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Continuously Infinite Commensurate–Incommensurate Phase Transition of a Two-Dimensional Competing Ising Model

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We consider the critical behavior of a two-dimensional competing axial Ising model including interactions up to third nearest neighbors in one direction. On the basis of a low-temperature analysis relating the transfer matrix of this model with the Hamiltonian of the $S = \frac{1}{2}$ XXZ chain, it is shown that the usual square root singularity dominating commensurate–incommensurate phase transitions of two-dimensional systems merges into a continuously infinite transition for certain relations among the coupling parameters. The conjectured equivalence between the maximum eigenstate of the transfer matrix associated with this model and the ground state of the XXZ chain is tested numerically for lattice widths up to 18 sites.

KEY WORDS: Competing axial Ising model; $S = \frac{1}{2}$ XXZ chain; commensurate–incommensurate phase transition.

Commensurate–incommensurate (C–IC) phase transitions in two-dimensions (2D) have been studied extensively, both from experimental and theoretical points of view.

The most common realization of these 2D phenomena is the adsorption of rare gas films on the surfaces of transition metals. In Xe physisorbed on Cu(110), monolayers have been reported[1] to order into a 2×2 structure and to display an axial IC phase at higher temperatures, namely, the monolayer contracts only in one direction and exhibits a continuously varying incommensurability. Similar situations have been observed in Ar physisorbed on MgO(100),[2] H_2 on Fe(110) or Pd(100),[3] and H_2 or D_2 adsorbed on graphite.[4]

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Theoretically, the absorbed monolayers can be modeled as 2D systems of interacting particles subject to a periodic external substrate field.

In the domain wall theory of C–IC phase transitions (see ref. 5 for review) monolayer particles are replaced by fluctuating domain walls and all fluctuations at small length scales are integrated out. The IC monolayer is visualized as an array of C domains separated by walls.

For the sake of simplicity, *low* temperatures will be considered in this work in the sense that the root mean square displacements of these walls are assumed to be of the order of the interatomic distance. In such regimes, the wall network may be viewed as a striped IC structure, i.e., domain walls do not intersect but run parallel on average.

In that case, the main contribution to the configurational entropy is given by the meander entropy of the walls. Basically, this description corresponds to the Pokrovsky–Talapov (PT) theory of 2D C–IC phase transitions[6] which, as is well known, gives rise to square root singularities in the thermodynamic potentials.

The purpose of this work is to investigate the effect of including short-ranged interactions between walls on the character of these transitions. Presumably these interactions, although small, could play a significant role in reality, as will be shown in the simplified system considered below.

The standard theoretical model describing uniaxial systems with competing C ground states is the 2D axial next-nearest-neighbor Ising or ANNNI model (see refs. 7 for reviews). Its Hamiltonian can be easily extended to include further-neighbor interactions.

The first step in this direction is to consider an axial third-nearest-neighbor Ising or A3NNI model with spins $S_{i,j} = \pm 1$ interacting through the Hamiltonian

$$H = -J_1 \sum_{i,j} S_{i,j}(S_{i,j+1} - XS_{i,j+2} - YS_{i,j+3}) - J_0 \sum_{i,j} S_{i,j}S_{i+1,j} \tag{1}$$

where X and Y denote the second- and third-neighbor competition ratios, respectively, i.e., $X = -J_2/J_1$, $Y = -J_3/J_1$ with $J_1, J_0 > 0$. Results for $J_1, J_0 < 0$ can be obtained from those of the former case by setting $J_3 \to -J_3$ and inverting the spin orientation in alternate columns.

This system has already been studied by means of Monte Carlo simulations[8] and domain wall analysis.[9] Also, the three-dimensional generalization was investigated using low-temperatures series methods[10] and mean field approximations.[11] So far, most of the interest has been focused on the case $Y = 0$.

