Transfer-matrix approach to estimating coverage discontinuities and multicritical-point positions in two-dimensional lattice-gas phase diagrams

N. C. Bartelt, T. L. Einstein, and L. D. Roelofs*
Department of Physics and Astronomy, University of Maryland, College Park, Maryland 20742
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We present a method of computing coverage discontinuities in two-dimensional lattice-gas phase diagrams using transfer matrices. By applying the method to Baxter's generalized hard-square model, we find good agreement with exact results. This method also can be used to estimate the position of multicritical points, and we again find good agreement with exact results and with previous work on the Ising metamagnet. We discuss the transfer-matrix eigenvalue spectrum around an Ising tricritical point and verify the prediction of conformal invariance that the finite-size scaling behavior of each of the leading eigenvalues is governed by a different critical exponent at the critical point. We show numerically that the finite-size convergence of the free energy at the (Ising-like) tricritical point of Baxter's model is consistent with a conformal anomaly of $\frac{7}{10}$. We show that the justification of a commonly used method to locate multicritical points using simultaneous scaling of the correlation length and the "persistence length" is misleading. Finally we suggest a method of estimating the position of multicritical points using information from only one strip width.

I. INTRODUCTION

Systems of atoms chemisorbed on single-crystal surfaces can be modeled as two-dimensional lattice gases. To compare models with experiment, temperature-coverage phase diagrams for the lattice gases must be computed. Phase diagrams for systems with attractive interactions usually have a low-temperature line of coexistence between dense and dilute phases which terminates at higher temperatures at a critical or multicritical point. Estimation of the coverage discontinuity[1-3] along the coexistence line and the location of the multicritical point[1-11] have been the subject of several recent studies. In this paper we demonstrate a different approach which appears to yield accurate results and to be simple to apply. Essentially, we extrapolate finite-size estimates of the appropriate "Onsager-Yang" magnetization, applying a method proposed by Hamer.[12] We locate the multicritical point directly by finding the temperature at which the discontinuity vanishes, in contrast to other methods[2,4,6-8,11] which look for the divergence of appropriate correlation lengths. An advantage of the method presented here is that from a single approach the entire temperature-coverage phase diagram can be computed.

The model we use to demonstrate the technique is the square lattice gas with nearest-neighbor repulsions and second-neighbor attractions. The Hamiltonian in the grand-canonical ensemble is

$$\mathscr{H}=-\mu\sum_i n_i+E_1\sum_{\langle ij\rangle_1} n_i n_j+E_2\sum_{\langle ij\rangle_2} n_i n_j \ . \tag{1}$$

The occupancy (0 or 1) of the ith site is n_i. The chemical potential μ determines the coverage. The sums over $\langle ij\rangle_n$ are sums over sites i and j which are nth nearest neighbors. Here we consider two specific cases with $E_2<0$: E_1 infinitely repulsive (interacting hard squares) and $E_2/E_1=-\frac{1}{2}$. In both cases there is a high-density $c(2\times2)$ ordered phase which coexists at low temperatures with a dilute disordered phase. The $c(2\times2)$ phase persists to higher temperatures than the coexistence line, which terminates at a tricritical point. In the first case, as Huse has pointed out,[13] the tricritical point, tricritical exponents, and the line of first-order transitions is known exactly from the work of Baxter.[14,15] This allows us to determine the accuracy of our approximation. As the second case has been studied with other techniques,[1,2,5,7,10] we can also make comparisons.

II. METHOD

First we discuss the problem of finding coverage discontinuities in the transfer-matrix formalism. The transfer matrix we consider is that between rows of a square lattice with N rows and M columns with periodic boundary conditions. Figure 1 shows the μ dependence of the three largest eigenvalues of the transfer matrix of the interacting hard-square system for $M=6$ at a temperature 10% below the tricritical temperature. The eigenvalues denoted by λ_{1+} and λ_{2+} have eigenvectors which are even under cyclic permutations of the columns of the lattice; λ_{1-} has an eigenvector which is odd under cyclic permutation. In the limit $N\to\infty$, M finite, only λ_{1+} contributes to the coverage:

$$\rho=\frac{kT}{M}\frac{\partial\ln\lambda_{1+}}{\partial\mu}=\langle 1+|\hat{\rho}|1+\rangle \ . \tag{2}$$

The density operator $\hat{\rho}$ is defined by

$$\hat{\rho}=\sum_i |i\rangle M^{-1}\sum_{k=1}^{M}(n_k)_i\langle i| \ , \tag{3}$$

where $(n_k)_i$ is the occupancy of the kth column of a row in state i. As M becomes large, a discontinuity in the

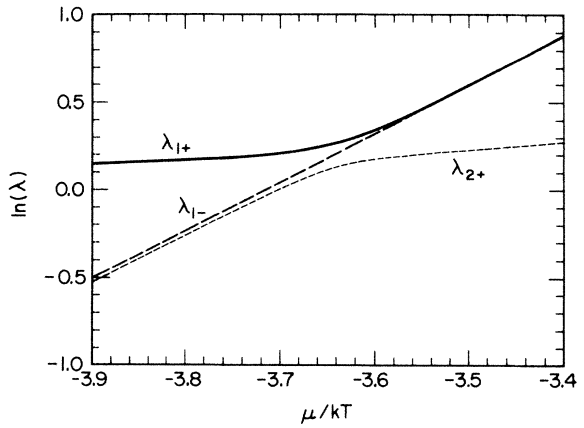

FIG. 1. Dependence of the largest eigenvalues of the transfer matrix of the interacting-hard-square problem on μ for $M=6$ and $T=0.9T_t$.

