BRIEF REPORTS

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Coexistence of excited states in confined Ising systems

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Using the density-matrix renormalization-group method we study the two-dimensional Ising model in an infinite strip geometry with free-boundary conditions. The renormalization scheme enables us to consider systems of width up to 300 (lattice spacings) and study the influence of the bulk magnetic field on correlation function structure for all temperatures. From our numerical results we have determined the crossover line for the correlation length related to the coexistence of the excited states. A detailed scaling study of this line is performed. Our numerical results support and further specify previous conclusions reached by Abraham, Parry, and Upton based on the bubble model of correlations.

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Understanding the statistical mechanics of classical systems in confined geometries has been a challenge for several years [1–3] with much interest concerning the behavior of fluids and simple magnets confined between parallel walls. Studies of such finite-size effects have not only been limited to the vicinity of the critical point, but have also focused on the first-order phase transition for which much less information is known [4]. In this Brief Report we consider a square-lattice two-dimensional Ising system in an infinite $L\times\infty$ strip geometry (with L the width of the strip) modeled by the Hamiltonian

$$\mathcal{H}=-J\sum_{\langle i,j\rangle}\sigma_i\sigma_j-H\sum_i\sigma_i, \tag{1}$$

where the coupling constant $J>0$, H is the bulk magnetic field, and $\sigma_i=\pm 1$. The first sum runs over all nearest-neighbor pairs while the second sum runs over all sites. Free boundary conditions are assumed, so that there are no symmetry breaking surface fields.

Below the bulk critical point this model is predicted to show an interesting crossover behavior in correlation function structure at a certain value $H_x(T;L)$ of the bulk field [4,5]. Specifically the borderline $H_x(T;L)$ separates quite distinct finite-size behaviors of the correlation length ξ. Using the approximate bubble model [6] Abraham *et al.* argued [5] that at subcritical temperatures

$$1/\xi=P(T)L|H|,\quad \text{for}\ \ 0<|H|\leqslant H_x, \tag{2}$$

$$1/\xi=R(T)+S(T)|H|^{2/3},\quad \text{for}\ \ |H|\geqslant H_x, \tag{3}$$

where $P(T)=2m/k_BT$, $R(T)=2\sigma_0/k_BT$ and $S(T)$ is an unknown positive coefficient. Here, m and σ_0 refer to the bulk spontaneous magnetization and the interfacial tension, respectively. The bubble model studies concluded that $H_x(T;L)$ scales towards the first-order line according to the form [5,7]

$$H_x(T;L)\approx A(T)L^{\alpha}+B(T)L^{\gamma}+C(T)L^{\delta}+\cdots, \tag{4}$$

where $\alpha=-1$, $\gamma=-5/3$, and $\delta=-7/3$.

This behavior is similar to the nonanalytic corrections to the Kelvin equation for the finite-size scaling of the shifted bulk coexistence field in a strip geometry with symmetry breaking surface fields which has been studied recently [8]. Using the density-matrix renormalization-group (DMRG) method [9,10] it was found that for a large range of surface fields and temperatures corrections are not compatible with the behavior predicted by the existing theory [11]. This discrepancy is one of the central motivations for our present study, since one may anticipate that the predicted nonanalytic correction terms for $H_x(T;L)$ are easier to observe because there is no length scale induced by a surface field [8].

Abraham *et al.* [5] argued that the correlation length crossover occurs because the class of dominating configura-

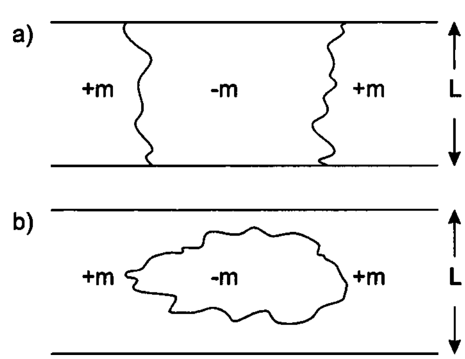

FIG. 1. The dominating configurations in strip geometry: (a) $0<|H|<H_x$, (b) $|H|>H_x$.

tions determining the behavior of correlation functions changes from a single connected loop for $|H|>H_x$ to two disconnected closed loops $|H|<H_x$ (which is allowed for both free- and periodic-boundary conditions). In our case, where the free boundaries are present, for $|H|<H_x$, the dominating configurations correspond to excitations in which the whole strip has the opposite magnetizations [12]. For $|H|>H_x$ the most important configurations between the spins contributing to the correlation function are again closed loops (domains) of opposite magnetizations (see Fig. 1).

