Structure factors associated with the melting of a (3×1) ordered phase on a centered-rectangular lattice gas: Effective scaling in a three-state chiral-clock-like model

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By computing the structure factor through the melting transition of a commensurate (3×1) phase in a version of Baxter's generalized hard hexagon model, we simulate what might be observed in diffraction experiments (especially those using low-energy electrons) on chemisorption systems which have similar Landau-Ginzburg-Wilson Hamiltonians. In the commensurate and disordered phases we observe that the shift of the peak of the critical scattering from the commensurate position is roughly proportional to the inverse correlation length in the reduced temperature range 0.015–0.15. The proportionality constant appears to depend on the position of the transition on the phase boundary (i.e., on the chemical potential). We see no sign of an incommensurate floating phase between the disordered and commensurate phases. Effective critical exponents are consistent with those expected from the three-state Potts model. To the precision of this calculation (a few percent), the structure factor scales over approximately 10% of the Brillouin-zone area.

I. INTRODUCTION

A single-scattering diffraction experiment on an adsorbed system measures the structure factor:

$$S(\mathbf{k})=\left\langle \left| \sum_{\mathbf{r}} n(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} \right|^2 \right\rangle , \tag{1}$$

where $\mathbf{r}$ denotes the possible positions of the adsorbed atoms, and $n(\mathbf{r})$ is the occupancy (0 or 1) of the binding site at $\mathbf{r}$. In the first paper of this series,[1] hereafter called I, we analyzed the behavior of the structure factor through the continuous disordering transitions of triangular lattice gases with $p(2\times2)$ and $(\sqrt{3}\times\sqrt{3})R30°$ ordered states. Our goal was to simulate what might be observed in low-energy electron diffraction (LEED) experiments on chemisorption realizations of these systems. In this paper we similarly examine a different type of system. In many adsorbed systems with commensurate ordered states, the peak of the structure factor in the disordered state need not be at the same $\mathbf{k}$'s as the δ functions of the commensurate state. The behavior of systems with this type of freedom [lattice gases with "chiral" terms in their Landau-Ginzburg-Wilson (LGW) Hamiltonians] has been the subject of much recent discussion.[2] One example of such a system is a centered rectangular lattice gas with an ordered (3×1) phase. A possible experimental realization was thought to be H/Fe(110).[3] Figure 1 shows a schematic picture of the (3×1) phase. The ground state is threefold degenerate. If one neglects gradient terms in the LGW Hamiltonian of this system, it is equivalent to the three-state Potts model. However, in the Potts model the interfaces between two phases are independent of the phases involved. In the 3×1 state there are three possible sublattices in which the system can order. Simple considerations[4] of interface energies for the 3×1 lattice gas show that $0\,|\,1$, $1\,|\,2$, and $2\,|\,0$ walls are not equivalent to $1\,|\,0$, $2\,|\,1$, and $0\,|\,2$ walls, where $n\,|\,n'$ represents a wall between a region ordered in sublattice n and a region ordered in sublattice n'. Thus there is a new uniaxial chiral term in the LGW Hamiltonian[4,5] which distinguishes this system from the Potts model.

A fundamental question is whether a transition is possible directly from the 3×1 commensurate state to the (incommensurate) fluid state if there is nonzero chirality. Mean-field arguments,[6] as well as some calculations for model systems,[7] suggest that there will be an intermediate incommensurate (floating) phase with algebraic decay of correlations (i.e., infinite correlation length) for any chirality. On the other hand, a study of the quantum version of the chiral clock model shows no floating phase for any size chirality.[8] Numerical studies of the chiral clock model, using Monte Carlo,[9] finite-size transfer-matrix scaling,[10,11] and Monte Carlo renormalization group,[12] all suggest that the floating phase does not appear until moderately large chirality (indicating a Lifshitz point). Huse and Fisher[4] argue that direct transitions are possible

