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Finite-size scaling of two-dimensional axial next-nearest-neighbor Ising models

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A finite-size-scaling analysis is applied to two axial next-nearest-neighbor Ising (ANNNI) models. By using the scaling behavior of both the correlation length and the modulation wave vector we are able to clearly identify and distinguish between the ordered commensurate phases, the lock-in fluid phases, and in particular, the two types of incommensurate (floating) phases occurring in the models. As expected, the brickwork ANNNI model does not have a floating-solid phase, but instead has a $q=\frac{1}{4}$ lock-in fluid phase above its $\langle 2 \rangle$ phase. On the basis of our results, we conclude that, in contrast to a recent suggestion, transfer-matrix methods can be a powerful tool in the study of two-dimensional models which exhibit incommensurate phases.

The study of two-dimensional spin systems exhibiting commensurate-incommensurate phase transitions has made a great deal of progress in recent years.[1] One model which has been used extensively in the study of this phenomenon is the axial next-nearest-neighbor Ising (ANNNI) model.[2–4] Several methods have been developed to handle the complicated phase structure occurring in the model. Examples of calculations performed on the two-dimensional ANNNI model include the free-fermion approximation,[5] interface free-energy calculations,[6] exact solution (on a special line) of an equivalent Hamiltonian,[7] Monte Carlo simulations,[8] and finite-size-scaling calculations and series-analysis techniques applied to the model's quantum Hamiltonian analogs.[9] The phase diagram of the model is widely accepted to be that shown in Fig. 5.

It is necessary, however, to take considerable care in numerical studies of the model, especially when attempting to distinguish between the floating-solid (algebraically decaying correlations) phase and the floating-fluid (exponentially decaying correlations) phase. Indeed, in a recent paper[10] Morgenstern suggests that numerical methods (both Monte Carlo and transfer-matrix scaling) may prove unreliable in the study of such problems. To support this suggestion, numerical studies on an exactly soluble mock ANNNI (brickwork ANNNI) model, which has no floating-solid phase, were compared with numerical studies on the true ANNNI model. The claim was that on the basis of numerical studies of these models it is not possible to distinguish convincingly between the two.

In this article we present a transfer-matrix-scaling[11] analysis of the ANNNI and brickwork ANNNI models. Using an analysis technique recently applied successfully to the three-state chiral clock model,[12] we calculate the phase diagrams of these two models. Our calculations show that it is possible to distinguish clearly between all of the phases occurring in the models, and hence that transfer-matrix scaling can provide a powerful method in the study of such systems.

The ANNNI model we study is defined by the Hamiltonian,

$$\mathscr{H}=-J_1\sum_{i,j}[S_{i,j}(S_{i,j+1}+S_{i+1,j})]+J_2\sum_{i,j}S_{i,j}S_{i+2,j}\ , \quad (1)$$

where i,j label the Cartesian coordinates of a square lattice and $S_{i,j}=\pm 1$. Both J_1 and J_2 are positive. The ratio $\kappa=J_2/J_1$ measures the degree of competition between the ferromagnetic nearest-neighbor bonds J_1 and the antiferromagnetic next-nearest-neighbor bonds J_2 [see Fig. 1(a)]. The brickwork ANNNI model differs from the ANNNI model in that every second-nearest-neighbor bond along the vertical (j) direction is removed and every second-nearest-neighbor bond along the horizontal (i) direction is increased in magnitude [see Fig. 1(b)]. The motivation for studying the brickwork ANNNI model is that it is exactly soluble by mapping it onto a 20-vertex dimer problem.[10,13]

The ground states of the two models are the same, the ground state for $\kappa<\frac{1}{2}$ being ferromagnetic, which we label $\langle \infty \rangle$. The ground state for $\kappa>\frac{1}{2}$ is a periodically extended (in the i direction) sequence of two up and two down ferromagnetic lines of spins [lying along the j direction in (1)], and we label this $\langle 2 \rangle$. The point $\kappa=\frac{1}{2}$, $T=0$ is the multiphase point[3] (a point of infinite ground-state degeneracy).