slope of the largest eigenvalue develops as the two largest even eigenvalues become degenerate: In the infinite-system limit the two largest even eigenvalues cross. Our problem is to estimate this discontinuity from results for finite M. Applying degenerate perturbation theory to the $M\rightarrow\infty$ limit, one finds that the two slopes, and thus the limits of the coverage discontinuity, are given by the solutions of

$$\begin{vmatrix} \langle a|\hat{\rho}|a\rangle-\rho & \langle a|\hat{\rho}|b\rangle \\ \langle b|\hat{\rho}|a\rangle & \langle b|\hat{\rho}|b\rangle-\rho \end{vmatrix}=0 , \tag{4}$$

where $|a\rangle$ and $|b\rangle$ are two even independent eigenvectors associated with the degenerate largest eigenvalue. The largest odd eigenvalue also becomes degenerate with the first even two. As the eigenvector of this eigenvalue is orthogonal to the even ones, it does not affect Eq. (4). The role of this eigenvalue will be discussed further below. The essential observation[12] is that the finite-size estimates of the matrix elements in Eq. (4) allow estimates of the coverage discontinuities to be made. Finite-size scaling at first-order transitions is discussed in detail by Privman and Fisher.[16] They consider the case of two coexisting phases and argue that the rounding of the discontinuity occurs for fields (chemical potentials) of the order $e^{-\sigma M/kT}$, where σ is the free energy per unit length of an interface between the two phases. In this problem we have three coexisting phases (two ordered and one disordered)—our coexistence line is a line of triple points—and two distinct interface free energies. Interfaces between ordered phases do not, however, significantly affect the coverage, so we expect the finite-size rounding of the transition in μ to be governed by the interface free energy between the disordered and ordered phases. At low temperatures the rounding is small, and accurate estimates of the coverage discontinuity can be made by inspection of the isotherms.[1,2] This cannot be done near the tricritical point. Figure 2 shows the dependence of $\langle 1+|\hat{\rho}|1+\rangle$, $\langle 1+|\hat{\rho}|2+\rangle$, $\langle 2+|\hat{\rho}|2+\rangle$, and $\langle 1-|\hat{\rho}|1-\rangle$. To estimate the triple-point chemical potential $\mu_{\rm TP}$, we find the chemical potential where $\langle 1+|\hat{\rho}|1+\rangle=\langle 2+|\hat{\rho}|2+\rangle$. As examination of Fig. 1 makes clear, this can only occur in the finite-size rounded region, and thus from the arguments above this method yields estimates $\mu_{\rm TP}(M)$, which approach $\mu_{\rm TP}$ exponentially in M. Making the identification $|1+\rangle=|a\rangle$ and $|2+\rangle=|b\rangle$, with the eigenvectors evaluated at $\mu_{\rm TP}(M)$, yields

$$\rho_{\pm}=\langle 1+|\hat{\rho}|1+\rangle\pm\langle 1+|\hat{\rho}|2+\rangle . \tag{5}$$

The μ dependence of $\langle 1+|\hat{\rho}|2+\rangle$ is shown in Fig. 2. It peaks at $\mu_{\rm TP}$ because it is proportional to the (reduced) compressibility κ: From perturbation theory,

$$\kappa=\frac{\partial\rho}{\partial\mu}\propto\sum_n\frac{|\langle 1+|\hat{\rho}|n+\rangle|^2}{\lambda_{1+}-\lambda_{n+}}\approx\frac{|\langle 1+|\hat{\rho}|2+\rangle|^2}{\lambda_{1+}-\lambda_{2+}} . \tag{6}$$

Since we expect the compressibility not to diverge as $\mu\rightarrow\mu_{\rm TP}$ ($\lambda_{1+}\rightarrow\lambda_{2+}$) in the large-$M$ limit, $\langle 1+|\hat{\rho}|2+\rangle$ must be peaked at $\mu_{\rm TP}$ with a width exponentially small in M. By comparing Figs. 2(a) ($M=6$) and 2(b) ($M=10$), this size dependence of the matrix elements can be qualitatively seen.

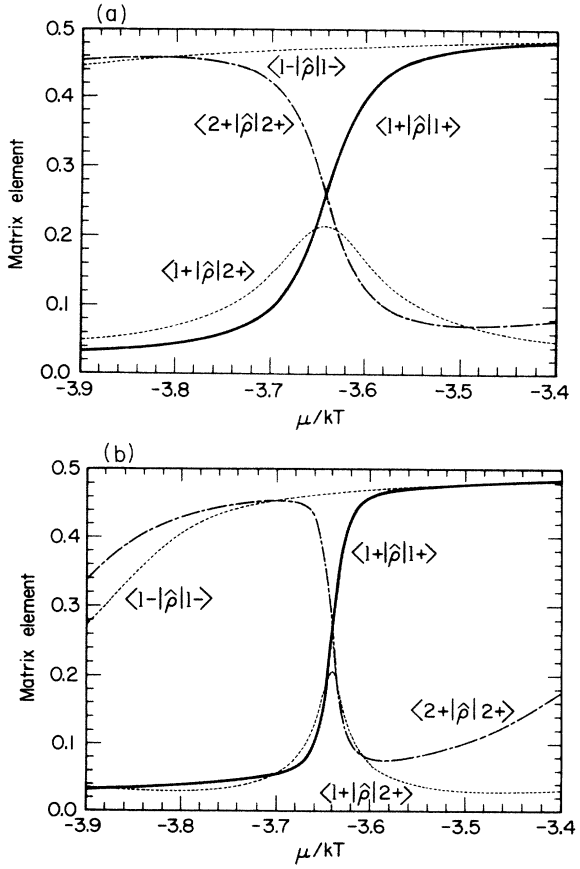

FIG. 2. μ dependence of the matrix elements for the interacting-hard-square problem at $T=0.9T_t$: (a) $M=6$ and (b) $M=10$.

