Interacting-fermion approximation in the two-dimensional axial next-nearest-neighbor Ising model

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We investigate the effect of including domain-wall interactions in the two-dimensional axial next-nearest-neighbor Ising model. At low temperatures this problem is reduced to a one-dimensional system of *interacting* fermions which can be treated exactly. It is found that the critical boundaries of the low-temperature phases are in good agreement with those obtained using a free-fermion approximation. In contrast with the monotonic behavior derived from the free-fermion approach, the wall density or wave number displays reentrant phenomena when the ratio of the next-nearest-neighbor and nearest-neighbor interactions is greater than $\frac{1}{2}$.

One of the simplest models where competing interactions lead to modulated structures is the axial next-nearest-neighbor Ising or ANNNI model.[1] Although this system seems to be too simple to describe quantitative results on specific materials, it may reproduce qualitative features observed in many physical systems describable by discrete models with effective short-range competing interactions. Examples of this class are magnetic systems of cerium monopnictides,[2] binary metal alloys,[3] ferroelectrics,[4] chemisorbed submonolayers,[5] and polytypes.[6]

Motivated by these findings the ANNNI model has been widely studied by numerous methods including Monte Carlo simulations,[7] series analysis,[8] mean-field calculations,[9] finite-size scaling transfer matrix studies,[10] interface calculations,[11] and free-fermion approximations.[12]

In this work we consider the effect of including domain-wall interactions in the two-dimensional version, which as it will be shown below, will give rise to important consequences on the wall density or wave number behavior. Our analysis closely follows a low-temperature calculation scheme introduced by Villain and Bak[12] for the same model, in which fluctuations around the ground states are represented by a set of alternating positive and negative domains bounded by solid-on-solid wandering threads or walls restricted to have no reentries. The summation of these paths is actually the discrete version of a path integral across the lattice. One of the central points of their calculation is that these walls are forced to have a hard-core behavior, namely, configurations containing nearest-neighbor walls are excluded. This constraint can be taken into account by making a simple scale transformation along the axial (competing) direction which straightforwardly transforms the problem onto a free-fermion approximation (FFA). Although at very low temperatures this calculation yields reliable results, as temperature increases the domain walls can no longer be represented only by the hard core, and finite first-neighbor interactions between them must be included. Certainly, other type of "defects" such as dislocations of the wall network may occur, but unlike wall-wall interactions they only play a relevant role in a high-temperature regime, close to the incommensurate-disordered transition.[7]

Let us consider the ANNNI model on a rectangular lattice of N columns and M rows with full periodic boundary conditions and with Ising spins $s = \pm 1$ interacting through the Hamiltonian

$$H = -J_1 \sum_{i,j} (s_{i,j}\, s_{i,j+1} - X s_{i,j}\, s_{i,j+2}) - J_0 \sum_{i,j} s_{i,j}\, s_{i+1,j} \, . \tag{1}$$

As usual, X denotes the competition ratio between the second- and first-neighbor interactions along the axial direction, i.e., $X = -J_2/J_1$. Results for $J_1 < 0$ can be obtained from those of $J_1 > 0$ by flipping every alternate column of spins, therefore we direct our attention to the latter case.

At $T = 0$ the regime of competing interactions can be divided into ferromagnetic ($X < \frac{1}{2}$) and a fourfold degenerate phase known as $\langle 2 \rangle$ ($X > \frac{1}{2}$) which is a periodic arrangement of two consecutive up spins followed by two neighboring down spins along the axial direction. At $X = \frac{1}{2}$ the ground state becomes infinitely degenerate. The vertical ordering is always ferromagnetic ($J_0 > 0$).

A simple analysis shows that the statistical weight W_r of an arbitrary row state with ν walls ($0 \leq \nu \leq N$) relative to the ferromagnetic phase ($\nu = 0$) is given by

$$W_r = A_\nu \exp\left(-4\beta X \sum_{j=1}^{N} n_j^r\, n_{j+1}^r\right) , \qquad (2)$$

where $A_\nu = \exp[2\beta\nu(2X-1)]$ and $\beta = J_1/T$. The index n_j^r denotes the presence ($n_j^r{=}1$) or absence ($n_j^r{=}0$) of a wall across the jth link of the rth row, therefore the sum contained on the right-hand side of Eq. (2) simply counts the number of times there are nearest-neighbor walls along a row, which is set to zero in the FFA.