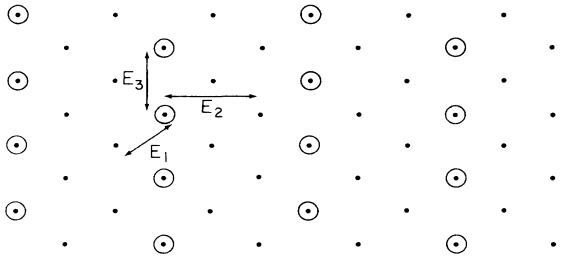

FIG. 1. The 3×1 phase on a centered ~~triangular~~ rectangular lattice studied in this paper, with the interactions producing the ordered array.

but in new universality classes. Much is known about the Potts model, and den Nijs has shown that the uniaxial chiral term is relevant,[13] in contrast to the triaxial chiral term which distinguishes the $(\sqrt{3}\times\sqrt{3})R30°$ lattice gas from the three-state Potts model,[1,4] so there is at least the possibility that the behavior is not Potts-like immediately away from the Potts point. So far, numerical work has been inconclusive. Kinzel *et al.*[14] and Kinzel[15] have studied a lattice gas similar to the one we introduce in Sec. II. Standard finite-size-scaling methods which work well at the Potts point worsen away from it.[16] Our Monte Carlo calculations are no more enlightening on this basic question; our purpose instead is to simulate what might actually be observed in LEED experiments on chemisorption systems.

The chiral term in the LGW Hamiltonian of the three-state Potts model is the following[4]:

$$\mathcal{H}_c = g_c \int d^2r \left[\psi \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x} \right] , \tag{2}$$

where $\hat{x}$ is the horizontal direction in Fig. 1 and $\psi(\mathbf{r})$ is the complex order parameter density: if we describe the three possible values of the local order by $n(\mathbf{r})=0$, 1, or 2 then $\psi(\mathbf{r}) \propto e^{i2\pi n(\mathbf{r})/3}$. To see how this term is related to the asymmetric domain wall energies, we write $\partial\psi/\partial x$ as $[\psi(\mathbf{r})-\psi(\mathbf{r}-a\hat{\mathbf{x}})]/a$. Equation (2) then becomes

$$\mathcal{H}_c = \frac{g_c}{a} \int d^2r [\psi^*(\mathbf{r})\psi(\mathbf{r}-a\hat{\mathbf{x}}) - \psi(\mathbf{r})\psi^*(\mathbf{r}-a\hat{\mathbf{x}})] . \tag{3}$$

Thus nonzero $\langle \mathcal{H}_c \rangle$ implies that

$$\langle \psi(\mathbf{r})\psi^*(r-a\hat{\mathbf{x}}) \rangle \neq \langle \psi^*(\mathbf{r})\psi(\mathbf{r}-a\hat{\mathbf{x}}) \rangle ,$$

leading to the domain wall asymmetries.[17]

II. MODEL SYSTEM

Our 3×1 structure on a centered rectangular lattice was created with E_1 (see Fig. 1) as infinitely repulsive and $E_3=-E_2$, with $E_2>0$. This is a version of Baxter's generalized hard hexagon model.[18–20] Baxter has computed the partition function of this model when

$$z = e^{\mu/k_BT} = \frac{(1-e^{-E_2/k_BT})(1-e^{E_2/k_BT})}{(1-e^{-E_2/k_BT}-e^{E_2/k_BT})} . \tag{4}$$

The critical point in Baxter's solution, which is three-state Potts-like, is located at

$$z_c/(1-z_c)^2 = (11+5\sqrt{5})/2 .$$

This gives $k_BT_c \approx 0.650E_2$ and $z_c \approx 0.741$. Also at this point the critical coverage is $(5-\sqrt{5})/10 \approx 0.276$. The special behavior along the line of exact solutions and its relationship with the rest of the phase diagram is discussed by Huse.[21] We have examined this model away from Baxter's solution, especially at $z=2.5$. (The corresponding critical coverage we find to be around 0.331.) As the activity increased the correlation time in the Monte Carlo simulations increased:[22] The reason we focused on the transition at $z=2.5$ was that the activity was sufficiently large so that behavior distinctly different from that at Baxter's point was observed, yet small enough so that obtaining good statistics was not a problem.