III. RESULTS

Our procedure for computing the coverage gap was to find the values of $\langle 1+|\hat{\rho}|2+\rangle$ and $\langle 1+|\hat{\rho}|1+\rangle$ when $\langle 1+|\hat{\rho}|1+\rangle$ equaled $\langle 2+|\hat{\rho}|2+\rangle$ for three different strip widths and then to extrapolate each to the infinite-system limit by fitting to the form $b+aM^{-x}$. A justification of this extrapolation will be given below. The 12-14-16 estimate of the interacting-hard-square system's T-ρ phase diagram is shown in Fig. 3. The matrix element $\langle 1+|\hat{\rho}|2+\rangle$ extrapolates to zero at $0.999\,85\,T_t$, where T_t is the exact value of the tricritical temperature,

$$E_2/\ln[(3-\sqrt{5})/4]\simeq 0.604\,02\,|E_2|$$

from Baxter's exact results. Except for values very close to T_t, the low-density side of the coverage gap of Baxter's result is reproduced. Baxter does not compute (at least explicitly) the high-density side. The estimates of ρ_t as 0.276 55 and $(\mu/kT)_t$ as -3.2543 are also close to the exact results $\rho_t=(5-\sqrt{5})/10=0.276\,39\ldots$ and $(\mu/kT)_t=-3.2538\ldots$. These estimates of the critical parameters are at least 2 orders of magnitude more accurate than the results from recent low-temperature-series expansions.[3,9] Above the tricritical temperature we estimated μ_c for each temperature as the μ where the maximum in $\langle 1+|\hat{\rho}|2+\rangle$ occurred. This method works because the compressibility [Eq. (6)] diverges along the critical line above T_t. At $1.2T_t$, this estimate of the critical line reproduced the results obtained by the standard method of scaling the leading correlation length. Similar results were obtained by estimating μ_c as the point where $\langle 1+|\hat{\rho}|1+\rangle-\langle 2+|\hat{\rho}|2+\rangle$ extrapolated to zero.

We applied the same procedure for the case $E_2=-E_1/2$. Measuring temperature in units of $|E_2|$, the T-ρ phase diagram is virtually indistinguishable from that of the interacting-hard-square phase diagram in Fig. 3. The 6-8-10 estimate of the tricritical temperature is $0.601\,23\,|E_2|$, very close to the value quoted above for the interacting-hard-square model. (The temperature of the tricritical point is insensitive to E_1: It appears to vary monotonically from the hard-square limit of $T_t\simeq 0.60\,|E_2|$ to $|E_2|/2\ln(1+\sqrt{2})\simeq 0.57\,|E_2|$ at $E_1=0$, when the two tricritical points merge at a "critical point of fourth order."[17] This is perhaps not surprising as E_2 is responsible for the existence of the coexistence line and thus sets the energy scale for its termination.) The estimates of $(\mu/kT)_t$ and ρ_t were $-1.9659\,|E_2|$ and 0.276 79, respectively. At low temperatures the coverage gap is consistent with Monte Carlo calculations[1] and with previous transfer-matrix estimates.[2] The estimate of the tricritical point is within the smaller error bars of the estimates from the correlation-length scaling of Ref. 2 (using the same strip widths).

Figure 4 shows the odd and even eigenvalue spectrum for $M=6$ at a temperature half of T_t. It strongly suggests that the second and third eigenvalues are degenerate in the infinite-system limit for chemical potentials smaller than the chemical potential of the triple point. Thus the second eigenvalue is parallel to the largest eigenvalue in the dense phase and so the matrix element $\langle 1-|\hat{\rho}|1-\rangle$ is an estimate of the high-coverage limit of the coverage discontinuity—extrapolating this matrix element in the manner described above yields essentially the same results as extrapolating ρ_+ of Eq. (5), as used to generate Fig. 3. As the tricritical point is approached, the "avoided crossing" involving the second, third, fourth, and fifth eigenvalues approaches the triple point (presumably in a way analogous to the approach of the avoided crossing at finite magnetic field of the second and third eigenvalues of the Ising model as the critical point is approached[16]). Thus near the tricritical point we expect the fourth eigenvalue to be degenerate with the largest in the $M\to\infty$ limit. This expectation will be verified below.

Privman and Schulman[18] suggest that the second-largest eigenvalue near a first-order transition gives the free energy of a metastable phase. The (near) degeneracy of the second and third eigenvalues at chemical potentials

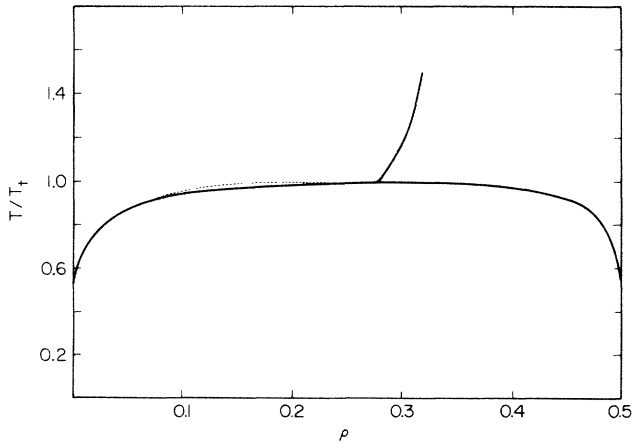

FIG. 3. Estimated T-ρ phase diagram for the interacting-hard-square problem compared with Baxter's exact results (dashed line) for the low-density side of the coexistence region. The critical line continues smoothly to $\rho\approx 0.368$ at $T=\infty$ (Ref. 4), the noninteracting hard-square limit.