Next we note that the energy required to create m single-step kinks between two succesive row states is $2mJ_0$ ($m = 0,1,\ldots,\nu$), hence we may sum up all low-temperature fluctuations by means of the following row-to-row symmetrical transfer matrix

$$\langle r|\hat{\Theta}|s\rangle = (W_r\, W_s)^{\frac{1}{2}}\ \gamma^{m_{rs}} , \qquad (3)$$

where $\gamma = \exp(-2J_0/T)$ and m_{rs} is the number of kinks between the row states $|r\rangle$ and $|s\rangle$.

Since two neighboring walls cannot cross or touch, we may associate the row configurations with collective states of ν spinless fermions allowing us to express the transfer matrix in terms of fermion operators $c, c^\dagger$ acting on a ferromagnetic vacuum state.

At low temperatures it is possible to neglect higher-order commutators and recover the matrix elements of Eq. (3) introducing a one-dimensional many-body Hamiltonian H_ν closely related with the transfer matrix, namely

$$\hat{\Theta} = A_\nu \exp(-H_\nu) , \qquad (4)$$

$$H_\nu = -\gamma \sum_j \left(c_j^\dagger c_{j+1} + \text{H.c.}\right) + 4\beta X \sum_j c_j^\dagger c_j c_{j+1}^\dagger c_{j+1} . \qquad (5)$$

The wall density or wave number $q = \nu/N$ ($0 \le q \le 1$) is obtained by minimizing the corresponding free energy $\mathcal{F}_q$ which in the limit $M \to \infty$ can be computed from the largest eigenvalue $\lambda_{\max}^{(q)}$ of $\hat{\Theta}$, i.e., $\mathcal{F}_q = -\frac{1}{N} T \ln \lambda_{\max}^{(q)}$. Therefore we are left with the calculation of the ground-state energy of the interacting fermion problem defined by H_ν.

As it is well known this system can be mapped onto an $S{=}\frac{1}{2}$ anisotropic Heisenberg chain in a uniform magnetic field by means of a Jordan-Wigner transformation,[13] hence H_ν can be rewritten as

$$H_\nu = -\frac{\gamma}{2} \sum_j \left(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta\, \sigma_j^z \sigma_{j+1}^z\right) + \beta X (2S^z + N) , \qquad (6)$$
$$S^z = \sum_j \sigma_j^z , \quad \Delta = -2\beta X/\gamma ,$$

where σ^x, σ^y, and σ^z are the usual spin-$\frac{1}{2}$ Pauli matrices. The relation between the magnetization per site $\mu = S^z/N$ (preserved by H_ν) and the "band-filling" q is simply

$$\mu = 2q - 1 \ , \ |\mu| \le 1 . \qquad (7)$$

From Eqs. (4) and (6) it follows that the free energy $\mathcal{F}_q$ can now be expressed as

$$\mathcal{F}_q/J_1 = \frac{2\gamma}{\beta} f(\Delta,\mu) + 2q - X , \qquad (8)$$

where $2f(\Delta,\mu)$ is the ground-state energy of the anisotropic Heisenberg chain with magnetization $\mu = 2q-1$ and anisotropy $\Delta = -2\beta X/\gamma$. This identification enables us to determine the critical boundaries of the $\langle 2\rangle$ and ferromagnetic states by studying the stability conditions of $\mathcal{F}_q$ around $\mu = 0$ and $\mu = -1$, respectively.

According to Eq. (8) it is clear that due to the inversion symmetry of the Heisenberg Hamiltonian, the free energy is unstable for all band-fillings greater than $\frac{1}{2}$, henceforth we will restrict our attention to the case $0 \le q \le \frac{1}{2}$.

The analytical properties of $f(\Delta,\mu)$ at and near $|\mu| = 1$ and $\mu = 0$ have already been studied by Yang and Yang[14] using a generalization of the Bethe-ansatz technique[15] providing us the necessary information to go further in our analysis. According to their work the expansion of $\mathcal{F}_q$ close to the ferromagnetic state results in

$$\mathcal{F}_q/J_1 = 2q\left(1 - 2X - \frac{\gamma}{\beta}\right) + O\left(q^3\right) . \qquad (9)$$

from which the standard FFA ferromagnetic boundary is obtained, namely $T_c \exp(-2J_0/T_c) = J_1 - 2J_2$, $X < \frac{1}{2}$. This coincidence is not surprising because at low wall-density regimes the short-ranged wall-wall interactions become irrelevant.