At $T = 0$ and $|Y| < 1$ the ground state may be (i) a ferromagnetic phase if $Y < (1 - 2X)/3$ for $X < 1/2$ and $Y < 1 - 2X$ for $X > 1/2$; (ii) a sixfold degenerate $\langle 3 \rangle$ state (periodic arrangement of three consecutive up spins followed by three neighboring down spins along the axial direction) if $Y > |1-2X|/3$; or (iii) the usual $\langle 2 \rangle$ ground state of the ANNNI model (fourfold-degenerate sequence of $\downarrow\downarrow\uparrow\uparrow \cdots$ spins) if $1-2X < Y < (2X-1)/3$ for $X > 1/2$.

It is convenient to work in the wall occupation number representation ($n_{r,j} = \frac{1}{2}[1 - S_{r,j} S_{r,j+1}]$), where the number of domain walls ν can be assumed to be conserved from row to row in the low-temperature regime, namely, dislocations such as overhangs and droplets are considered unlikely to occur. Walls attract or repel each other at first- and second-nearest-neighbor distances, depending on whether the second- and third-neighbor couplings are ferro- or antiferromagnetic, respectively.

Along the $\langle 2 \rangle : \langle 3 \rangle$ and $\langle 2 \rangle$:ferromagnetic boundaries, the ground state becomes infinitely degenerate but in such a way that configurations containing nearest-neighbor walls are forbidden, i.e., $n_j n_{j+1} \equiv 0$. The ordering along the noncompeting direction is always ferromagnetic.

We will restrict ourselves to considering a set of coupling parameters (X, Y) *close* to $(1/2, 0)$, within a region defined by

$$|J_3|,\ |J_1 + 2J_2| \ll T \ll J_0 \tag{2}$$

In this regime, fluctuations around all possible ground states can be reliably represented in terms of *interacting* "hard-core" walls ($n_j n_{j+1} \equiv 0$) wandering across the lattice and restricted to having no reentries. *A posteriori*, we will test numerically the extent to which this analysis is reliable by calculations on a finite system.

The summation of the wall contours may be implemented through the transfer matrix formalism, which is actually the discrete version of a path integral across the lattice. We point out only the relevant results here, referring the reader to ref. 9 for a more detailed calculation.

Within these approximations it is straightforward to build up a close relation between the transfer matrix $\hat{\Theta}$ of the 2D A3NNI model and the Hamiltonian of an $S = 1/2$ anisotropic Heisenberg–Ising or XXZ chain with anisotropy Δ in a uniform magnetic field h, namely

$$\hat{\Theta} = \exp[\tfrac{2}{3}\beta N(2Y + 2X - 1)] \exp(-\mathscr{H}_\nu)$$

$$\mathscr{H}_\nu = -\frac{\gamma}{2} \sum_{j=1}^{N-\nu} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z) - h S^z \tag{3}$$

$$S^z = \sum_{j=1}^{N-\nu} \sigma_j^z, \qquad \Delta = -2\beta Y/\gamma, \qquad h = \tfrac{2}{3}\beta(Y/2 + 2X - 1)$$

where $\beta = J_1/T$, $\gamma = \exp(-2J_0/T)$, and σ^x, σ^y, σ^z are the usual spin-1/2 Pauli matrices. The chain is ferro- or antiferromagnetic, depending on the sign of J_3.

Note that to take into account the hard-core constraint the actual length of the XXZ chain is reduced by a factor $(1-q)$, where $q = \nu/N$ is the density of domain walls in the original system $(0 \leqslant q \leqslant 1/2)$. The conservation of S^z simply indicates that dislocations are excluded in this description.

Defining $2f(\Delta, \mu)$ as the ground-state energy of the XXZ chain within a subspace of magnetization μ, the free energy $\mathscr{F}_q$ of the 2D A3NNI model with wall density q results in

$$\begin{aligned} \frac{\mathscr{F}_q}{J_1} &= 2\frac{\gamma}{\beta}(1-q)\, f(\Delta, \mu) - 2q\left(\frac{Y}{2} + 2X - 1\right) - Y \\ \mu &= \frac{3q-1}{1-q}, \qquad |\mu| \leqslant 1 \end{aligned} \tag{4}$$

Therefore, we are left with the calculation of the analytical properties of $f(\Delta, \mu)$, which has already been studied by Yang and Yang[12] using the Bethe ansatz[13] technique (see also des Cloizeaux and Gaudin[14]).