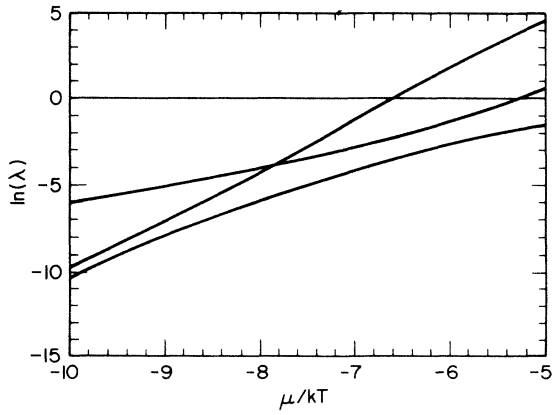

FIG. 4. The seven largest eigenvalues for the interacting-hard-square system at $T=0.5T_t$ as a function of $(M=6)$. The heavy lines denote pairs of eigenvalues which are degenerate on this scale.

smaller than that of the triple point is consistent with the picture of a metastable phase with $c(2\times2)$ order at these chemical potentials.

We now discuss the generalization of the above treatment of coverage discontinuities to other lattice-gas systems. In the treated models the $c(2\times2)$ state breaks the translational symmetry of the lattice and is characterized by a degeneracy of the two largest eigenvalues of the transfer matrix. In general, we characterize the states having broken translational symmetry by the δ functions occurring in their structure factors. For every independent δ function there will be an eigenvalue degenerate with the largest eigenvalue. For example, in the $p(2\times2)$ ordered state, the largest four eigenvalues become degenerate in the infinite-system limit [eigenvalues associated with $\mathbf{k}=(\pi/a,\pi/a),(\pi/a,0),(0,\pi/a)$ become degenerate with the largest eigenvalue[19]]. Near a position in a phase diagram associated with a coverage discontinuity, we expect that these three eigenvalues will have the same qualitative behavior as λ_{1-} in Fig. 1. Thus the eigenstate which plays the role of $2+$ in Eq. (5) does not necessarily correspond to the third-largest eigenvalue or even the second-largest eigenvalue which is invariant under lattice translations in the finite lattice direction. It will be the invariant eigenstate with the largest eigenvalue not degenerate with λ_{1+} in the ordered state.

IV. CONVERGENCE PROPERTIES

To discuss the convergence of the matrix elements to the infinite-system discontinuity, we first give an alternate derivation of Eq. (5). At low enough temperatures we expect[16] the dominant configurations of the strip at the transition point of the infinite-system limit to have the features indicated in Fig. 5: regions of dense or dilute phase are separated by narrow domain walls. The average distance between domain walls, $\xi_{||}$, is determined by the interfacial tension between the dense and dilute phases. For $x\gg\xi_{||}$, we thus expect the density-density correlation function to have the limit

$$\lim_{x\gg\xi_{||}}\langle\rho(0)\rho(x)\rangle=\left[\frac{\rho_++\rho_-}{2}\right]^2. \tag{7}$$

For $x\ll\xi_{||}$ but $x\gg\xi_\infty^\pm$, where $\xi_\infty^\pm$ are the correlation lengths in the single phases (which diverge at the tricritical point), we expect the correlation function to have the limit

$$\lim_{\substack{x\ll\xi_{||}\\ x\gg\xi_\infty}}\langle\rho(0)\rho(x)\rangle=\frac{\rho_+^2+\rho_-^2}{2}. \tag{8}$$

In the transfer-matrix formalism the row-row density-density correlation function can easily be shown to be

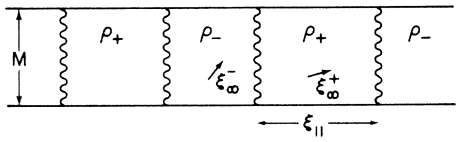

FIG. 5. Expected dominant configurations of the strip at the triple point showing only domain walls between phases of different density.

$$\langle\tilde\rho(0)\tilde\rho(x)\rangle=\langle 1+|\hat\rho|1+\rangle^2+\sum_{n=2}\left[\frac{\lambda_{n+}}{\lambda_{1+}}\right]^x|\langle 1+|\hat\rho|n+\rangle|^2 \tag{9}$$

(distinguishing the row density from the site density by placing a tilde over the ρ). Identifying[16] ξ_n^{-1} with $\ln(\lambda_{1+}/\lambda_{n+})$ and assuming that $\xi_\infty^\pm\ll x$ with $(|\lambda_{3+}|/\lambda_{1+})^x\ll1$, we reproduce Eq. (5). The important observation now is that ρ_+ and ρ_- are expected[16] to differ from their values in the $M\to\infty$ limit by terms proportional to (some power of) e^{-M/ξ_∞}. Thus we expect the estimates of Eq. (5) to converge exponentially in M. For this case our power-law extrapolation can also be shown analytically to converge exponentially; our numerical results are consistent with such rapid convergence. Far beneath T_t, where there is no problem with convergence, fits directly to an exponential improved the convergence to the exact results, but such fits gave much poorer results near T_t.

At the tricritical point we anticipate power-law convergence of the coverage discontinuity to zero. For these Ising-like tricritical points, along the line of triple points the coverage discontinuity is expected[13] to vanish as $(1-T/T_t)^\omega$ with $\omega=\frac{1}{4}$ and the inverse correlation length as t^ν with $\nu=\frac{5}{4}$. Thus finite-size scaling theory predicts that at the tricritical point

$$\frac{\rho_+-\rho_-}{2}=|\langle 1+|\hat\rho|2+\rangle|=aM^{-\omega/\nu}=aM^{-1/5}. \tag{10}$$

For the interacting-hard-square system, our 12-14-16 extrapolations at the estimated tricritical point yield $\omega/\nu=0.20021$. For the case $E_2=-E_1/2$ we find $\omega/\nu=0.1953$ from 6-8-10 extrapolations.

