following trick is used. We shift the excitation energy levels E_l in (27) downwards into the complex E-plane: $E_l \to E_l - i\gamma$, where the width γ describes phenomenologically the decay rate of one-domain states $|\phi_l\rangle$. Decay of these states should be caused by the interaction term (21) in the same manner as the false vacuum decay.

As the result, the metastable vacuum energy gains the imaginary part

$$\operatorname{Im} E \simeq -\pi g(h)\, |\langle\phi_l| V |0_+\rangle|^2_{E_l=0}, \tag{28}$$

where

$$g(h) = \operatorname{Im} \cot\left[\frac{f(\pi) - i\pi\gamma}{2|h|\, M}\right]. \tag{29}$$

The metastable vacuum relaxation rate Γ is determined then in the usual way (17). It is evident from (28), (17) that Γ oscillates in h^{-1} with the period Δh^{-1} given by

$$\Delta h^{-1} = 2\pi M / f(\pi). \tag{30}$$

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^{-1} vanish and relations (28), (17) transform to the Fermi's golden rule:[24, 25]

$$\Gamma = 2\pi\, |\langle\phi_l| V |0_+\rangle|^2_{E_l=0}. \tag{31}$$

Let us now calculate the matrix element in (28):

$$\begin{aligned}\langle\phi_l| V |0_+\rangle &= \frac{1}{2}\int_{-\pi}^{\pi} \frac{d\theta}{2\pi}\, \phi_l^*(\theta)\, \langle 0_+|\, \psi(-\theta)\, \psi(\theta)\, V\, |0_+\rangle \\ &\simeq \int_{-\pi}^{\pi} \frac{d\theta}{2\pi}\, \varphi_l^*(\theta)\, \langle 0_+|\, \psi(-\theta)\, \psi(\theta)\, V\, |0_+\rangle.\end{aligned} \tag{32}$$

Expanding operator V in the h-power series

$$\langle 0_+|\, \psi(-\theta)\, \psi(\theta)\, V\, |0_+\rangle = \sum_{j=1}^{\infty} \langle 0_+|\, \psi(-\theta)\, \psi(\theta)\, \mathscr{H}^{(j)}\, |0_+\rangle$$

and keeping in it only the leading ($j=1$) term one obtains from (8), (13), (14):

$$\langle 0_+ |\, \psi(-\theta)\, \psi(\theta)\, V\, |0_+\rangle \simeq \langle 0_+ |\, \psi(-\theta)\, \psi(\theta)\, \mathscr{H}^{(1)}\, |0_+\rangle$$

$$= \langle 0_+ |\, \psi(-\theta)\, \psi(\theta)\, U\, |0_+\rangle \frac{\omega(\theta)}{\sinh \omega(\theta)}$$

$$= -2i\mathcal{N}\, |h|\, M \frac{d \ln \epsilon(\theta)}{d\theta} \cdot \frac{\omega(\theta)}{\sinh \omega(\theta)}.$$

Thus, the matrix element (32) can be approximately represented as

$$\langle \phi_l |\, V\, |0_+\rangle \simeq -i\mathcal{N}\, |h|\, M \int_{-\pi}^{\pi} \frac{d\theta}{\pi} \frac{\omega(\theta)}{\sinh \omega(\theta)}\, \varphi_l^*(\theta) \frac{d \ln \epsilon(\theta)}{d\theta}. \tag{33}$$

Substitution of (33), (28), (24) into (16) yields the final expression for the imaginary part of the free energy F_{ms} in the limit $h \to -0$:

$$\operatorname{Im} F_{ms} \simeq \frac{\pi}{2} |H|\, M g(h) \left| \int_{-\pi}^{\pi} \frac{d\theta}{\pi} \frac{\omega(\theta)}{\sinh \omega(\theta)} \frac{d \ln \epsilon(\theta)}{d\theta} \exp\left[\frac{i f(\theta)}{2\, |h|\, M} \right] \right|^2. \tag{34}$$

This expression generalizes formula (18) of ref. 20 to arbitrary anisotropy J_1/J_2 and all temperatures $0 < T < T_c$.