Based on these exact results, we may proceed to study the wall density behavior close to the $\langle 3 \rangle$ $(q = 1/3)$ and $\langle 2 \rangle (q = 1/2)$ C phases, expanding $f(\Delta, \mu)$ around $\mu = 0$ and 1^-, respectively. The crux of the analysis lies in the recognition that in these expansions the second-order term *is lacking*, i.e., $\partial^2 f(\Delta, \mu)/\partial\mu^2|_{\mu=0,1} \equiv 0$ for $\Delta < -1$. The physical meaning of this lack is the appearance of square root singularities dominating the C–IC phase transition.

A similar calculation may be carried out for $q = 0^+$, although close to the ferromagnetic boundary the IC phases are believed to be unstable with respect to the disordered state, so wall dislocations are expected to play a relevant role near the ferromagnetic line.

Upon minimizing the free energy $\mathscr{F}_q$ in the neighborhood of the $\langle 3 \rangle$ state, following Yang and Yang, we found

$$\begin{aligned} \left(\frac{3q-1}{1-q}\right)^2 &= \frac{2}{3}\left(\frac{\partial^3}{\partial\mu^3} f(\Delta, \mu)\bigg|_{\mu=0}\right)^{-1} \left[f(\Delta, 0) + \left(\frac{Y}{2} + 2X - 1\right)\frac{\beta}{\gamma} \right. \\ &\qquad \left. \mp 3\frac{\partial}{\partial\mu} f(\Delta, \mu)\bigg|_{\mu=0} \right] + \mathcal{O}(3q-1)^3 \end{aligned} \tag{5}$$

where $f(\Delta, \mu)$ and its derivatives at $\mu = 0$ are given by

$$f(\Delta, 0) = \frac{1}{4}\cosh\lambda - \sinh\lambda\left(\frac{1}{2} + 2\sum_{n>0}\frac{1}{1+\exp(2\lambda n)}\right)$$

$$\left.\frac{\partial}{\partial\mu} f(\Delta, \mu)\right|_{\mu=0} = \frac{1}{2}\sinh\lambda \sum_{-\infty}^{+\infty} \frac{(-1)^n}{\cosh(n\lambda)} \tag{6}$$

$$\left.\frac{\partial^3}{\partial\mu^3} f(\Delta, \mu)\right|_{\mu=0} = 2\pi^2 \sinh\lambda \frac{\sum_{-\infty}^{+\infty} (-1)^{n+1} n^2/\cosh(n\lambda)}{[\sum_{-\infty}^{+\infty} (-1)^n/\cosh(n\lambda)]^2}$$

with $\cosh\lambda = -\Delta$, $\lambda > 0$, and $Y > |2X-1|/3$.

The upper and lower signs of Eq. (5), which result from the spin inversion symmetry of the XXZ Hamiltonian, correspond to the cases $q = \frac{1}{3}^+$ and $\frac{1}{3}^-$, respectively.

In the neighborhood of $q = \frac{1}{2}^-$, close to the $\langle 2 \rangle$ state, the expansion of $f(\Delta, \mu)$ around $\mu = 1^-$ yields

$$\left(\frac{1-2q}{1-q}\right)^2 = \frac{\beta}{\gamma\pi^2}(3Y + 1 - 2X) + \frac{2}{\pi^2} + \mathcal{O}(1-2q)^3 \tag{7}$$

with $1 - 2X < Y < (2X-1)/3$, $X > 1/2$.