In both models, for $\kappa\neq\frac{1}{2}$, the $\langle \infty \rangle$ and $\langle 2 \rangle$ phases persist over a range of temperatures before melting into less ordered phases. In both the ANNNI model and the brickwork ANNNI model the $\langle \infty \rangle$ phase melts directly into a lock-in fluid, a phase with exponentially and monotonically decaying pair correlations. At a still higher temperature, the lock-in fluid becomes a floating fluid. The floating-fluid phase also has exponentially decaying correlations, but now these correlations are oscillatory with a wave vector which varies continuously with temperature and κ. The line dividing the lock-in fluid and the floating fluid is called a disorder line.[14]

For $\kappa>\frac{1}{2}$ however, the two models exhibit qualitatively different behavior. The brickwork ANNNI model

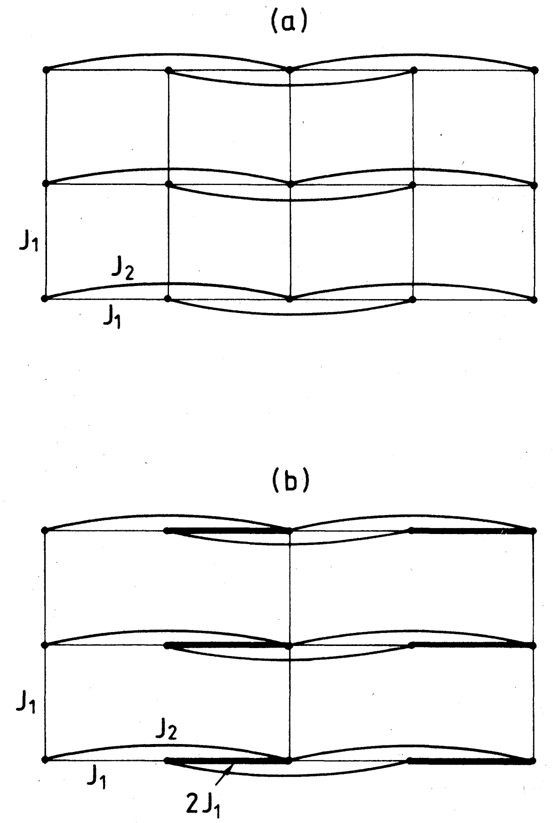

FIG. 1. Interactions in (a) the ANNNI model and (b) the brickwork ANNNI model. The nearest-neighbor couplings are ferromagnetic and the next-nearest-neighbor couplings are antiferromagnetic.

behaves in the same manner as it does for $\kappa < \frac{1}{2}$, the only difference being that the lock-in fluid phase now has wave vector $q = \frac{1}{4}$ rather than $q = 0$. In the ANNNI model however, the $\langle 2 \rangle$ phase melts into a floating-solid phase. This is a phase with algebraically decaying and oscillating pair correlations. The wave vector of the oscillations varies continuously with changes in κ and T. The floating-solid phase melts into a floating-fluid phase.

It is clear from the above discussion that two fundamental quantities occurring in the pair correlation function are the correlation length and the characteristic wave vector of the modulation. It is possible to calculate both of these quantities from the two largest eigenvalues of the transfer matrix, and then to use a scaling analysis to determine the phase boundaries.

This technique (transfer-matrix scaling, or the phenomenological renormalization group)[11] depends on the hypothesis that the correlation length of an infinite strip of finite width L will depend on L in a manner characteristic of the phase of the limiting two-dimensional system. The correlation length is expected to behave as follows: In an ordered phase it grows exponentially with L as $L \to \infty$; in a fluid phase it is asymptotically independent of L; finally, in a phase with quasi-long-range order or at a second-order critical point, it grows algebraically with L as $L \to \infty$. To study systems with floating phases we define a quantity which clearly differentiates between these behaviors,[12,15]

$$Y_L = \frac{\ln(\xi_L / \xi_{L-1})}{\ln[L/(L-1)]} . \tag{2}$$

In a fluid phase, Y_L decays exponentially to zero as $L \to \infty$. In an ordered phase, Y_L increases linearly with L as $L \to \infty$. At a critical point or in a phase with quasi-long-range order, Y_L is asymptotically independent of L as $L \to \infty$.

