Square-lattice-gas model with repulsive nearest- and next-nearest-neighbor interactions

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The square-lattice gas with several ratios (R) of next-nearest-neighbor coupling to nearest-neighbor coupling is studied by finite-size scaling using transfer-matrix methods. Results are obtained for the phase diagram and critical exponents for the 2×1 and 2×2 order-disorder transitions, for the case $R=1$. While the correlation length exponent ν seems to be nonuniversal, weak universality appears to hold for the (2×2) transition and possibly for the 2×1 transition. Reentrant behavior is observed for the 2×1 transition line but appears to decrease with increasing strip width. The variation of the 2×1 transition line with different values of R $(R=1,\ 2,\ 5,\ \infty)$ is also studied.

INTRODUCTION

Recently, various two-dimensional lattice gas models have been the subject of intensive theoretical studies. These models are of interest as models of chemi- and physisorbed systems, as well as displaying a rich variety of phase transitions and critical phenomena. One such model which has received considerable attention is the simple square-lattice model with competing nearest-neighbor and next-nearest-neighbor repulsive interactions. This model is of particular interest for the case $R>0.5$ (where R is the ratio of the next-nearest-neighbor coupling J_2 to the nearest-neighbor coupling J_1). For these values of R, this model exhibits two phases, namely, the (2×1) and (2×2) ordered structures.[1,2] The order-disorder transitions for these phases are thought to belong to the universality class of the X-Y model with cubic anisotropy.[3] As such, they should exhibit variable (nonuniversal) critical exponents.

This model has recently been studied with use of a number of different techniques, including Monte Carlo simulations,[1] transfer-matrix finite-size scaling,[2] and the interfacial free-energy method,[4] with somewhat different results. The Monte Carlo simulations $(R=1)$ gave a good overall estimate of the phase diagram, but missed the disordered region between the (2×1) and (2×2) ordered phases. In addition, the critical exponents were calculated in a small region of the (2×1) transition line, and it was found that the exponents did indeed vary slightly both with R and external magnetic field H. However, the reduced critical exponents $[\hat{\gamma}=\gamma/\nu,\ \hat{\beta}=\beta/\nu,\ \text{and}\ \hat{\phi}=(2-\alpha)/\nu]$ were found to be virtually indistinguishable from the $R=0$ (Ising) values. Thus, in this study, Suzuki's weak universality[5] was held to be valid, at least for the region of the phase diagram which was studied.

In a later transfer-matrix study[2] an entire phase diagram was calculated for the $R=1$ case. A disordered region between the (2×1) and (2×2) ordered phases was found and, somewhat surprisingly, reentrant behavior was found for the (2×1) transition line. It was not clear whether this reentrant behavior was due to finite-size effects or whether it was a genuine property of the model. Also, no estimates of the critical exponents were given.

In a more recent study by Slotte[6] the interfacial free-energy technique[4] was used to study the phase diagram for all values of R. In this study, the (2×1) transition line was found to be independent of R, for $R>0.669$ (with temperature and field scaled in units of J_2, the next-nearest-neighbor interaction). In addition, this transition line did not exhibit reentrant behavior. Also, an estimate was given for the critical value of the chemical potential at a second-order phase transition of the hard-square-lattice gas, which was considerably higher than the currently accepted value.[7]

In light of the previous results it was found useful to conduct a more detailed study, both of the exponents and of the phase diagram, with use of transfer-matrix scaling. Our results, which we discuss in more detail below, are as follows. We find that the correlation length critical exponent ν varies throughout the phase diagram and is nonuniversal. Our results for the correlation function exponent η (based on the Derrida-deSeze conjecture) indicate that weak universality holds for the (2×2) transition line, and that it may possibly hold for the (2×1) transition as well. We find that the (2×1) transition line varies as R is varied $(R>0.669)$ in contrast to the results of Slotte. (This is particularly evident in comparing the critical temperature at $H=0$ for the $R=1$ case with that for the $R=\infty$ case.) Finally, we find that the reentrant behavior of the (2×1) transition line tends to decrease with increasing strip width.