Following Yang and Yang, the free energy close to the $\langle 2\rangle$ phase can be expanded as

$$\mathcal{F}_q/J_1 = 4X \tanh\lambda \left(\varepsilon_0 (1-2q) + \frac{\pi^2 \varepsilon_2}{3\varepsilon_0^2}(1-2q)^3\right) + \frac{2\gamma}{\beta} f(\Delta,0) + 2q - X + O\left((1-2q)^4\right) , \qquad (10)$$

where ε_0, ε_2, and $f(\Delta,0)$ are given by

$$\varepsilon_0 = \frac{1}{2} + \sum_{n>0} \frac{(-1)^n}{\cosh(n\lambda)}, \quad \varepsilon_2 = \sum_{n>0} \frac{(-1)^{n+1} n^2}{2\cosh(n\lambda)} , \qquad (11)$$
$$f(\Delta,0) = \frac{1}{4}\cosh\lambda - \sinh\lambda\left(\frac{1}{2} + 2\sum_{n>0}\frac{1}{1+\exp(2\lambda n)}\right) ,$$
$$\cosh\lambda = -\Delta, \quad \lambda > 0 .$$

The stability condition of phase $\langle 2\rangle$ now reads

$$4X\varepsilon_0 \tanh\lambda > 1, \quad X > \tfrac{1}{2} . \qquad (12)$$

Note that in the low-temperature limit (high anisotropy regime), we can expand this equation up to first order in $1/\Delta$ and recover the FFA boundary, i.e., $T_c \exp(-2J_0/T_c) = J_2 - \frac{1}{2}J_1$, $X > \frac{1}{2}$.

It is interesting to point out that even at higher temperatures the agreement with the FFA result is quite good as can be seen in Fig. 1 where both approximations

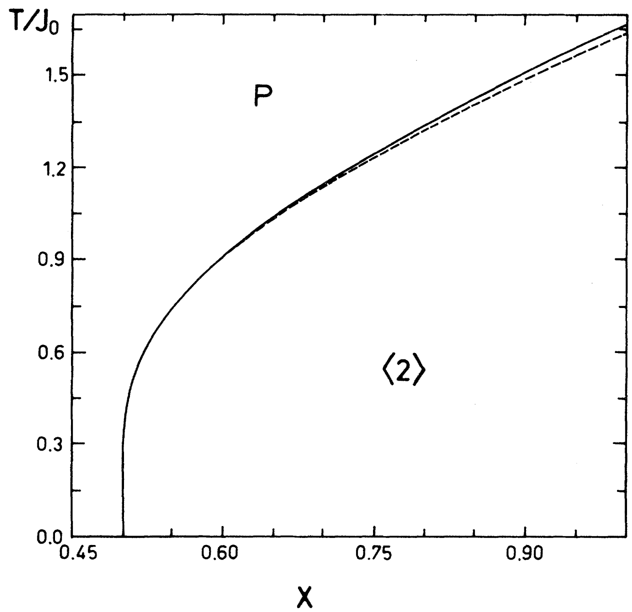

FIG. 1. Critical boundaries of the ⟨2⟩ phase for $J_0 = J_1$. The solid line denotes the free-fermion calculation. The dashed line indicates the interacting-fermion approximation result.

are compared. Since our approach has less entropy restrictions it yields a lower transition temperature, as it should.

Due to the lack of the quadratic term in Eq. (10), it follows that slightly above the ⟨2⟩ state the wall density behaves as

$$q = \frac{1}{2} - \frac{1}{8\pi X}\left(\left.\frac{d\varepsilon_0}{d\lambda}\right|_{\lambda=\lambda_c} + \left(4X\sinh^2\lambda_c\right)^{-1}\right)^{\frac{1}{2}} \times \left(\frac{1+2J_0/T_c}{\varepsilon_2(\lambda_c)}\right)^{\frac{1}{2}} \coth^{\frac{3}{2}}\lambda_c \left(\frac{T-T_c}{T_c}\right)^{\frac{1}{2}}, \tag{13}$$

where T_c and λ_c are determined from Eq. (12). This is in agreement with the general theory of Pokrovskii and Talapov[16] on commensurate-incommensurate phase transitions in two-dimensional systems, according to which the wave number of the incommensurate phase should display a square-root singularity on approaching a commensurate state of type $p \times 1$ provided that $p^2 > 8$ (the ⟨2⟩ structure has a period $p = 4$).

Next let us consider the wave-number behavior derived from the minima of Eq. (8). After solving numerically the full Yang and Yang integral equations for arbitrary band-fillings, we found that for $X < \frac{1}{2}$ the wave number properties are in qualitative agreement with those obtained using the free-fermion approach. However, for $X > \frac{1}{2}$ the wave number exhibits a reentrant feature in contrast with the monotonic FFA behavior. This suggests the possibility of reentrant phenomena within the incommensurate phase which is known to be stable with respect to paramagnetism if $X > \frac{1}{2}$.[17] These results are shown in Fig. 2.