A similar quantity can be defined for the scaling behavior of the modulation wave vector q,[14]

$$Z_L = \frac{-\ln(\delta q_L / \delta q_{L-1})}{\ln[L/(L-1)]} . \tag{3}$$

The quantity δq_L is the deviation of q from the zero-temperature commensurate value. In an incommensurate region Z_L will decay to zero as $L \to \infty$. In a commensurate region Z_L increases with L as $L \to \infty$. In a

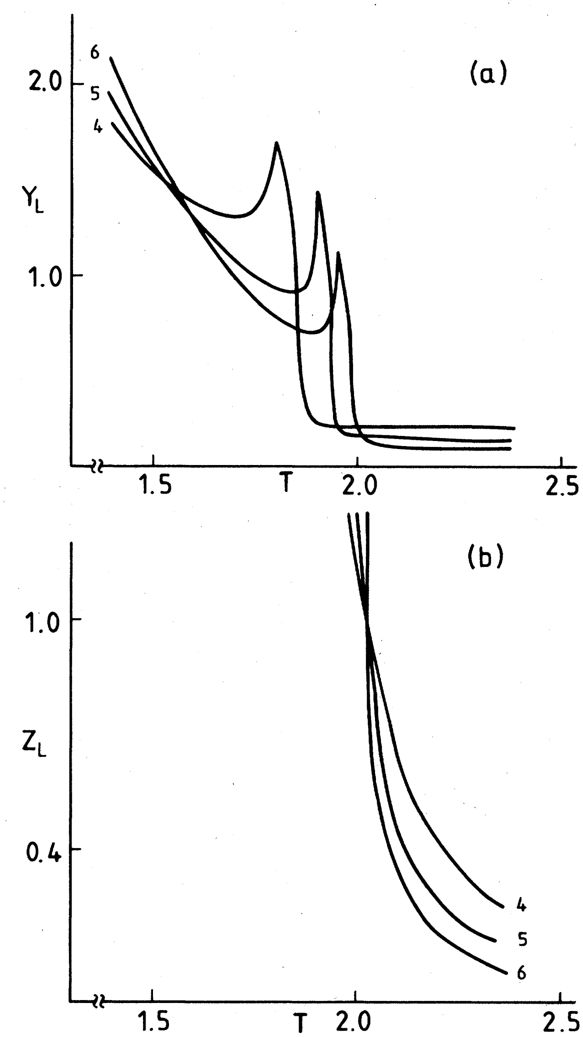

FIG. 2. Scaling functions for the ANNNI model for $\kappa = 0.25$ and $L = 4$, 5, and 6: (a) the correlation-length scaling function, Y_L [see Eq. (2)]; (b) the wave-vector scaling function, Z_L [see Eq. (3)]. T is in units of J_1/k_B in this and all subsequent figures.

commensurate-to-incommensurate transition or at a disorder line, Z_L is asymptotically independent of L as $L \to \infty$.

The quantities Y_L and Z_L also enable one to determine whether the phase transition is anisotropic or not. This is especially relevant to the commensurate-solid to incommensurate-solid transition where an anisotropic phase transition[15] has been predicted. Thus, if one does not allow for anisotropic scaling in systems with modulated phases, the floating-solid phase will not be correctly located.