We computed the structure factor given by Eq. (1) using the Monte Carlo techniques described in I. The centered rectangular lattice had rectangular boundaries with periodic boundary conditions. The number of columns, which must be a multiple of six to support the 3×1 phase, was chosen to be three times the number of sites in a column, as illustrated in Fig. 1. In the ordered state the number of unit cells is the same in both principal directions, and thus the number of points in $\mathbf{k}$ space is enhanced along the incommensurate direction [the direction of $\bar{\Delta}$ in Fig. 2 or the $\hat{\mathbf{x}}$ direction of Eq. (2)]. Most of the simulations were performed on lattices with 3888 sites which, again, we feel typifies the size of defect-free regions on metal surfaces prepared using standard methods.

Figure 2 shows the surface Brillouin zone of the centered rectangular lattice with the lines along which $S(\mathbf{k})$ was computed. The point on the $\bar{\Delta}$ line corresponding to the δ-function position of the ordered, commensurate (3×1) phase (not a point of high symmetry) we denote by $\bar{\Delta}_c$. Notice that $\bar{\Delta}_c$ does not even lie on the zone boundary, and thus the Lifshitz condition is not satisfied.[23] If the Lifshitz condition is not satisfied, then mean-field theory says that a continuous transition from the commensurate state is possible only to an incommensurate state[6,23] with algebraic decay of correlations (a "floating" state), and thus these types of systems were omitted from early LGW classification schemes.[24] The oblique line through $\bar{\Delta}_c$ connects $\bar{\Gamma}+\mathbf{g}_1-\mathbf{g}_2$ and $\bar{\Gamma}+\mathbf{g}_2$; $\bar{S}$ the intersection of this line with the edge of the zone, is a high-symmetry point.

III. ANALYSIS OF MONTE CARLO DATA

Figure 3 shows the form of the data obtained from the Monte Carlo calculations at $z=2.5$ for a 36×108 lattice: It shows the structure factor 5% below T_c, close to T_c, and 5% and 10% above T_c. Figure 4 depicts the temperature dependence of $S(\mathbf{k})$ at $\bar{\Delta}_c$.

Assuming a single commensurate-to-disorder transition, the structure factor in the limit $\delta\mathbf{k}=\mathbf{k}-\bar{\Delta}_c$ and $t=|T-T_c|/T_c$ small is expected to have the form

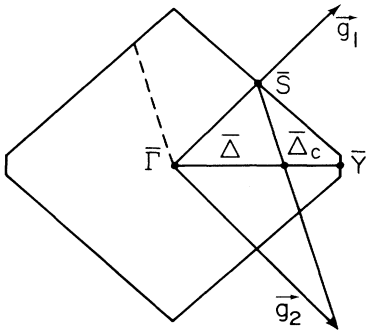

FIG. 2. Surface Brillouin zone of the centered rectangular lattice, along with the positions where $S(\mathbf{k})$ was computed.

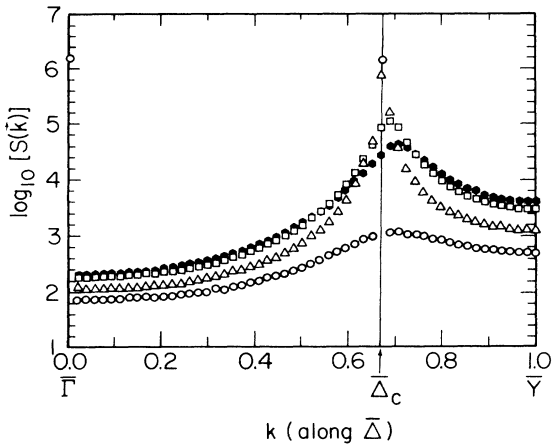

FIG. 3. Plots of $S(\mathbf{k},T)$ for a 36×108 lattice at temperatures approximately 5% below T_c (○), at T_c (△), 5% above T_c (□), and 10% above T_c (●).