METHOD AND RESULTS

The well-known transfer-matrix scaling technique[8–11] involves studying the scaling properties of the correlation length for semi-infinite strips of width N for different values of N. The ratio of the largest eigenvalue λ_0 to the next-largest eigenvalue (in magnitude) λ_1 of the transfer matrix gives the correlation length

$$\xi^{-1}=\ln\left(\frac{\lambda_0}{|\lambda_1|}\right) . \quad (1)$$

From (1) one obtains the correlation length $\xi(T,\ 1/N)$ as a function of temperature T and strip width N. In the limit $N\rightarrow\infty$ one assumes the scaling behavior $\xi(t,1/N)=b\,\xi(b^{y_t}t,b/N)$, where $t=(|T-T_c|)/T_c$, and T_c is the critical temperature. From this one obtains, at the critical temperature,

$$\xi_N/N=\xi_{N'}/N' . \quad (2)$$

Similarly, one has for the thermal exponent y_r ($=1/\nu$)

$$y_T=\ln\left(\frac{\partial\xi_N/\partial t}{\partial\xi_{N'}/\partial t}\right)\left[\ln\left(\frac{N}{N'}\right)\right]^{-1}-1 \ . \tag{3}$$

To obtain the critical exponent η we have used the following relation conjectured by Derrida and deSeze[12]:

$$\eta=N/\pi\xi_N \text{ (at } T_c) \ . \tag{4}$$

This relation has been shown to hold for the Ising and X-Y models and it is believed to hold for several isotropic systems in two dimensions.[12]

Since for a strip of width N, the transfer matrix has dimensions $2^N\times2^N$, we found it necessary in our study to use an additional technique for reducing the size of the transfer matrix. This consisted essentially of using the translational symmetry of the finite strip to block diagonalize the matrix into N different blocks, each corresponding to a different symmetry class.[13] This permitted a reduction of the dimension of the matrix to approximately $2^N/N$ and thus a $1/N^2$ reduction in computer storage space.

In Fig. 1 we show our finite-size scaling results for $R=1$ as obtained from Eq. (2) for (6-8) [where, for example, (6-8) denotes $(N=6,\ N'=8)$] and (10-12) scalings. The differences between these two scaling results for the (2×1) transition line are small for $0<H/J_1<3.5$, suggesting that finite-size effects are small in this region. In the region $H/J_1>3.5$, reentrant behavior is observed, in contrast to Slotte's results, which show no reentrant behavior. However, the temperature at which the reentrant behavior begins decreases by 11% as one goes from the (6-8) scaling results to the (10-12) results. At the same time, the width (in field) of the reentrant region is reduced by approximately 20%. Thus, although reentrant behavior is observed, it appears to be decreasing with increasing strip width. [A similar but smaller decrease in reentrant behavior was also seen when comparing (4-6) scaling results with (6-8) results.] We note that, with the exception of the reentrant portion of the (2×1) transition line, the finite-size effects seem to be larger for the (2×2) transition line.

Figure 2(a) shows the behavior of the exponent y_T for $R=1$ as a function of the field H/J_1 for (6-8) and (10-12) scalings. A smooth variation is observed for both scalings, along the (2×1) and (2×2) transition lines. This is in agreement with the prediction of nonuniversal, variable exponents for these transitions.[3] However, it is clear that there are still strong finite-size effects in the region near $H/J_1=4$. This is further indicated by the appearance of nonphysical negative values for y_T (not show in figure) in the lower half of the (2×1) reentrant region. We note, however, that the temperature at which negative values for y_T are obtained is smaller for (10-12) scaling than for (6-8) scaling. Thus it would appear that the nonphysical negative values of y_T disappear with increasing strip width.

Figure 2(b) shows the behavior of the quantity $N/\pi\xi_N$, which we are using as an estimate for η, as a function of field for both scalings. While some variation in our calculated value of η is observed for the (2×1) part of the phase diagram, we observe that in the (2×2) transition region [(10-12) scaling] η is virtually constant. Thus we may conclude that in the (2×2) region, Suzuki's weak universality holds, while in the (2×1) region it appears to hold up to $H/J_1=3$ and may possibly hold for the entire phase diagram. This is in agreement with the suggestion made by Binder and Landau.[1] We note that our value $\eta=0.23\pm0.02$ for the nonreentrant portion of the (2×1) transition line is somewhat below the Ising value of 0.25 and significantly below the previously estimated value $\eta=0.29\pm0.15$.[1] In addition, we note that our result $\eta\approx0.025$ for the (2×2) transition line (for which there was no previous estimate) is extremely small.