The correlation length and wave vector of the finite-width strips are calculated by finding the leading eigenvalues of the transfer matrix. For the models studied here, the transfer matrix is a $4^L \times 4^L$ matrix. We use a representation of the transfer matrix as a product of L sparse matrices to reduce the size of the computations.[16] If the two largest eigenvalues of the transfer matrix are denoted by λ_1 and λ_2, then the correlation length is given by

$$\xi_L = \frac{1}{\ln(\lambda_1 / |\lambda_2|)} , \tag{4}$$

and the modulation wave vector is given by

$$q_L = \frac{1}{2\pi} \arctan \left[\frac{\mathrm{Im}(\lambda_2)}{\mathrm{Re}(\lambda_2)} \right] . \tag{5}$$

The functions Y_L and Z_L for the ANNNI model for $\kappa = 0.25$ are displayed in Fig. 2. The presence of the sharp peaks in the correlation-length function Y_L, are a consequence of the cusp in the inverse correlation length that occurs at a disorder point. This behavior in the correlation length is evident in Fig. 3, where the scaled correlation length is plotted as a function of temperatures at $\kappa = 0.25$. Returning to Fig. 2, we thus suggest that the two crossings of the function Y_L that occur because of the sharp peak are spurious and should disappear in the large-L limit. Indeed, the size of the peaks should scale to zero with large L. For finite L, the location of the peaks provides estimates of the position of the disorder point in the inifinite lattic.

Having identified the crossings in Y_L near the sharp peak as being due to finite-lattice effects, we now focus discussion on the true scaling point in the function Y_L [at $T = 1.55$ in Fig. 2(a)] and the wave vector (Z_L) scaling point in Fig. 2(b). It is evident that Z_L scales (is independent of L) at a *higher* temperature than Y_L. This indicates that the wave vector locks in to a commensurate value at a higher temperature than the thermodynamic phase boundary indicated by the correlation-length scaling. At $\kappa = 0.25$ in the ANNNI model we thus find that there exists a direct transition from the ordered $q = 0$ ferromagnetic phase to a $q = 0$ lock-in fluid phase. This transition occurs at the point where the correlation length scales. At a higher temperature the $q = 0$ lock-in fluid phase becomes a $q \neq 0$ floating-fluid phase. The disorder point is the point at which the wave vector scales. The location of the disorder point indicated by the wave vector scaling is in good agreement with that indicated by the peaks in Y_L (see Fig. 2). We have performed the same analysis for several values of κ, and a similar behavior to that discussed above was found for all $\kappa < \frac{1}{2}$.

The functions Y_L and Z_L for the ANNNI model at $\kappa = 0.60$ are presented in Fig. 4. It is evident that now Z_L scales at a *lower* temperature than Y_L. At the temperature where Y_L scales, the system undergoes a thermodynamic phase transition while the wave vector remains finite. The Y_L curves then remain approximately parallel to the T axis over a range of temperature. This behavior

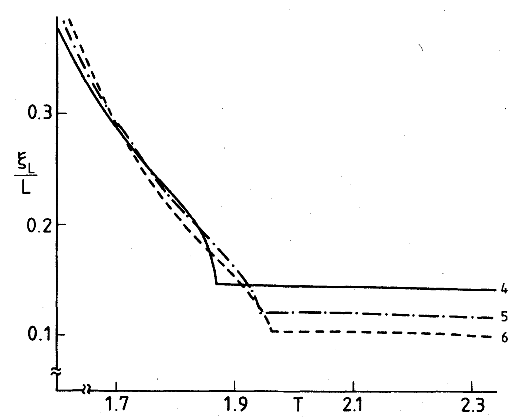

FIG. 3. Scaled correlation lengths for the ANNNI model for $\kappa = 0.25$ and $L = 4$ (solid curve), $L = 5$ (dashed-dotted curve) and $L = 6$ (dashed curve).