The density-density correlation function at large r decays to ρ^2 as $Ar^{-\eta}$ in the infinite system at the tricritical point. Using conformal invariance the constant A can be related to the constant a, defined above, which determines the convergence of $\langle 1+|\hat\rho|2+\rangle$. To do this we first recall[20,21] that a pure, refined, scaling operator $\phi(\mathbf{r})$ which has scaling dimension η and spin s has correlation functions in the strip given by

$$\langle\tilde\phi(0)\tilde\phi(x)\rangle=\left[\frac{2\pi}{M}\right]^\eta\sum_{n,n'=0}^{\infty}b_nb_{n'}e^{-\pi(\eta+2(n+n'))x/M}\frac{1}{M^2}\sum_{m,m'=1}^{M}e^{2\pi i(s+n-n')(m-m')/M}, \tag{11}$$

where $\phi(\mathbf{r})$ is normalized by $\langle\phi(0)\phi(\mathbf{r})\rangle = r^{-\eta}$, and where

$$b_n = \frac{\Gamma(\eta/2+n)}{\Gamma(\eta/2)n!} . \tag{12}$$

However, the site density operator is not refined or normalized; for example, it contains a part proportional to the critical energy operator[22] (for a discussion of the refinement of critical operators, see Ref. 23). We can expand the density operator in terms of refined critical operators ϕ_i,[23]

$$\rho(\mathbf{r}) = a_I I(\mathbf{r}) + \sum_j a_j \phi_j(\mathbf{r}) . \tag{13}$$

We define the ϕ_j so that at criticality $\langle\phi_j\rangle = 0$; the identity operator is necessary because $\langle\rho\rangle \neq 0$. Thus

$$\langle\rho(0)\rho(\mathbf{r})\rangle = a_I^2 + \sum_{j,j'} a_j a_{j'} \langle\phi_j(0)\phi_{j'}(\mathbf{r})\rangle . \tag{14}$$

Conformal invariance predicts[21] that $\langle\phi_j(0)\phi_{j'}(\mathbf{r})\rangle$ is zero unless ϕ_j and $\phi_{j'}$ are in the same conformal block of operators. If they are in the same block, then

$$\langle\phi_j(0)\phi_j(r)\rangle = B_{jj'} r^{-\eta-n_j-n_{j'}}$$

with η the lowest-scaling dimension in the block (the scaling dimension of the primary operator) and n_j an integer. If, for the moment, we consider only primary operators, the site-site density-density correlation function will have the form

$$\langle\rho(0)\rho(\mathbf{r})\rangle = \rho^2 + \sum_n \frac{A_n}{r^{\eta_n}} , \tag{15}$$

where η_n are the primary-operator critical dimensions. Applying the same arguments of conformal invariance to this sum as were used to derive Eq. (11) yields an expression for the row-row densities in the strip:

$$\langle\tilde{\rho}(0)\tilde{\rho}(x)\rangle = \rho^2 + \sum_n A_n \langle\tilde{\phi}_n(0)\tilde{\phi}_n(x)\rangle , \tag{16}$$

with $\langle\tilde{\phi}_n(0)\tilde{\phi}_n(x)\rangle$ given by Eq. (11). We identify each term of the sums of Eqs. (11) and (16) with a term in Eq. (9). Each inverse correlation length, $\ln(\lambda_{1+}/\lambda_{n+})$, is associated with a different η even though they all have the same symmetries. If r is measured in lattice constants, comparison of Eq. (9) with Eq. (11) yields

$$|\langle 1+|\hat{\rho}|2+\rangle| = \left[\frac{2\pi}{M}\right]^{\eta/2} (A_{2+})^{1/2} . \tag{17}$$

(We have implicitly verified this prediction for the spin-spin correlation function of the Ising model.[24]) Thus $a = (2\pi)^{1/5}(A_{2+})^{1/2}$. We find that $A_{2+} = 0.040\,65$ for the interacting-hard-square system. Of course, A_{n+} is a nonuniversal quantity. That $\langle 1+|\hat{\rho}|3+\rangle$ is nonzero means that A_{3+} is nonzero; by extrapolating this matrix element in the same way as $\langle 1+|\hat{\rho}|2+\rangle$, we can estimate A_{3+} and η_{3+}. At the tricritical point of the interacting-hard-square problem, we find that the site-site density-density correlation function has the form (assuming now the known value—see below—of the scaling dimension of η_{3+}):

$$\langle\rho(0)\rho(\mathbf{r})\rangle \approx \rho^2 + \frac{0.04}{r^{2/5}}\left[1 + \frac{0.3}{r^2} + \cdots\right] . \tag{18}$$

The prediction of Eqs. (9), (11), and (16) that

$$\ln\left[\frac{\lambda_{1+}}{\lambda_{2+}}\right] = \frac{\pi\eta_{2+}}{M} \tag{19}$$

for $M = 16$ yields an estimate of the smallest η contributing to the density-density correlation function of 0.4006 (with ξ_{2+} evaluated at the estimated tricritical point). Table I lists the M dependence of $M/\pi\xi$ derived from the largest eight even and odd eigenvalues (only the even ones contribute to the density because $\langle 1+|\hat{\rho}|n-\rangle = 0$) evaluated at the exact tricritical point. They reproduce the list in Ref. 25 of known zero-spin scaling dimensions for the Ising tricritical point. In addition, there are two dimensions (~ 4.4 and ~ 4.2) not associated with any primary operators. They are consistent, however, with the higher-order terms of Eq. (11). Equations (9) and (11) would then predict that

$$\langle 1+|\hat{\rho}|4+\rangle / \langle 1+|\hat{\rho}|2+\rangle = \eta_{2+}/2 .$$