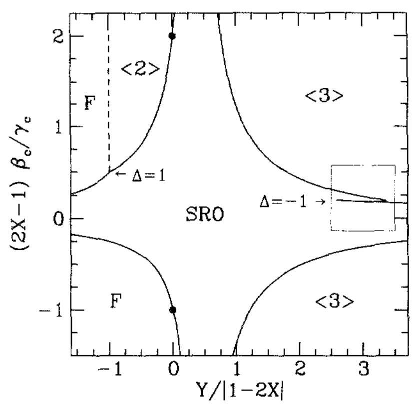

Fig. 1. Phase diagram of the 2D A3NNI model close to the regime defined by Eq. (2) in the text. Temperature increases on approaching zero from both sides of the vertical scale. The solid line separates long-range-order commensurate phases from quasi-long-range incommensurate states with algebraically decaying spin–spin correlation functions. At higher temperatures the incommensurate state is unstable with respect to a short-range order paramagnetic phase; the corresponding boundary cannot be obtained with the present low-temperature approach. The $\langle 2 \rangle$ and ferromagnetic (F) phases coexist along the dashed line up to maximum temperature associated to the fully isotropic ferromagnetic XXZ chain. The dots denote the critical temperatures of the ANNNI model ($Y = 0$). The region inside the square on the right is associated to the isotropic antiferromagnetic XXZ chain and indicates the region of main interest in this work.

Critical temperatures can be evaluated by setting $q = 1/3$ and $1/2$ in Eqs. (5) and (7), respectively. The resulting phase boundaries are shown in Fig. 1 as a function of the scaled variables $Y/|1-2X|$ and $(2X-1)\beta/\gamma$, which is an appropriate set of parameters to describe this model within the region defined by Eq. (2).

Expanding the right-hand side of Eqs. (5) and (7) up to first order in $T - T_c$, it is clear that the domain wall density goes continuously to the corresponding C values as $|T - T_c|^{1/2}$ in agreement with the PT theory.[6] The free energy remains regular on the C side, but behaves singularly as $|T - T_c|^{3/2}$ in the IC state. Hence the specific heat diverges with a critical exponent $\alpha = 1/2$.

Certainly, invoking universality, a PT transition can be expected in the 2D A3NNI model; the details of the interactions between spins are not essential. Nevertheless, the validity of the previous conclusions depends strongly on the fact that $f(\Delta, \mu)$ and its derivatives must be *analytic* functions of Δ and μ.

There is a particular regime where this statement is no longer valid and the effective forces between domain walls give rise to a completely different critical behavior. Indeed this is the situation at $\Delta = -1$, which corresponds to the top of the $\langle 3 \rangle$ phase for a given value of $Y > 0$. This region is enlarged in Fig. 2.

Within $(2\ln 2 - 1)^{-1} < Y/(2X-1) < 3.3676$, three C–IC transitions occur. At some transition temperature T_1 the $\langle 3 \rangle$ phase is unstable against IC states with $q > 1/3$; as temperature is increased, the system reenters the

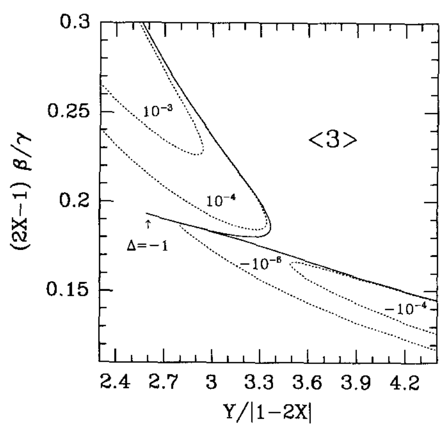

Fig. 2. Neighborhood of $\Delta = -1$. At this point the system undergoes a continuously infinite commensurate–incommensurate phase transition. Temperature increases from top to bottom. The dotted lines denote contours of constant wall density $q = 1/3 + \varepsilon$.

$\langle 3 \rangle$ phase at $T_2 > T_1$ and is finally favored by IC phases with $q < 1/3$ at $T_3 > T_2$.

If $Y/(2X-1) \simeq 3.3676$ ($\Delta \simeq -1.2538$), then $T_1 = T_2$ and no reentrance takes place, namely, the critical amplitudes associated to the square root singularities of the wall densities are strictly zero and the free energy becomes regular. The amplitudes corresponding to $T_1(X)$ and $T_2(X)$ are displayed in Fig. 3a for a fixed value of $Y = 0.1$.

When $(2X-1)/Y \to (2\ln 2 - 1)$, both T_2 and T_3 coalesce at a common transition temperature T^* (which is still in the low-temperature regime) defined by $-\Delta = 2\beta^* Y/\gamma^* = 1$, with a vanishing critical amplitude, as shown in Figs. 3a and 3b. However, at this point the free energy is no longer regular. Let us now discuss the correct critical behavior at T^*.