One way of analyzing this problem beyond the bubble model approximation is to use transfer-matrix (TM) methods [13]. However, it is well known that to obtain satisfactory finite-size scaling results, one should consider large enough systems [14]. This may, in turn, complicate calculations or even make them impossible. To overcome this problem we have applied the DMRG method for two-dimensional systems based on the TM approach. It is possible to develop a very efficient algorithm for the construction of the effective transfer matrices for large L and this method has been successfully employed for a number of problems (for which no exact solutions are available; e.g., for nonvanishing bulk fields) [15–18]. Using this method we have been able to analyze the present system in the full range of temperature and bulk magnetic field for strips of widths up to $L=300$. For a comprehensive review of the background, achievements, and limitations of the DMRG method, see Ref. [19].

We first calculated the free-energy levels

$$f_i(H,T;L)=-\frac{k_BT}{L}\ln[\lambda_i(H,T;L)], \tag{5}$$

for $i=0,1,2,\ldots$, where λ_i are the eigenvalues of the TM arranged in order of decreasing magnitude. We note that because the inverse (longitudinal) correlation length can be defined as

$$1/\xi(L)=\log(\lambda_0/\lambda_1), \tag{6}$$

and the lowest free-energy level does not cross others, especially important are the values of the bulk magnetic field $H_x(T;L)$, where the first- and second-excited states cross each other. In such a case we can observe the crossover in the behavior of the correlation length.

Let us first analyze the structure of the TM low-lying levels as a function of the bulk magnetic field H at fixed T. At very low temperature they should behave essentially in the same way as the ground-state energy. Therefore, it is worthwhile considering the ground-state properties of the system. To begin we label the configuration of a row for the strip as $|\sigma_1,\sigma_2,\ldots,\sigma_{L-1},\sigma_L\rangle$, where the values of σ_i are denoted $\pm$ for simplicity. For zero magnetic field H the two states with all spins positive $|++\cdots++\rangle$ or negative $|--\cdots--\rangle$ have the same energy. The extra magnetic field term splits both states and the energy per spin is

$$\epsilon_{1,2}=-J\left(2-\frac{1}{L}\right)\pm H. \tag{7}$$

Assuming $H>0$ the $|++\cdots++\rangle$ state is always the singlet ground state. In order to find the first-excited states we have to flip the first or the last column ($i=1,L$) in the previous configurations. In this way we get the four states $|-+\cdots++\rangle$, $|++\cdots+-\rangle$, $|+-\cdots--\rangle$, and $|--\cdots-+\rangle$. The magnetic field splits this level into two doublets and for the two first states their energy decreases when the H increases according to the equation

$$\epsilon_{3,4}=-J\left(2-\frac{3}{L}\right)-H\left(1-\frac{2}{L}\right). \tag{8}$$

Therefore, we expect the crossing of the singlet state $|--\cdots--\rangle$ with the doublet $|-+\cdots++\rangle$, $|++\cdots+-\rangle$ at a value of the bulk magnetic field given by

$$H_x(T=0;L)=\frac{J}{L-1}. \tag{9}$$

Note that for $T\to 0$, Eq. (4) reduces to Eq. (9) provided $A(T)\to J$ and $B(T),C(T)\to 0$.

At finite temperatures we do not have any real crossing points but, instead, so-called ''regions of avoided level crossing.'' At $H=0$ the first two levels are separated according to $f_1-f_0\sim\exp(-\sigma_0L/k_BT)$, so they are asymptotically degenerate for $L\to\infty$. The region of avoided level crossing continues for nonzero magnetic fields up to $|H|\sim\exp(-\sigma_0L/k_BT)$. In order to determine the behavior of ξ, we have to consider the second and third eigenvalues of the transfer matrix [4,5], where asymptotic degeneracy is also present for f_1 and f_2 [20]. It is assumed that the difference f_2-f_1 and the avoided level crossing region centered on H_x are of order $\exp(-CL)$, where the coefficient C may be H and T dependent. Given this it is still sensible to discuss the algebraic shift of the value $H_x(T;L)$ for $L\to\infty$. In order to find out the value of H_x in finite temperatures at fixed L, we identify H_x with the value of the bulk magnetic field where the second free-energy level f_1 has a maximum and the separation f_2-f_1 is minimal. The curves $H_x(T;L)$ represent the