A word of caution should be added on interpreting these results. Our calculations are reasonable in the floating incommensurate phase provided that the density of local defects is negligible, while these figures extend up to infinite temperatures. Nevertheless, note that the reentrance behavior could take place at "intermediate" regimes which according to Monte Carlo simulations[7] can be almost considered as dislocation free.

At very low temperatures ($\Delta \to -\infty$) it is possible to recover the wall densities computed by Villain and Bak

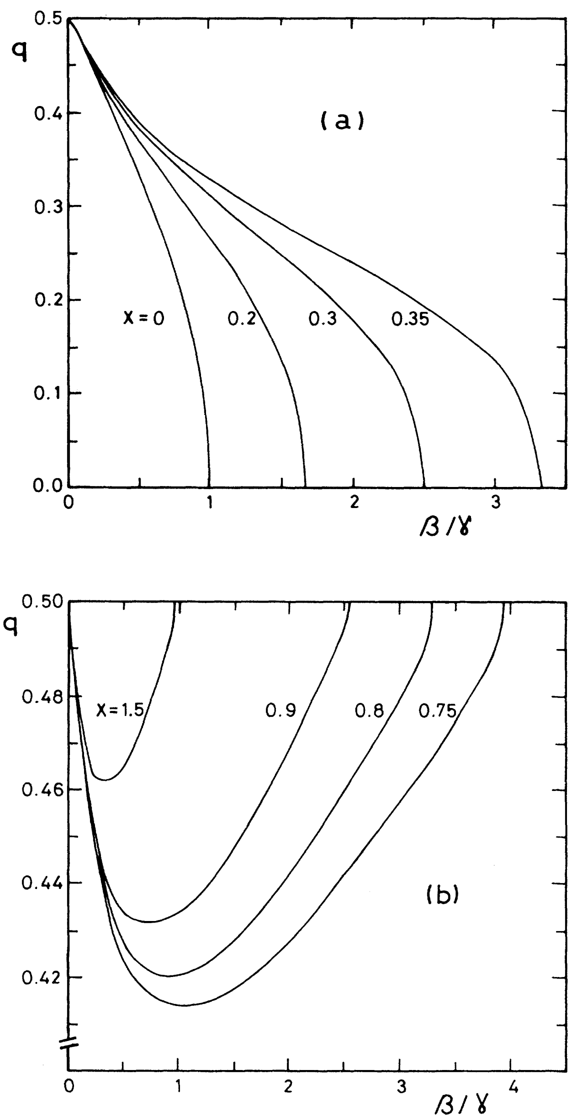

FIG. 2. Wall densities resulting from the interacting-fermion approach as a function of the temperature parameter $\beta/\gamma = (J_1/T)\exp(2J_0/T)$. (a) $X < \frac{1}{2}$; (b) $X > \frac{1}{2}$. In both cases the free-fermion approximation yields a monotonic behavior with a limiting value of $q_0 \approx 0.301$.

noting that[14]

$$f(\Delta,\mu) = -\frac{1}{4}\Delta + \frac{1}{2}\Delta(1-\mu) - \frac{1+\mu}{2\pi}\sin\left(\pi\frac{1-\mu}{1+\mu}\right) + O\left(\Delta^{-1}\right) . \tag{14}$$

The minimization of $\mathcal{F}_q$ in Eq. (8) is then satisfied by the following wall densities

$$\frac{1}{1-q}\cos\left(\frac{\pi q}{1-q}\right) - \frac{1}{\pi}\sin\left(\frac{\pi q}{1-q}\right) = (1-2X)\,\beta/\gamma\,, \tag{15}$$

which is precisely the FFA result.

In conclusion, we have shown that the domain-wall interactions of the two-dimensional ANNNI model are describable by an interacting-fermion theory which reproduces the FFA results at the low-temperature limit. On such a regime the deviations from the hard-core wall picture are exponentially small [of the order $O\left(\Delta^{-1}\right)$] and therefore the FFA description is quite appropriate. However, as temperature increases the wall interactions become very important in the thermodynamic description giving rise to the possibility of reentrant phenomena within the incommensurate phase, as is shown by the wall density behavior obtained in this work.

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[16] V. L. Pokrovskii and A. L. Talapov, Zh. Eksp. Teor. Fiz. **75**, 1151 (1978) [Sov. Phys. JETP **48**, 579 (1978)].

[17] It is an open problem whether the incommensurate phase extends up to arbitrarily large values of X or only up to some finite X_L implying the existence of a Lifshitz-type multicritical point. On the ferromagnetic side the incommensurate state is believed to be unstable with respect to the disordered phase.