In the complex plane $f(\Delta, 0)$ has a branch cut at $-1 \leqslant \Delta < 1$, across which no analytical continuation is possible, although on the real axis $f(\Delta, 0)$ ands all its derivatives are continuous at $\Delta = -1$.[12,14] On the other hand, $\partial f(\Delta, \mu)/\partial\mu|_{\mu=0}$, $\partial^3 f(\Delta, \mu)/\partial\mu^3|_{\mu=0}$, and higher-order derivatives display essential singularities at $\Delta = -1$. The corresponding asymptotic expansions given by Yang and Yang around this singular point turn out to be

$$
\begin{aligned}
f(\Delta, 0) &\sim \frac{1}{4} - \ln 2 + (\Delta+1)\left(\frac{1}{3}\ln 2 - \frac{1}{12}\right) + \mathcal{O}(\Delta+1)^2 \\
\left.\frac{\partial}{\partial\mu} f(\Delta, \mu)\right|_{\mu=0} &\sim 2\pi \exp\left(-\frac{\pi^2}{(8\,|\Delta+1|)^{1/2}}\right) \\
\left.\frac{\partial^3}{\partial\mu^3} f(\Delta, \mu)\right|_{\mu=0} &\sim \frac{\pi^3}{4} \exp\left(\frac{\pi^2}{(8\,|\Delta+1|)^{1/2}}\right)
\end{aligned}
\tag{8}
$$

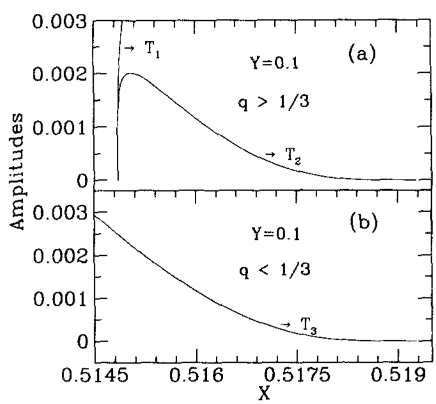

Fig. 3. Critical amplitudes as a function of X for $Y = 0.1$. (a) Amplitudes accompanying the first (T_1) and second (T_2) transitions (upper and intermediate solid lines of Fig. 2, respectively). (b) Amplitude of the third transition (T_3) (lower solid line of Fig. 2).

These results provide us the necessary information to go a further step in our analysis. According to Eq. (5), it is straightforward to show that near T^* the wall density actually behaves as

$$\left(q-\frac{1}{3}\right) \propto \mp \exp\left(-\mathscr{A}\left|\frac{T-T^*}{T^*}\right|^{-1/2}\right)\left|\frac{T-T^*}{T^*}\right|^{1/2}$$
$$\mathscr{A}=\frac{\pi^2}{8(J_0/T^*+1/2)^{1/2}} \tag{9}$$

where the upper and lower signs correspond to $T>T^*$ and $T<T^*$, respectively.

Therefore, at $X=1/2+(\ln 2-1/2)\,Y$ the free energy is signaled by a infinite-order singularity of the form

$$|T-T^*|^{3/2}\exp\left(-\mathscr{A}\left|\frac{T-T^*}{T^*}\right|^{-1/2}\right)$$

and the C–IC transition becomes continuously infinite in accordance with the essential singularity actually found in the ground-state energy of the XXZ chain.

We would like to point out that this transition is not of the Kosterlitz–Thouless[15] (KT) type, although it shares some common features. For instance, in the ANNNI model, wall *dislocations* become bound in pairs and destablize the floating IC state through a continuously infinite KT transition. Their positional entropy finally leads to the melting of the IC phase.[16] In contrast, here dislocations are assumed to have a negligible density in bulk, so the wall network is still well defined at $\Delta=-1$. However, Eq. (9) indicates that at this singular point of the phase diagram the effective *repulsions* between walls wash out square root singularities and lead to a continuously infinite C–IC transition.