For $M = 16$ we find that this ratio of matrix elements is 0.194 compared with the predicted 0.200. In general, the terms of Eq. (14) involving secondary operators will also be associated with eigenstates of Eq. (9).[21] They will have the same eigenvalues as those associated with nonzero n

TABLE I. The M dependence of the scaling dimension estimates $\eta_{n\pm} = M/\pi\xi_{n\pm}$ at the tricritical point of the interacting-hard-square system. The extrapolations come from a three-point power-law fit of the final three entries in each column.

M	1−	2+	2−	3+	3−	4+	5+
6	0.148 980	0.391 853	1.929 327	2.466 734	5.305 349	5.377 699	6.832 993
8	0.149 880	0.395 154	1.871 208	2.431 161	4.752 832	4.847 429	6.345 874
10	0.150 238	0.396 798	1.841 740	2.416 987	4.546 002	4.646 002	6.185 444
12	0.150 391	0.397 729	1.823 935	2.410 157	4.440 540	4.569 160	6.112 401
14	0.150 455	0.398 306	1.812 002	2.406 451	4.377 664	4.518 692	6.073 647
16	0.150 478	0.398 688	1.803 436	2.404 271	4.336 354	4.487 602	6.050 909
Extrap.	0.1505	0.400 04	1.758	2.3992	4.195	4.404	5.9984
Refs. 21,25	$\frac{3}{20}$	$\frac{2}{5}$	$\frac{7}{4}$	$\frac{12}{5}$	$\frac{3}{20}+4$	$\frac{2}{5}+4$	6

and n' in Eq. (11). As the amplitudes of the secondary operators in Eq. (13) are nonuniversal, this would mean ratios like

$$\langle 1+|\hat{\rho}|4+\rangle/\langle 1+|\hat{\rho}|2+\rangle$$

would also be nonuniversal. However, the amplitude of these terms would be proportional to $M^{-\eta/2-2n}$ rather than $M^{-\eta/2}$; thus, in the large-M limit the ratio of the matrix elements can be computed using Eq. (11), as is evidently observed. The first four of these scaling dimensions have been estimated numerically before using Monte Carlo renormalization-group techniques.[5] The result for the second eigenvalue, which couples to the $c(2\times2)$ order-order correlation function, has been noted before.[3] The eigenvalue λ_{2+} gives the η associated with the density-density correlation function; λ_{2-} is related to the "cubic" field, which when applied creates a critical end point;[26] and λ_{3+} gives the η associated with the energy-energy[22] correlation function. The value of 6 is consistent with corrections to scaling in zero staggered field found in an analysis by Huse[27] of Baxter's exact results. Huse postulated that it might be an irrelevant field linear in the lattice cutoff. Looking at the eigenvalues associated with eigenvectors which transformed like $e^{2\pi im/M}$ gave estimates of the scaling dimensions differing from the ones listed in Table I by m (or $M/2-m$ in the case of the odd block), which is consistent with the predictions of Eq. (11).

Recently, arguments of conformal invariance were used[28] to predict

$$\frac{\ln(\lambda_{1+})}{M}\approx f-\frac{\pi c}{6M^2}\ , \tag{20}$$

where c, the conformal anomaly, characterizes a universality class. Fitting the results from strips of width 12, 14, and 16 to this form, we find $c=0.70003$, consistent with the identification of $c=\frac{7}{10}$ with the Ising tricritical point by Friedan *et al.*[25]

Above the tricritical point one expects the density-density correlations to be governed by the energy-energy correlation function of the Ising model ($\eta=2$). Thus above T_t [cf. Eq. (17)], $|\langle 1+|\hat{\rho}|2+\rangle|\propto M^{-1}$; above T_t the coverage discontinuity vanishes with a different power from that at T_t. To summarize, at low temperatures $\langle 1+|\hat{\rho}|2+\rangle$ converges to the coverage discontinuity exponentially. At the tricritical point it vanishes with increasing strip width with an exponent characteristic of the tricritical point, and far above T_t it vanishes with an exponent characteristic of the Ising critical line. Between each of these three regimes there is crossover from one behavior to another. Using only three strip widths at one temperature, this crossover cannot be detected—thus the inaccuracies in the phase diagram of Fig. 3 just below (not at) the tricritical point. (A method of extrapolation allowing for the crossover would be better.)

V. RESULTS WITH A STAGGERED FIELD

On the coexistence line beneath T_t, three phases coexist: two dense $c(2\times2)$ phases and a dilute disordered phase. Thus, as remarked earlier, the coexistence line is a line of triple points.[17] Consider a staggered field (h_s) which prefers one $c(2\times2)$ sublattice over the other. At chemical potentials greater than that of the triple point, there is a single discontinuity in the "staggered magnetization" at $h_s=0$ as h_s is varied with T fixed. At chemical potentials less than that of the triple point there are two first-order transitions: For large positive h_s there is a dense phase with long-range order in one sublattice, for small $|h_s|$ there is a dilute phase with small staggered magnetization, and for large negative h_s there is a dense phase with long-range order in the other sublattice. Using the above methods we can estimate the magnitude of the discontinuities of staggered magnetization and directly locate the position of the triple point at a given temperature.