In order to study the behavior of the (2×1) transition line as a function of R, we have plotted, in Fig. 3, the phase diagram for four different values of R. We note that there is a significant variation in the (2×1) transition line for different values of R, not only in the region near $H/J_2=4$, but in the low-field region as well. In particular, at $H=0$, we note that the transition temperature (k_BT_c/J_2) increases

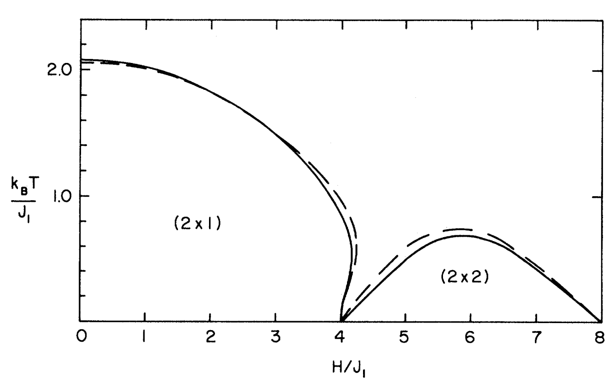

FIG. 1. Phase diagram for the $R=1$ case. The dashed line indicates (6-8) scaling; solid line refers to (10-12) scaling. The reentrant region is that portion of the (2×1) transition line for which $H/J_1>4$.

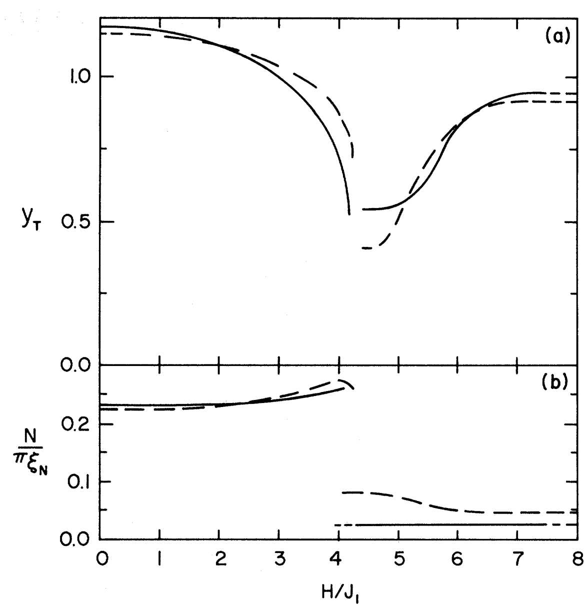

FIG. 2. Exponents y_T and η $(R=1)$. Dashed line indicates (6-8) scaling results. Solid line indicates (10-12) scaling. The exponent η is given by $N/\pi\xi_N$ (at T_c) if the Derrida-deSeze conjecture holds.

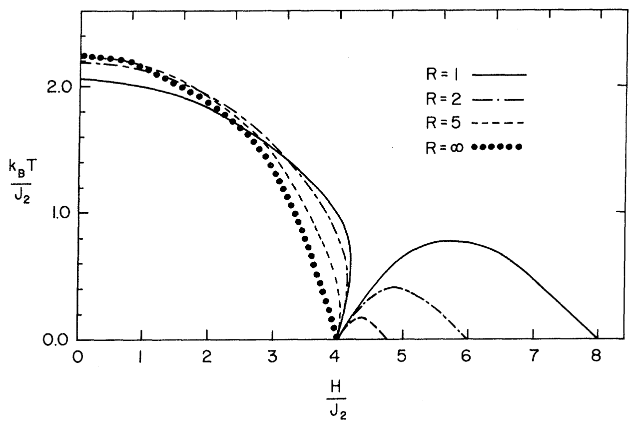

FIG. 3. Phase diagram for four different values of R [(4-6) scaling].

monotonically [for (4-6) scaling], from a value of 2.05 for the $R = 1$ case to a value of 2.26 (close to the Ising value) for the $R = \infty$ (antiferromagnet) curve. This is in contrast to the R-independent behavior (for $R > 0.669$) found via the interfacial free-energy method. As a further test of the correct transition temperature at $H = 0$ for the $R = 1$ case, we have performed a scaling analysis for T_c. Using the results from (4-6), (6-8), and (10-12) scalings, and the Binder-Landau Monte Carlo results, we estimate the ($N = \infty$) value for T_c to be 2.11 ±0.02. This is clearly below the Ising value (2.269) obtained by Slotte.[6] Thus we find clear evidence that the transition temperature at $H = 0$ varies, i.e., increases monotonically as R is increased.

Finally, we have measured the zero-temperature slope at high field of the (2×2) transition line, which may be used to obtain an estimate of the critical chemical potential $(\mu/k_B T_c)_c$ for the hard-square-lattice gas with first- and second-neighbor exclusion.[7,14,15] This is given[6] as

$$\left(\frac{\mu}{k_B T_c}\right)_c = -2\left(\frac{\partial Hc}{\partial(k_B T)}\right)_{T=0} .$$

From this we have obtained a value of 4.70 for the critical chemical potential. This is within 4% of the value (4.91) obtained by Slotte.[7,14,15]

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