The last (exponent) factor of the integrand in (34) oscillates with high frequency in the considered case of small $|h|$. Therefore, in the limit $|h| \to 0$, the integral in the right-hand side of (34) is determined by the saddle point of $f(\theta)$: $\theta = \theta_1 \equiv -i \ln z_1$, $\omega(\theta_1) = 0$, and asymptotically equals to

$$\operatorname{Im} F_{ms} \simeq B\, |H|\, g(h) \exp\left[-\frac{A}{|H|} \right], \tag{35}$$

where

$$A = \frac{|f(\theta_1)|}{M\beta}, \tag{36}$$

$$B = \frac{\pi M}{18}. \tag{37}$$

4. DISCUSSION

First, let us establish equivalence of expressions (2) and (36) for the amplitude A, which are given by the phenomenological droplet theory and by our transfer-matrix calculations.

The droplet equilibrium shape in the $d=2$ Ising model is determined by the equation

$$a_1 \cosh(\beta\lambda x_1) + a_2 \cosh(\beta\lambda x_2) = 1, \tag{38}$$

obtained by Zia and Avron.[27] Here x_1, x_2 denote Descartes coordinates of a point on the droplet boundary, the scale parameter λ determines the droplet size, and

$$a_1 = \frac{\tanh(2K_2)}{\cosh(2K_1)}, \qquad a_2 = \frac{\tanh(2K_1)}{\cosh(2K_2)}.$$

It is remarkable, that Eq. (38) can be rewritten in terms of the Ising model excitation spectrum (7) first obtained by Onsager:[28]

$$x_2 = \pm\frac{1}{\beta\lambda}\,\omega(i\beta\lambda x_1). \tag{39}$$

Integrating in x_1 this equation we find the area of the equilibrium-shaped droplet $S(\lambda) = W/\lambda^2$, where

$$W = \frac{2}{\beta^2}\,|f(\theta_1)|.$$

It follows from Wulff's theorem[27] that the surface energy $\Sigma(\lambda)$ also can be expressed in W: $\Sigma(\lambda) = 2W/\lambda$. Therefore, $\hat{\Sigma}^2 = 4W$, and

$$A = \frac{\beta\hat{\Sigma}^2}{8M} = \frac{|f(\theta_1)|}{M\beta}$$

in exact agreement with (36).

Our expression $\pi M/18$ for the amplitude B is the same as that obtained previously in the extreme anisotropic limit.[20] As it was mentioned in the introduction, this expression is very close to the Voloshin's result (3). The latter is expected to be exact in the critical region, where fluctuations are isotropic and universal. It is likely, that the small discrepancy between (37) and (3) is caused by approximations used in our modified perturbation theory. We hope to clarify this question in future.

Let us compare obtained expressions for the amplitude B with the numerical results by Baker and Kim[21] which they calculated for the symmetric case $J_1 = J_2 \equiv J$ of the Ising model . These authors considered the power series for the magnetization $M(h)$ at a fixed temperature below T_c:

$$M(h) = M(0) - 2 \sum_{n=1}^{\infty} (-2h)^n a_n,$$

and calculated numerically 12 coefficients a_n in this expansion at $u = 0.1u_c$, and 24 coefficients at $u = 0.9u_c$. Here $u = \exp(-4\beta J)$; $u_c = 3 - \sqrt{8}$ corresponds to the critical temperature. On the other hand, Lowe and Wallace[14] demonstrated by use of the dispersion relation, that Eq. (1) leads to the following asymptotic formula for the coefficients a_n:

$$a_n \xrightarrow[n \to \infty]{} \frac{B}{2\pi} (2A\beta)^{-n} \frac{(n+1)!}{n}. \tag{40}$$

So, the ratio

$$R_n = \frac{B(n+1)!}{2\pi n a_n (2A\beta)^n} \tag{41}$$

should approach to unity at large n, if we put in it the correct values of amplitudes A and B . We plot in Fig. 2 this ratio, where coefficients a_n are taken from paper[21] by Baker and Kim. The left pair of curves corresponds to the low temperature case $u = 0.1u_c$, the right pair of curves corresponds to the higher temperature $u = 0.9u_c$. The amplitude A in (41) is taken from (36). Solid and dashed curves differ by choice of the amplitude B in (41). In solid curves, it is chosen as $B = \pi M/18$ according to our result (37); in dashed curves $B = M/(2\pi)$ according to Voloshin's result.[18] All four curves in Fig. 2 seems to stabilize at large n to the values, which are rather close to unity. This indicates a remarkable good agreement of numerical results[21] with expressions (3) or (36). Though, agreement with Voloshin's value seems somewhat better, saturation in curves is not achieved, and further numerical calculation are desirable to distinguish between (3) and (36).