Let us now check the reliability of the main assumptions of this work. Although we cannot prove them on a rigorous basis, we can nevertheless test their validity for a finite system.

According to Eq. (3), the eigenstate $|\psi_{\max}\rangle$ corresponding to the maximum eigenvalue of the *actual* transfer matrix of the 2D A3NNI model must contain all the ground-state microscopic functions of the XXZ chain. Indeed, this is a strong conjecture which should be verified.

In order to extract this information from $|\psi_{\max}\rangle$, we need first to *project* this state on a subspace with a well-defined number of walls. The idea is to measure the extent to which $|\psi_{\max}\rangle$ is immersed in this subspace as long as we approach the region defined by Eq. (2).

Following Villain and Bak,[16] the hard-core wall constraint can be taken into account by introducing a set of fictitious coordinates $\{\xi_1, \xi_2,..., \xi_\nu\}$ defined in such a way that the actual wall positions $\{x_1, x_2,..., x_\nu\}$ of an arbitrary row state are transformed as

$$\begin{gathered} \xi_p = x_p - p, \qquad x_{p+1} - x_p \geqslant 2, \qquad \xi_{p+1} - \xi_p \geqslant 1 \\ p = 1, 2,..., \nu, \qquad \nu + 1 \equiv 1 \end{gathered} \tag{10}$$

Note that the width of the effective system in the corresponding subspace has $N' = N - \nu$ sites. Then we can define wall number operators $\hat{n}_\xi$ associated with these coordinates and construct wall–wall correlation functions W_r of the form

$$W_r = \frac{1}{N'} \sum_{\xi=1}^{N'} \langle \psi_{\max} | (2\hat{n}_\xi - 1)(2\hat{n}_{\xi+r} - 1) | \psi_{\max} \rangle \tag{11}$$

In particular, within the $\langle 3 \rangle$ phase $(N' = \frac{2}{3}N)$ these functions should converge to the *actual* ground-state spin–spin correlation functions C_r of the XXZ chain with zero magnetization, namely

$$C_r = \frac{1}{N'} \sum_{j=1}^{N'} \langle \psi_0 | \sigma_j^z \sigma_{j+r}^z | \psi_0 \rangle \tag{12}$$

We have found a quite remarkable agreement between these functions which in principle arise from completely different operators. This can be seen in Fig. 4, which shows the results obtained for $\Delta = -1$ after

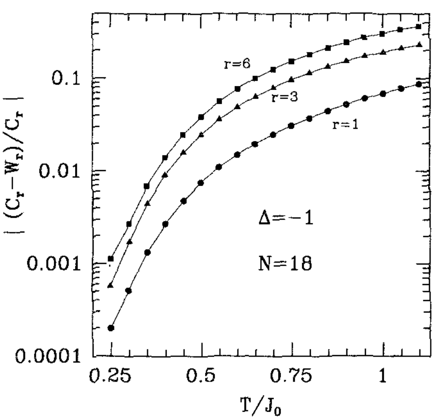

Fig. 4. Relative error of the wall–wall correlation functions W_r for a strip of $N = 18$ sites with respect to the ground-state spin–spin correlation functions C_r of an XXZ chain with $N' = 12$ spins and $\Delta = -1$ as a function of temperature. The actual value of C_r are $C_1 \simeq -0.5986$, $C_3 \simeq -0.2211$, and $C_6 \simeq 0.1426$. Data for $r = 2, 4, 5$ are not shown in order to improve the clarity of the figure.

diagonalizing exactly an XXZ chain of 12 spins and an A3NNI strip of 18 sites with periodic boundary conditions. Here we set $J_1 = J_0$, $Y(T/J_0) = \gamma/2\beta$, and $X = 1/2 + (\ln 2 - 1/2) Y$. Results of comparable accuracy were obtained for other values of Δ, as long as we approach the region defined by Eq. (2).

In conclusion, the overlap between the W_r and C_r correlation functions strongly supports the hypothesis that at low-temperature regimes dislocations do not play a central role in the C–IC transition. This evidence gives us confidence in the main results of this work, in particular for the existence of a continuously infinite C–IC phase transition, which contrasts with the usual PT behavior.

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