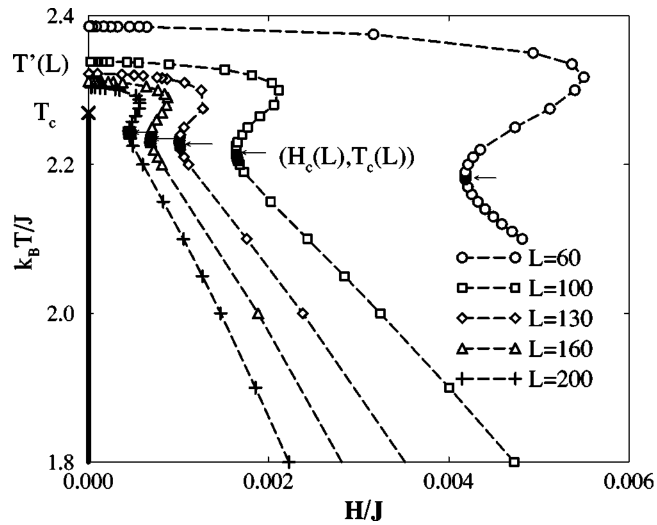

FIG. 2. The lines of coexistence of the excited states for different strip width L. Here T_c is the bulk critical point and the thick solid line denotes the bulk first-order line phase boundary. The arrows point at the inflection points where $H_x(T;L)$ has a local minimum as a function of the temperature. $T'(L)$ describes the point where $H_x(T;L)$ ends on the $H=0$ axis. The dashed lines are used as guides for the eye.

TABLE I. Scaling exponents for $H_x(T;L)$ as extrapolated from the DMRG data.

T	α	$\gamma+1$	$\delta+5/3$
1.00	$-0.9994(5)$	$-0.668(1)$	$-0.66(4)$
1.50	$-0.9990(5)$	$-0.667(1)$	$-0.64(1)$
1.75	$-1.000(1)$	$-0.668(2)$	$-0.64(1)$
2.00	$-0.998(1)$	$-0.667(1)$	$-0.67(1)$
2.15	$-1.028(3)$	$-0.67(1)$	$-0.67(2)$
2.20	$-1.002(6)$	$-0.69(1)$	$-0.68(3)$

coexistence of the excited states and are shown in Fig. 2. As $L\rightarrow\infty$ the coexistence lines of the excited states shift towards the $H=0$ axis, which is intuitively clear at $T=0$. To see this, note that as the width of the strip increases the energy of configurations, in which only one column of spins is flipped, decreases and approaches the energy of configurations with all spins pointed in one direction. Thus in the $L\rightarrow\infty$ limit one necessarily has $H_x=0$.

We now turn to the scaling of the coexistence line $H_x(T;L)$ close to the bulk first-order line (Fig. 2). To verify the bubble model predictions [Eq. (4)] we have tabulated the values of $H_x(T=\text{const};L)$ for $L=20,40,\ldots,200$ and for temperatures ranging from $T\approx0.44T_c$ up to $T\approx0.99T_c$.

Table I shows the values of scaling exponents obtained from the DMRG data. Using the powerful extrapolation technique of Bulirsch and Stoer (BST) [21], we have obtained excellent agreement with the predictions of Abraham *et al.* [5].

In order to get the coefficient A in Eq. (4) one can compare Eqs. (2) and (3). They have to agree at the value $H=H_x$ in the thermodynamic limit, which implies the following relation [7]:

$$A(T)=\sigma_0(T)/m(T). \tag{10}$$

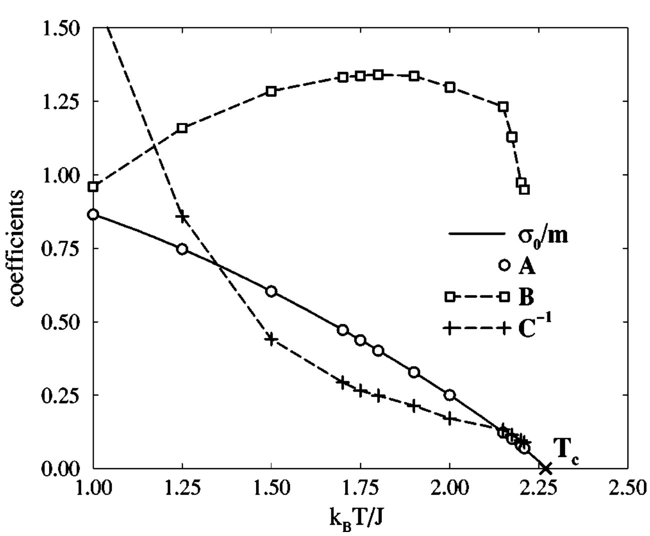

FIG. 3. Coefficients appearing in the scaling of the coexistence line $H_x(L;T)$ close to the bulk first-order phase boundary. The solid line denotes the analytical result determined in the bubble model. The symbols describe our numerical results. The dashed lines are guides for the eye.