Expression (35) differs from (1) by the oscillating factor $g(h)$. We interpret this factor as the correction caused by the discrete-lattice effects.[29] Mathematically oscillations arise from avoided crossing[19, 17] of the metastable vacuum energy $E = 0$ with the discrete energy levels (26) in

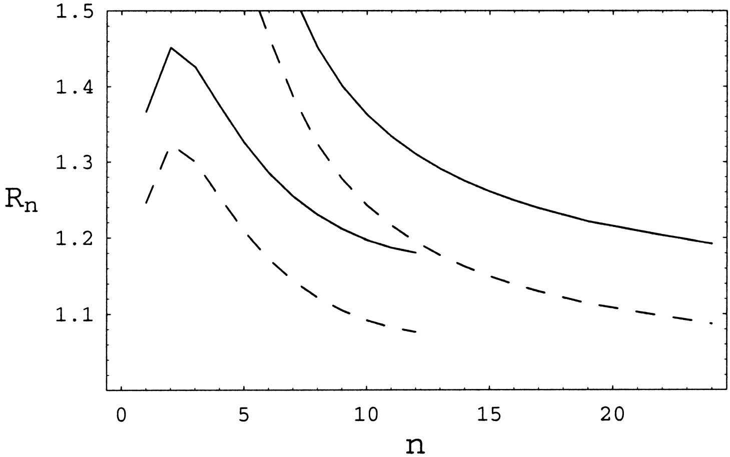

Fig. 2. Plot of R_n given by (41) versus n. Coefficients a_n in (41) are taken from ref. 21; amplitude A is taken from (36); amplitude B is taken either from (37) (solid curves), or from (3) (dashed curves). Two left curves correspond to $u = 0.1u_c$, two right curves correspond to $u = 0.9u_c$.

the two-fermion sector. The oscillation period in h^{-1} is given by Eq. (30), which can be written as

$$\Delta h^{-1} = M/\langle \omega(\theta) \rangle. \tag{42}$$

In the zero-temperature limit Eq. (42) leads to the asymptotics

$$K\Delta h^{-1} = \tfrac{1}{2} + O(K^{-1}), \tag{43}$$

since $M = 1$ and $\omega(\theta) = 2K$ in the limit $K \to \infty$. Asymptotics (43) was obtained previously by Günther *et al.* from simple physical arguments.[17] These authors observed avoided crossing oscillations in the numerical constrained transfer matrix calculations of the imaginary part of the (constrained) free energy. It turns out, that the zero-temperature result (43) describes within 3% accuracy the numerical transfer matrix calculations up to $T = 1.2J$, i.e., to $K = 0.833$.

A naive extrapolation of (43) to finite temperatures leads to the expression[32]

$$K\Delta h^{-1} = KM/\sigma, \tag{44}$$

where $\sigma = \omega(\theta)|_{\theta=0}$ is the domain wall surface tension. The right-hand side of (44) grows with increasing T and even diverges at $T \to T_c$. In particular,

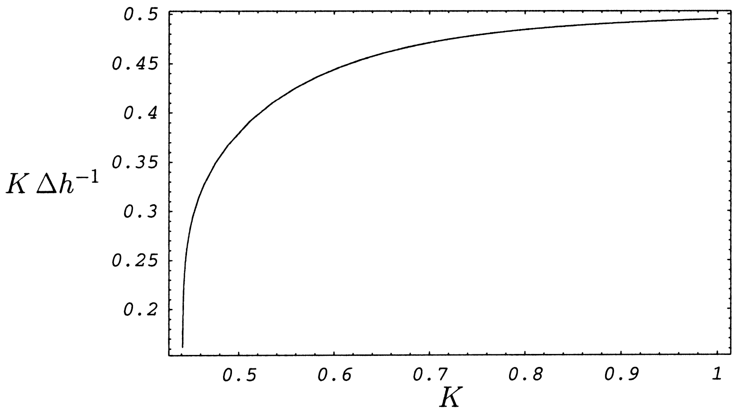

Fig. 3. Oscillation period Δh^{-1} multiplied by K versus K in the symmetric case.

it takes the values 0.5783 at $K=1$ and 0.6951 at $K=0.833$, which are rather far from $1/2$ value observed in numerical calculations.[17]