$$S(\mathbf{k},T)=a_1 t^{-\gamma}X_{\pm}(a_2 t^{-\nu}\delta\mathbf{k}) , \tag{5}$$

where $X_{\pm}(\mathbf{w})$ are universal, but the constants a_1 and a_2 depend on the microscopic details of the system. The three-state Potts model is characterized by a symmetric scaled structure factor $X_{\pm}(\mathbf{w})=X_{\pm}(|\mathbf{w}|)$. As emphasized by Huse and Fisher,[4] the scaled structure factor may no longer be symmetric with the chiral term present. As the scaled structure factor is a characteristic of the universality class, this would indicate a new, non-Potts, universality class.

To address this question we performed a least-squares fit of the data above T_c to the form of Eq. (5). We parameterized the function X_+ by the constants c_n and d_n defined by

$$X_+(w_x\hat{\mathbf{x}}+w_y\hat{\mathbf{y}})=[\,1+(w_x-w_0)^2+c_3(w_x-w_0)^3 +c_4(w_x-w_0)^4+d_2w_y^2+d_4w_y^4]^{-1} , \tag{6}$$

where the $\hat{\mathbf{y}}$ direction is perpendicular to the $\hat{\mathbf{x}}$ direction defined above. Including a c_5 or d_6 term does not appreciably improve the fits or change the results. A similar expansion for the scaled structure factor of the Ising model[25] using the c_n from the known small-w expansion reproduces the exact scaling function to 5% for $w\lesssim 11$. Adjusting the c_n in a least-squares fit, as we do here, would have given even better accuracy. (We estimate, *a posteriori*, that our data scales to 5% for w's up to around 15.) For large $|\delta\mathbf{k}|$ or t (and also for small t, because of the finite lattice size), the data does not scale. Performing the fit, we find that Eq. (5) can account for the data[26] with $0.015<t<0.15$ and with $\delta\mathbf{k}$ less than $\frac{1}{3}$ of $\bar{\Delta}_c\bar{S}$, less than $\frac{1}{4}$ of $\bar{\Delta}_c\bar{Y}$, and less than $\frac{1}{2}$ of $\bar{\Delta}_c\bar{\Gamma}$ and $\bar{\Delta}_c(\bar{\Gamma}+\bar{g}_2)$. At small t the data does not scale because of finite-size effects; at large t and $|\delta\mathbf{k}|$ it does not scale because of corrections to scaling. From a least-squares fit using the data that does scale we find $(T_c)_{\text{eff}}=0.787\pm0.007E_2$, $\gamma_{\text{eff}}=1.35\pm0.10$, $\nu_{\text{eff}}=0.85\pm0.10$, and $w_0=1.0\pm0.2$. The given uncertainties are our estimates of those due only to the statistical error in our Monte Carlo data. The effective critical exponents are consistent with those expected from the three-state Potts model (where $\gamma=\frac{13}{9}\approx1.44$ and $\nu=\frac{5}{6}\approx0.83$), and Fig. 5 shows some of the data above T_c scaled with three-state Potts exponents. The satisfactory scaling of the data with three-state Potts exponents is consistent with other studies[14,27] of similar models. Here, however, the effective scaling function is clearly asymmetric, with a peak at nonzero w_0.

The situation beneath T_c is different in that there is no extended data range over which Eq. (5) is satisfied. This is consistent with our observations in I: For these models the amplitudes of corrections to scaling seem to be greater beneath T_c. Fixing T_c to the value estimated from the data above T_c, and choosing arbitrarily the reduced temperature range 0.015 to 0.15 to analyze, we find the manifestly *effective* exponents $\gamma'_{\text{eff}}=1.15\pm0.2$ and $\nu'_{\text{eff}}=0.6\pm0.1$ with $w_0=0.5\pm0.1$. This type of deviation from the pure three-state Potts model exponents is consistent with what we observed in I for a transition in the three-state Potts model universality class.