Figure 6 shows the eigenvalue spectrum of the interacting-hard-square system at $0.8T_t$ and at a chemical potential clearly less than that of the triple point. (The eigenvalues are labeled by their symmetry properties at $h_s=0$.) There is an avoided crossing at finite h_s which gives rise to a discontinuity in the staggered magnetization. As before, an estimate of its magnitude is

$$m_s^{\pm}=\langle 1+|\hat{m}_s|1+\rangle\pm\langle 1+|\hat{m}_s|1-\rangle\ . \tag{21}$$

The transition h_s was determined from $\langle 1+|\hat{m}_s|1+\rangle=\langle 1-|\hat{m}_s|1-\rangle$, the analogue of the criterion used to estimate the transition chemical potential when $h_s=0$. Figure 7 shows the resulting μ-m_s phase diagram. As the triple point is approached, the avoided crossing of Fig. 6 approaches $h_s=0$. The matrix element $\langle 1+|\hat{m}_s|1-\rangle$ changes from a double-peaked function of h_s to a single-peaked function. This chemical potential serves as (another) estimate of the triple point. For $M=12$, $T=0.8T_t$, this occurs at $\mu/kT=-4.1187$ compared with $\mu/kT=-4.1178\ldots$ from Baxter's exact solution. Above this chemical potential there is a single transition at $h_s=0$ with $\langle 1+|\hat{m}_s|1+\rangle=0$ and $m_s=\langle 1+|\hat{m}_s|1-\rangle$. As μ

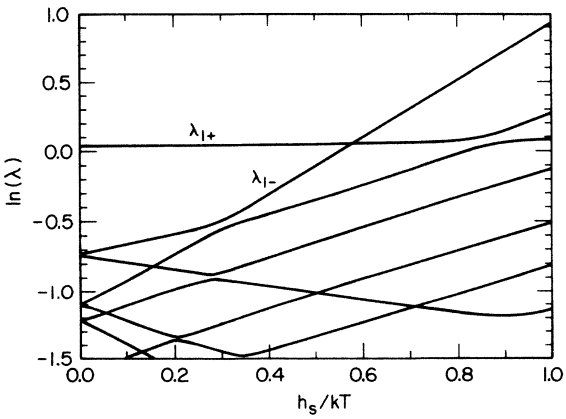

FIG. 6. Eigenvalue spectrum for the interacting-hard-square system at $T=0.8T_t$ and $\mu/kT=-4.7$ as a function of staggered field ($M=10$). λ_{1+} and λ_{1-} do not cross; the avoided crossing is indiscernable on this scale.

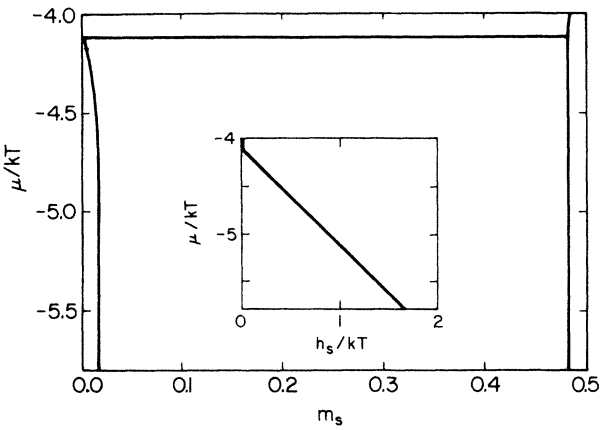

FIG. 7. μ-m_s phase diagram for the interacting-hard-square problem at $T=0.8T_t$. The inset depicts the corresponding μ-h_s phase diagram.

becomes more negative, the transition h_s becomes larger. As h_s becomes large the occupancy of one of the sublattices becomes small. At $\mu/kT=-5.2$ we estimate the value of h_s/kT at the transition to be 1.063, and the occupancy is small enough that the discontinuity in m_s agrees to three decimal places with what one would expect if one of the sublattices had zero occupancy (using the known magnetization of the Ising model at this temperature).

VI. COMPARISON WITH CORRELATION-LENGTH SCALING

Finally, we compare the methods of Refs. 2, 7, 10, and 11 for locating the position of the tricritical point with ours. References 2 and 11 state that the correlation length ξ_{2+} associated with λ_{2+} (called $\hat{\xi}$ or the persistence length) does not diverge along the critical line above T_t. This is not true: ξ_{2+} is proportional to $M/\pi\eta$, with η the critical dimension of the energy-energy correlation function[29] ($\eta=2$ for the Ising model). Thus the success of Ref. 2 in locating T_t as a single temperature where ξ_{2+} is proportional to M is due to the crossover from one amplitude to another and the exponential divergence below T_t rather than because there exists one temperature (the tricritical point) where $\xi_{2+}\propto M$. (Compare the discussion at the end of Sec. IV.) As an example of the danger in this approach, in Ref. 7 the case $|E_2/E_1|=\frac{1}{50}$ is studied. The temperature where both ξ and $\hat{\xi}$ scale linearly with system size is found not to be at a tricritical point. This is interpreted as meaning that the tricritical point decomposes into two critical endpoints at small $|E_2/E_1|$. The present calculation locates a tricritical point at all negative values of E_2/E_1.

Looking at matrix elements gives an analogous situation because at T_t and above $\langle 1+|\hat{\rho}|2+\rangle$ converges to zero. Thus the tricritical point cannot be located with just the criterion that $\langle 1+|\hat{\rho}|2+\rangle$ converge to zero (or that $\langle 1+|\hat{\rho}|1+\rangle-\langle 2+|\hat{\rho}|2+\rangle$ converge to zero). Near the tricritical point there is crossover between the powers of the convergence rather than its amplitudes in the correlation-length method. A disadvantage of the matrix-element method is that it needs information from at least three different strip widths. (For any particular M, $\langle 1+|\hat{\rho}|2+\rangle$ is nonzero for all T, so an extrapolation is crucial.)