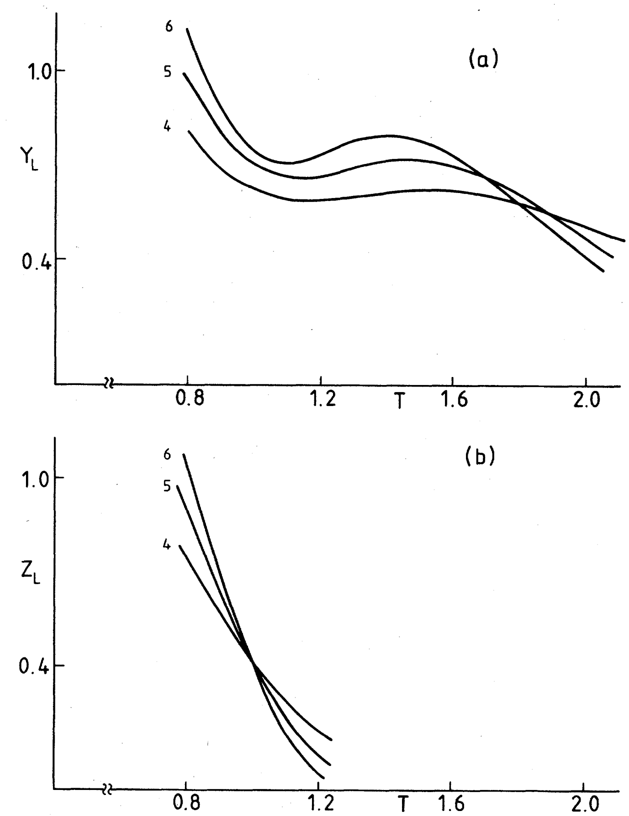

FIG. 4. Scaling functions for the ANNNI model for $\kappa = 0.60$ and $L = 4, 5, 6$: (a) the correlation length scaling function, Y_L [see Eq. (2)]; (b) the wave-vector scaling function, Z_L [see Eq. (3)].

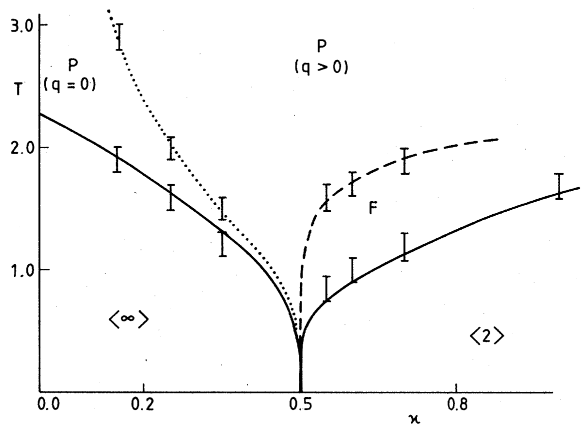

FIG. 5. Phase diagram of the ANNNI model. The symbols ⟨ ∞ ⟩ and ⟨2⟩ indicate the ordered commensurate phases. The $P(q=0)$ and $P(q>0)$ phases are fluid phases with and without modulation, respectively. The phase F is a floating-solid phase with quasi-long-range order. The error bars indicate estimates of the transition temperatures from the finite-size scaling analysis. The solid lines are the melting temperature of the commensurate phases from interface free-energy calculations (Ref. 18). The dotted and dashed lines are guides to the eye.