To explore the behavior of the structure factor in more

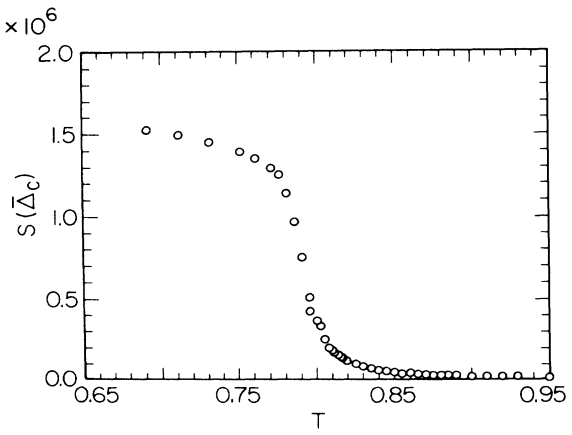

FIG. 4. Temperature dependence of $S(\bar{\Delta}_c)$. T here and below in units of E_2.

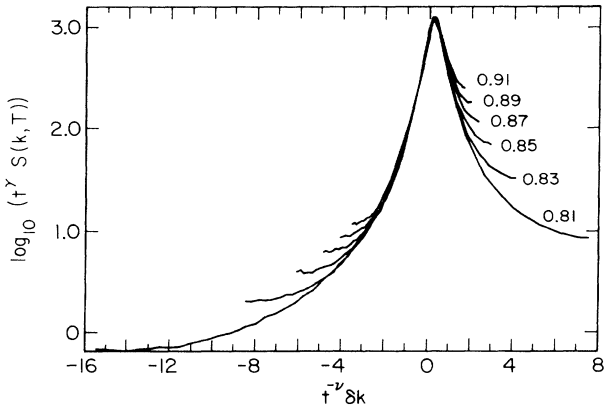

FIG. 5. Structure factor above T_c, scaled with three-state Potts exponents. Notice the peak of the scaled structure factor is evidently not at $t^{-\nu}\delta\mathbf{k}=\mathbf{0}$.

detail, we computed the correlation lengths and susceptibilities explicitly. At each temperature we performed a least-squares fit of the structure factor to a Lorentzian:

$$L(\mathbf{k},T)=\frac{\chi}{1+\xi_x^2(\delta k_x-q)^2+\xi_y^2 k_y^2} \ . \tag{7}$$

We used data with the same $\delta\mathbf{k}$ which scaled in the preceding analysis. The units of k_x and k_y were chosen so that $\mathbf{g}_1\cdot\hat{\mathbf{x}}=2\pi/a_x=\mathbf{g}_1\cdot\hat{\mathbf{y}}=2\pi/a_y=1$. Only when the data was obviously above T_c did we use the point at $\delta\mathbf{k}=\mathbf{0}$. By fitting the structure factors to Lorentzians we are not claiming that the scaled structure factor is purely Lorentzian: Indeed, deviations of the scaled structure factor from Lorentzian behavior are evident at large $|\delta\mathbf{k}|$. We are just finding the Lorentzians which best describe the structure factors. From Eq. (5) the correlation lengths ξ_x and ξ_y defined in this way will be proportional to $t^{-\nu}$ (and given in units of a_x and a_y) and the susceptibility χ will be proportional to $t^{-\gamma}$, as usual. (These definitions of the correlation length and susceptibility are not standard choices, however.[27]) If the scaling function is anisotropic, then q will be proportional to ξ^{-1}. Baxter[20] observes that $q\propto\xi^{-2}$ along his line of exact solutions, which Huse and Fisher[4] interpret as meaning that the chirality vanishes at the transition of the solved model. That $q\propto\xi_x^{-2}$ at the Potts point can be viewed as a lattice-constant effect: An atomic form factor which is not spherically symmetric would lead to the same behavior because $(1+b\delta k_x)X(\xi_x\delta k_x)$ has a q which goes to zero as ξ^{-2}. As in I, we obtain effective exponents from log-log plots.[28] From log-log plots of ξ_x and χ (see Fig. 6), we find that $\nu_{\rm eff}=0.87\pm0.08$ and $\gamma_{\rm eff}=1.55\pm0.12$, respectively, with $(T_c)_{\rm eff}=0.789\pm0.006\ E_2$. Defining $\bar{\beta}$ by $q\propto t^{\bar{\beta}}$, we similarly find $\bar{\beta}_{\rm eff}=0.97\pm0.10$. Analysis of ξ_y gives $\nu_{\rm eff}=0.95\pm0.09$. These results are consistent with the analysis presented above which simultaneously used all the data.