Reference 10 proposes that the tricritical point can be estimated as the temperature where the compressibility $\kappa(M)$, is proportional to a power of M. Near the tricritical point the free energy has the scaling form[13]

$$f(\mu,T)\approx t^{2-\alpha}X_{\pm}(gt^{-\phi}) , \tag{22}$$

where the scaling fields t and g depend analytically on T and μ. For the (Ising-like) tricritical point studied here, $\alpha=-\frac{1}{2}$ and $\phi=\frac{9}{4}$.[13] The compressibility along the line $g=0$ (the line of triple points beneath T_t) thus diverges as

$$\kappa\propto\frac{\partial^2 f}{\partial\mu^2}\sim t^{2-\alpha-2\phi}=t^{-2} . \tag{23}$$

Similarly, the correlation length along $g=0$ diverges as $t^{-\nu}$ with $\nu=(2-\alpha)/d=\frac{5}{4}$, so one expects $\kappa(T_t,\mu_t,M)=M^{(2-\alpha-2\phi)/\nu}=M^{8/5}$. Equivalently, one can directly argue that $\kappa\propto M^{2-\eta}$, with η the scaling dimension of the density-density correlation function ($\frac{2}{5}$ from Table I). We have verified this behavior: comparing $M=14$ with $M=16$ yields the estimate of $(2-\alpha-2\phi)/\nu$ as 1.601. Above T_t, κ diverges like the specific heat, so $\kappa\propto\ln(M)$.

In more complicated lattice gases, the transfer matrix becomes large with increasing strip width. Thus the techniques of locating a multicritical point discussed above can be difficult to apply because they require two or three strip widths. This problem is encountered in Ref. 10, for example. To get around this difficulty, we suggest yet another technique of estimating the position of (multi-) critical points which needs only one strip width. In the Ising model in zero field beneath T_c the third eigenvalue provides an estimate of the (standard) correlation length because the first two eigenvalues are degenerate. (In the picture analogous to Fig. 5, the third eigenvalue estimates ξ_∞.) Above T_c, the third eigenvalue, because of its eigenvector's even symmetry under spin inversion, gives the correlation length associated with the energy-energy correlation function. Thus the third eigenvalue peaks close to T_c (in the finite-size rounded region) and thus provides an estimate of T_c—from a single strip width. (It actually peaks exactly at T_c, but this is presumably a special property of the Ising model.) We expect similar behavior along the line of phase transitions in the lattice-gas models discussed above. On the line of first-order transitions, the fourth eigenvalue gives an estimate of ξ_∞. [See Fig. 5. Because of the degeneracy of the first three eigenvalues, the fourth gives both density-density and $c(2\times2)$ order-order correlation lengths.] This correlation length increases as the multicritical point is approached. If the value of η associated with this eigenvalue is greater on the line of second-order transitions than at the multicritical point, then from Eq. (19) there will be a maximum in the associated correlation length. The position of this peak provides an estimate of the location of the

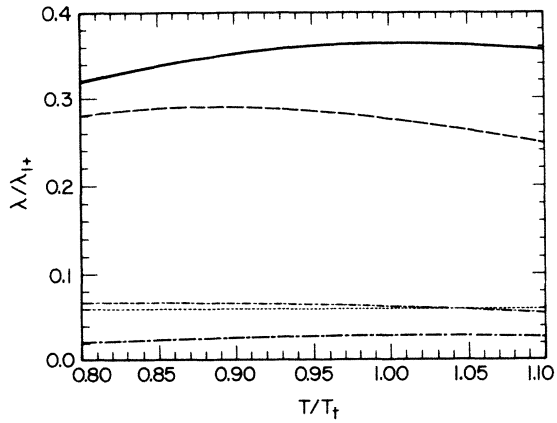

FIG. 8. Dependence of the fourth and smaller eigenvalues on temperature along the line of transitions of the interacting-hard-square system.

multicritical point. This indeed happens with the fourth eigenvalue at the Ising tricritical point (where $\eta_{T_t}=\frac{7}{4}$ and $\eta_{T_c>T_t}\geq 2$), as shown in Fig. 8: The correlation lengths of a narrow strip ($M=6$) associated with the fourth and smaller eigenvalues are plotted along the line of transitions determined from $\langle 1+|\hat{\rho}|1+\rangle=\langle 2+|\hat{\rho}|2+\rangle$. The correlation length associated with the fourth eigenvalue peaks at $0.9996T_t$ and the one associated with the fifth peaks at $0.881\,51T_t$. The accuracy of the fifth increases with increasing system size, but is already acceptable for the narrow widths where this method would be applied. We emphasize that this method of estimating the position of the multicritical point only requires information from one strip width. Notice that neither the susceptibility, the compressibility, nor the specific heat of the finite systems peaks at the multicritical point.

VIII. CONCLUSION

We have shown how matrix elements obtained from transfer matrices can be successfully used to estimate coverage discontinuities in square lattice gases when the dense phase has $c(2\times 2)$ order. Extension to other lattice gases, as described in the text, is straightforward and should yield the same exponential convergence. The tricritical points of the square lattice-gas models are also located precisely by this method. However, whether or not similar accuracy can be expected in locating the multicritical points of more complicated models is hard to know, *a priori*. For example, as we show, the Ising-like tricritical point studied here has many special properties predicted by conformal invariance, while the multicritical point of general (anisotropic) lattice gases need not be conformally invariant.

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*Permanent address: Dept. of Physics, Haverford College, Haverford, PA 19041.

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