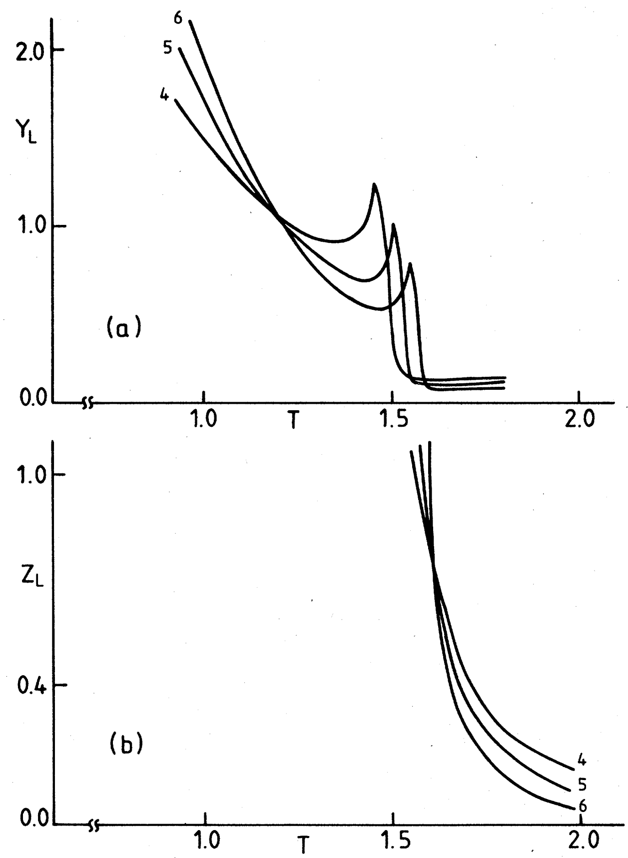

FIG. 6. Scaling functions for the brickwork ANNNI model for $\kappa=0.35$ and $L=4$, 5, and 6: (a) the correlation length scaling function, Y_L [see Eq. (2)]; (b) the wave-vector scaling function, Z_L [see Eq. (3)].

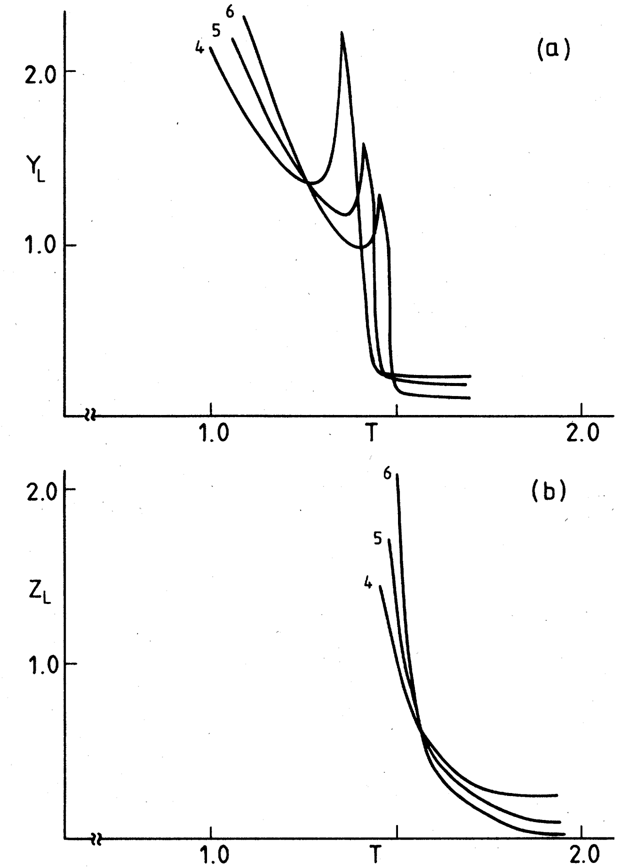

FIG. 7. The scaling functions for the brickwork ANNNI model for $\kappa=0.70$ and $L=4$, 5, and 6: (a) the correlation length scaling function, Y_L [see Eq. (2)]; (b) the wave-vector scaling function, Z_L [see Eq. (3)].