A substantially different temperature dependence for the oscillation period Δh^{-1} is given by our expression (42) due to the averaging of $\omega(\theta)$ over the quasi-momentum θ. This averaging results from localization of domain wall eigenfunctions in applied magnetic field, as it was explained in Section 3.1. In Fig. 3 we plot the quantity $K\Delta h^{-1}$ versus K in the symmetric case $K \equiv K_1 = K_2$, where Δh^{-1} is taken from (42). As one can see from the figure, $K\Delta h^{-1}$ holds almost constant value $K\Delta h^{-1} \approx 1/2$ down to $K = 0.8$. Our values for $K\Delta h^{-1}$ at $K=1$ and at $K=0.833$ are 0.495 and 0.487, respectively. This is in very good agreement with numerical transfer-matrix results reported by Günther *et al.*[17]

The oscillation amplitude is governed by the phenomenological parameter γ in Eq. (29), which calculation remains beyond the scope of the present paper. It is natural to expect, however, that $\gamma(T)$ decreases with decreasing temperature, providing significant oscillations at low temperatures, and negligible ones in the critical region. Perhaps, such increase of the oscillation amplitude at low temperatures could explain a strong Arrhenius-like temperature dependence of the prefactor $B(K)$, $B(K) = k\exp(-CK)$, $1 < C < 2$ observed in the interval $0.5 < K < 2.5$ in numerical constrained transfer matrix and Monte Carlo calculations, see Fig. 13 of ref. 17. Such a strong dependence of $B(K)$ is in evident disagreement with our Eq. (37) predicting almost constant value of the prefactor $B(K)$ in this temperature interval. This discrepancy could result from different definitions of the parameter $B(T)$ in the present paper and in ref. 17. Really, if one determines $B(T)$ drawing a line through the minima of the oscillating curve

Im $F(H, T)$ (see Fig. 4 of ref. 17), this could effectively decrease $B(T)$ at smaller T, since these minimums become deeper as T decreases. So, the oscillating factor (29) and its probable temperature dependence should be taken into account when interpreting numerical calculations of the imaginary part of the metastable free energy and nucleation rates at low temperatures.

APPENDIX: FERMIONIZATION

In this Appendix we present fermionic representations of spin operators, which are used in Section 2. Consideration is restricted to the ferromagnetic phase $T < T_c$ in the thermodynamic limit $\mathcal{N} \to \infty$. In this limit the Jordan–Wigner transformation can be written as[23]

$$P_n = \sigma_n^3 \sigma_{n-1}^1 \sigma_{n-2}^1 \cdots, \qquad Q_n = -i\sigma_n^2 \sigma_{n-1}^1 \sigma_{n-2}^1 \cdots. \tag{A1}$$

Here P_n and Q_n are the fermionic operators satisfying the following anti-commutational relations:

$$\{P_n, P_{n'}\} = 2\delta_{nn'}, \qquad \{Q_n, Q_{n'}\} = -2\delta_{nn'}, \qquad \{P_n, Q_{n'}\} = 0.$$

Let us define the another set of fermionic operators p_n, q_n, which are related with P_n , Q_n by the duality transformation:[31]

$$p_n = iQ_n, \qquad q_n = -iP_{n+1}. \tag{A2}$$

Operators p_n, q_n obey the same anticommutational relations as P_n , Q_n, span an orthogonal space of free fermion field, and generate the Clifford algebra.[23]

Fermionic creation and annihilation operators $\psi(\theta)$, $\psi^\dagger(\theta)$ introduced in Section 2 are related with p_n, q_n by

$$\begin{aligned} 2i\psi(\theta) &= e^{-i\alpha(\theta)} p(\theta) - e^{i\alpha(\theta)} q(\theta), \\ 2i\psi^\dagger(-\theta) &= e^{-i\alpha(\theta)} p(\theta) + e^{i\alpha(\theta)} q(\theta), \\ p(\theta) &= \sum_{n \in \mathbb{Z}} e^{-in\theta} p_n, \qquad q(\theta) = \sum_{n \in \mathbb{Z}} e^{-in\theta} q_n, \end{aligned} \tag{A3}$$

where

$$\begin{aligned} e^{2i\alpha(\theta)} &= -\tanh K_2 \left[\frac{(e^{i\theta} - z_1)(e^{i\theta} - z_2^{-1})}{(e^{i\theta} - z_2)(e^{i\theta} - z_1^{-1})} \right]^{1/2}, \\ e^{2i\alpha(0)} &= -1, \end{aligned} \tag{A4}$$

parameters z_1, z_2 are defined by (12).