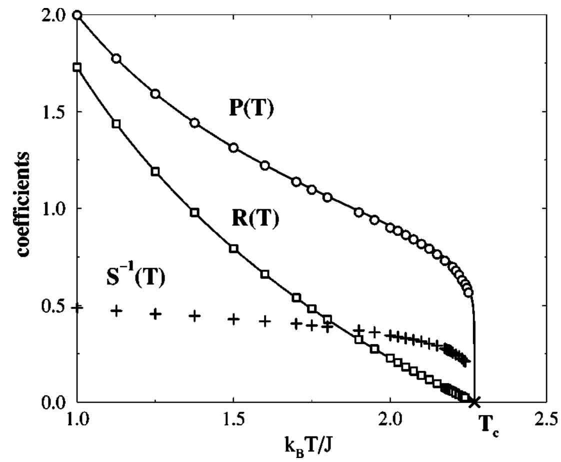

FIG. 4. The coefficients of the correlation length in Eqs. (2) and (3). Solid lines denote the bubble model results: $P(T)=2m/k_BT$ and $R(T)=2\sigma_0/k_BT$. The symbols describe the corresponding DMRG results.

In Fig. 3 our data match this curve very well. To the best of our knowledge, the coefficients $B(T)$ and $C(T)$ in Eq. (4) have not been yet determined, but our numerical results can predict their temperature behavior.

Close to T_c the validity of Eq. (4) is limited because the scaling of points on the H_x curve is governed by the bulk critical region. In order to study it in detail we have considered characteristic points of the upper part of the H_x curve: the inflection points $(H_c(L),\ T_c(L))$ and the end points $T'(L)$ (see Fig. 2), where the following scaling is expected:

$$\tau_c(L)=[T_c-T_c(L)]/T_c\sim L^{-y_T},$$

$$H_c(L)\sim L^{-y_H}. \tag{11}$$

Here, $y_T=1$ and $y_H=15/8$ are the thermal and magnetic exponents of the two-dimensional Ising model.

To verify the scaling to the critical point $(H=0,\tau=0)$ we determined the inflection points and the end points for $L=30$, 60, 100, 130, 160, and 200 using the BST technique. We have examined the scaling form (11) for $L\rightarrow\infty$ and found very good agreement. For example, we find

$$\tau_c=0.00006(6) \quad \text{and} \quad y_T=1.005(5),$$

$$H_c=-0.0006(6) \quad \text{and} \quad y_H=1.876(8),$$

$$\tau'=0.0000(3) \quad \text{and} \quad y_T=1.006(6).$$

Note that for $T\rightarrow T_c$ and $L\rightarrow\infty$ we can reproduce the scaling form (11) from Eq. (4) by assuming that $A(T)\rightarrow0$, $B(T)\rightarrow0$, and $C(T)\rightarrow\infty$. This is in agreement with our numerical estimations for scaling coefficients as depicted in Fig. 3. Of course, this relation is not valid at T_c.

In order to analyze the behavior of the correlation length we have determined $1/\xi$ for L between 100 and 300 for temperatures below $T_c(L)$. To examine the form of Eq. (2) first we have confirmed the linear dependence of the coefficient on L. Next we compared our numerical results with the coefficients $P(T)$ and $R(T)$ in Eqs. (2) and (3). Furthermore, we can also calculate the temperature dependence of the $S(T)$ coefficient which was not determined in the bubble model (see Fig. 4).

As the temperature increases, more and more complex configurations on the Ising strip contribute to the free energy in contrast to the assumption of the bubble model [5]. Consequently, for high temperatures the validity of Eqs. (2) and (3) is limited to a very narrow range of magnetic fields. The bubble model predictions are also invalid for very strong bulk magnetic fields. This is why, for higher temperatures, a smaller value of H is necessary to recover the linear dependence of $1/\xi$ on H, as in Eq. (2). Similarly, when $T \to T_c(L)$ the regime with the $H^{2/3}$ dependence of $1/\xi$ [Eq. (3)], close to the right side of the coexistence line, shrinks to zero.

In conclusion, we have used the density-matrix renormalization-group method to obtain reliable information about the two-dimensional Ising model in nonzero bulk magnetic field. We have confirmed the crossover behavior predicted for the correlation length on the basis of the bubble model [5]. In contrast to the bubble model, however, our study has not been limited to subcritical temperatures and small bulk fields. We have confirmed the predictions of Abraham *et al.* [5] for the scaling of the first-order line in the subcritical region. Moreover, we have established the precise scaling form for the bulk magnetic field by numerically determining the coefficients $B(T)$ and $C(T)$ in Eq. (4). Furthermore, we have extended the analysis of the bubble model to *the critical region*, verifying that the scaling behavior is governed by the bulk critical point. Finally, we have numerically confirmed the magnetic field dependence of the correlation length, simultaneously extracting the temperature dependence of the previously unknown coefficient $S(T)$ appearing in Eq. (3). The above results again demonstrate that for two-dimensional classical systems the DMRG technique provides a highly reliable accurate method for studying the equilibrium properties of large systems in a *nonvanishing* bulk magnetic field.

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