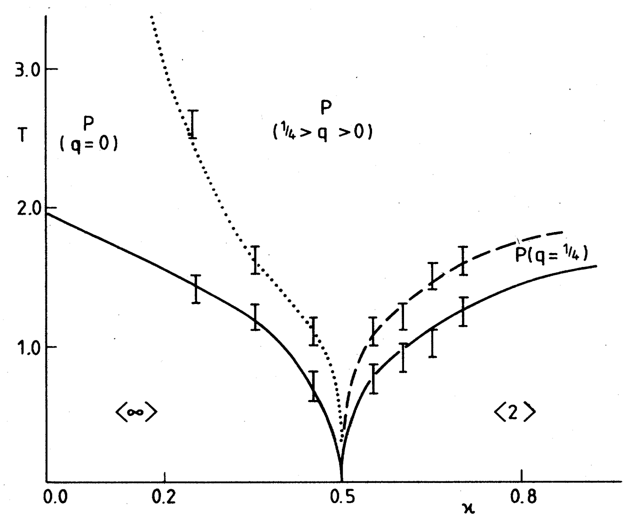

FIG. 8. The phase diagram of the brickwork ANNNI model. The three fluid phases are denoted $P(q=0)$, $P(0<q<\frac{1}{4})$, and $P(q=\frac{1}{4})$. All lines are guides to the eye.

signals the presence of a phase with quasi-long-range order. The point at which Z_L scales determines the point at which the wave vector locks in. This and the corresponding sharp increase in Y_L indicates a transition to a commensurate ordered phase. This type of behavior was found for all $\kappa > \frac{1}{2}$ in the ANNNI model.

By performing the analysis discussed in the preceding three paragraphs for a range of κ values, we arrive at the ANNNI model phase diagram given in Fig. 5, which is in good agreement with previous analytic and numerical calculations.[5–9,17,18] We now perform this analysis for the exactly soluble[10,13] brickwork ANNNI model, which is known to have no quasi-long-range-ordered phase, and which should provide a test of our method. The scaling functions Y_L and Z_L for the brickwork ANNNI model at $\kappa = 0.35$ and $\kappa = 0.70$ are shown in Figs. 6 and 7, respectively. At both of these values of κ, the correlation-length scaling function Y_L exhibits the sharp peaks indicative of a disorder point. This behavior is the same as that found in the ANNNI model for $\kappa < 0.5$ (see Fig. 3). Again there are two spurious crossings in the scaling function due to the presence of the peaks. We again concentrate on the true correlation-length scaling points and the wave-vector scaling points.

In both cases (Figs. 6 and 7), Z_L scales at a *higher* temperature than Y_L, the same behavior as found for the ANNNI model for $\kappa < \frac{1}{2}$. At no values of κ did the brickwork ANNNI model exhibit the behavior indicative of a quasi-long-range-ordered phase, and on the basis of our analysis, the phase diagram given in Fig. 8 is deduced. Note that the quasi-long-range-ordered phase which lies above the $\langle 2 \rangle$ phase in the true ANNNI model (see Fig. 4) is replaced by a $q = \frac{1}{4}$ lock-in fluid phase in the brickwork ANNNI model.

The analysis used in this work has combined wave-vector scaling with the standard correlation-length scaling to plot out the phase diagram of two ANNNI models. The combination of the two analyses has been especially useful in these models, as the correlation-length scaling along exhibits some puzzling features. First, at a disorder point, the inverse correlation length has a cusp (see Fig. 3), and this results in a sharp peak in the function Y_L (see Fig. 2), and in the occurrence of two spurious crossings in this function. Second, at the commensurate-solid to incommensurate-solid phase boundary in the ANNNI model, the function Y_L does not scale on finite lattices (see Fig. 4), and it is necessary to locate the phase boundary from the wave-vector scaling alone. These features emphasize the necessity for care in analyzing the data from numerical studies on two-dimensional systems with modulated order.

In conclusion, a finite-size-scaling analysis of the ANNNI model generates a phase diagram in excellent agreement with the combined predictions of other methods. We are able to identify clearly all of the phases present in the model by using the scaling properties of both the correlation length and the modulation wave vector. The commensurate-solid, lock-in fluid and floating-fluid and floating-solid phases all have distinctive signatures in the scaling behavior of these two quantities. In the case of the brickwork ANNNI model we find that, in agreement with previous work, no quasi-long-range-ordered phase exists in the phase diagram of the model. These results show that, in disagreement with a recent suggestion,[10] transfer-matrix scaling is a powerful method in the study of models with modulated phases.

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