Relations (A1), (A2) express operators p_n, q_n in terms of Pauli matrices. The inverse transformation reads as

$$\sigma_n^1 = p_n q_{n-1},$$

$$\sigma_n^2 = p_n (p_{n-1} q_{n-2})(p_{n-2} q_{n-3}) \cdots, \tag{A5}$$

$$\sigma_n^3 = i q_{n-1} (p_{n-1} q_{n-2})(p_{n-2} q_{n-3}) \cdots. \tag{A6}$$

Brackets in Eqs. (A5), (A6) are shown to indicate, that σ_n^2 and σ_n^3 are the products of odd number of fermionic operators, i.e., σ_n^2 and σ_n^3 are the odd elements of the Clifford group.

Following Jimbo *et al.*,[23] let us introduce operator $\bar{\sigma}_n^3$, which represent σ_n^3 under the boundary condition $\sigma_n^3 \to 1$ for $n \to -\infty$:

$$\bar{\sigma}_n^3 = (q_{n-1} p_{n-1})(q_{n-2} p_{n-2}) \cdots.$$

This operator is an even element of the Clifford group. Due to the obvious identity $\bar{\sigma}_n^3 \bar{\sigma}_{n'}^3 = \sigma_n^3 \sigma_{n'}^3$, operators σ_n^3 and $\bar{\sigma}_n^3$ produce the same correlation functions, which makes reasonable to identify them in the thermodynamic limit. Accordingly, we shall replace σ_n^3 by $\bar{\sigma}_n^3$ in the operator U:

$$U \mapsto h \sum_{n=1}^{\mathcal{N}} \bar{\sigma}_n^3. \tag{A7}$$

Operators $\bar{\sigma}_n^3$ are characterized up to ± 1 factor by the following commutation relations:

$$\bar{\sigma}_n^3 q_{n'} \bar{\sigma}_n^3 = \varkappa(n'-n)\, q_{n'}, \qquad \bar{\sigma}_n^3 p_{n'} \bar{\sigma}_n^3 = \varkappa(n'-n)\, p_{n'}, \tag{A8}$$

where

$$\varkappa(n) = \begin{cases} 1 & \text{for} \quad n \geqslant 0 \\ -1 & \text{for} \quad n < 0 \end{cases}.$$

Thus, $\bar{\sigma}_n^3$ induces a linear orthogonal transformation of the linear space of free fermions. As it was shown by Jimbo *et al.*[23] in Appendix 1, such an operator can be expressed as the normally ordered exponent

$$\bar{\sigma}_n^3 = \langle \bar{\sigma}_n^3 \rangle \, :\exp(\rho_n/2):. \tag{A9}$$

Here operator ρ_n is quadratic in free fermionic variables p_n and q_n, $\langle \bar{\sigma}_n^3 \rangle$ is the vacuum expectation value of $\bar{\sigma}_n^3$, i.e., the spontaneous magnetization $\langle \bar{\sigma}_n^3 \rangle = M = [1-k^2]^{1/8}$. The explicit expression for ρ_n reads as

$$\begin{aligned}\frac{\rho_n}{2} &= -\sum_{j<n} \psi_j^{(+)} \psi_j^{(-)}, \\ \psi_j^{(+)} &= -\int_{-\pi}^{\pi} \frac{d\theta}{2\pi}\, e^{ij\theta} U_+(-\theta)\, p(\theta), \\ \psi_j^{(-)} &= \int_{-\pi}^{\pi} \frac{d\theta}{2\pi}\, e^{ij\theta} U_-(\theta)\, q(\theta),\end{aligned} \tag{A10}$$

where the functions

$$U_\pm(\theta) = [\epsilon(\theta)]^{\mp 1} \exp[i\alpha(\theta)]$$

provide the Wiener-Hopf factorization of $\exp[2i\alpha(\theta)]$:

$$\exp[2i\alpha(\theta)] = U_+(\theta)\, U_-(\theta).$$

Functions $U_+(\theta)$ and $U_-(\theta)$ are analytical in $z = e^{i\theta}$ outside and inside the unit circle, respectively. Rewriting $\psi_j^{(+)}$ and $\psi_j^{(-)}$ in terms of creation and annihilation operators $\psi^\dagger(\theta)$, $\psi(\theta)$ by use of (A3) one obtains from (A7), (A9), (A10) the desired fermionic representation (8) of the U operator.

In deriving (A10) we have chosen the free fermion basis $p(\theta)$, $q(\theta)$ and applied the theorem, presented by Jimbo *et al.* in pages 137, 138 of their article.[23] In our case, the kernel functions for matrices P, E introduced in this theorem read as (compare with Eqs. (3.15), (3.16) in the same article):

$$\begin{aligned}P(\theta, \theta') &= \frac{e^{i(n-1)(\theta-\theta')}}{1-e^{-i(\theta-\theta'-i0)}}, \\ E(\theta, \theta') &= \begin{pmatrix} 0 & \exp[-2i\alpha(\theta)] \\ \exp[2i\alpha(\theta)] & 0 \end{pmatrix} 2\pi\delta(\theta-\theta').\end{aligned}$$

To illustrate convenience of representations (8), (A9), (A10), we shall apply them to derive a compact Fredholm determinant formula for the zero-field correlation function $\langle \sigma_{0,0}\sigma_{m,n} \rangle$ in the ferromagnetic phase. Let us first write this correlation function by use of (A9), (8) in the form

$$\begin{aligned}\langle \sigma_{0,0}\sigma_{m,n} \rangle &= \langle 0_+ |\, \bar{\sigma}_0^3 \exp(-m\mathscr{H}^{(0)})\, \bar{\sigma}_n^3\, | 0_+ \rangle \\ &= M^2 \langle 0_+ | :\exp(\rho_0/2) : \exp(-\mathscr{H}^{(0)} m) : \exp(\rho_n/2): | 0_+ \rangle,\end{aligned} \tag{A11}$$

where

$$\frac{\rho_0}{2} \mapsto \frac{1}{2} \iint_{-\pi}^{\pi} \frac{d\theta_1 d\theta_2}{(2\pi)^2} e^{-\frac{i}{2}(\pi+\theta_1+\theta_2)} D(\theta_1, \theta_2)\, \psi(\theta_1)\, \psi(\theta_2),$$

$$\frac{\rho_n}{2} \mapsto \frac{1}{2} \iint_{-\pi}^{\pi} \frac{d\theta_1 d\theta_2}{(2\pi)^2} e^{\frac{i}{2}(\pi+\theta_1+\theta_2)} e^{-in(\theta_1+\theta_2)} D(\theta_1, \theta_2)\, \psi^\dagger(\theta_1)\, \psi^\dagger(\theta_2),$$

$$D(\theta_1, \theta_2) = \frac{1}{2\sin[(\theta_1+\theta_2)/2]} \left[\frac{\epsilon(\theta_1)}{\epsilon(\theta_2)} - \frac{\epsilon(\theta_2)}{\epsilon(\theta_1)} \right].$$

We have dropped all creation operators $\psi^\dagger$ in $\rho_0/2$, and all annihilation operators ψ in $\rho_n/2$, since the normally ordered exponents of $\rho_n/2$ and $\rho_0/2$ act in (A11) on the vacuum states. In the well-known holomorphic representation[33] of fermionic operators, the matrix element (A11) takes the form of the Gaussian continual integral over Grassnann variables, which integration yields immediately:

$$\langle \sigma_{0,0} \sigma_{m,n} \rangle = M^2 \det(1 - D_{mn}) \tag{A12}$$

$$= M^2 \exp\left(-\sum_{j=1}^{\infty} \frac{\mathrm{Sp}\, D_{mn}^{2j}}{2j} \right). \tag{A13}$$

Here D_{mn} denotes a linear integral operator acting on the function $f(\theta)$ as follows:

$$D_{mn} f = \int_{-\pi}^{\pi} \frac{d\theta'}{2\pi} D(\theta, \theta') \exp\left\{ -\frac{in(\theta+\theta')}{2} - \frac{m[\omega(\theta)+\omega(\theta')]}{2} \right\} f(\theta').$$

Equation (A12) is a compact form of the well-known exact representation of the two-point correlation function in the Ising model obtained by Wu *et al.*[34] (see Eqs. (2.9)–(2.13) in the referred article). The latter representation can be reduced to (A13) by explicit integration in the right-hand side of Eq. (2.12) in $\phi_1, \phi_3, \phi_5, \ldots$. On the Fredholm determinant representation of correlation functions see Palmer and Tracy.[30]

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