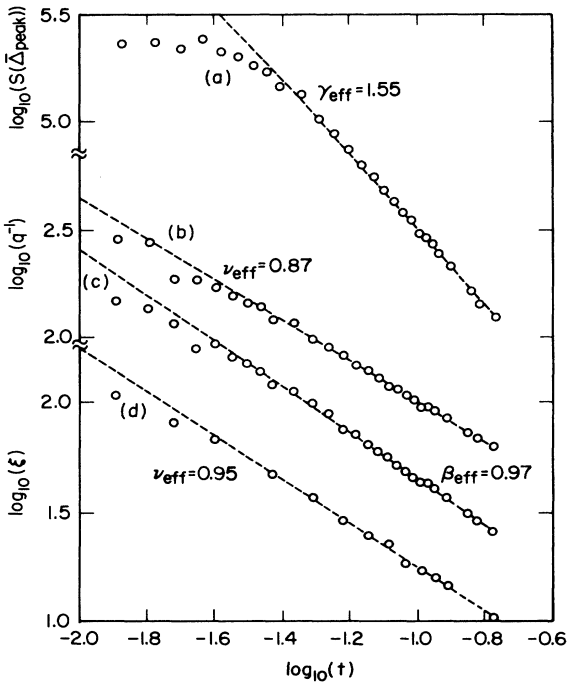

FIG. 6. Log-log plots above T_c at $z=2.5$ with $T_c=0.787E_2$ for the quantities characterizing the structure factor: (a) χ, (b) ξ_x, (c) q^{-1}, and (d) ξ_y. The units of q and ξ differ slightly from Eq. (7) and Table I.

In order to explicitly compare the behavior of q and ξ_x, Fig. 7 shows $q\xi_x$ as a function of T for $z=2.5$ and two other activities. It appears that $q\xi_x$ approaches a constant as T_c is approached from above or below. There is no sign of it tending to vanish as it would in a Potts-like transition.

The behavior of $q\xi_x$ versus T also contrasts with what one expects for a double transition with an intermediate incommensurate phase. In such a floating phase q is finite, whereas ξ_x is infinite, and thus $q\xi_x$ would be expected to diverge as the floating phase is approached from the disordered phase. We see no sign of this occurring. Moreover, ξ_x appears to diverge as a power law rather than exponentially in t, the behavior expected in approaching a floating phase from a disordered phase.[29]

The observed behavior is evidently independent of lattice size for the, lattice sizes we have studied: We varied the system size from 12×36 to 72×216 and see only small finite-size effects in $q\xi_x$ 10% above T_c at $z=2.5$. Table I lists q, ξ_x^{-1}, $q\xi_x$, and ξ_x/ξ_y at $(T,z)=(0.855\ E_2, 2.5)$ as a function of system size; we estimate the uncertainty in ξ and q due to statistical error to be around 5%. Plots of $q\xi_x$ are roughly independent of system size approximately 1.5% above T_c for systems of sizes greater than 36×108. In an incommensurate floating phase ξ_x (and $q\xi_x$) would increase linearly with system size. We see no sign this occurs for an extended temperature range. The finite-size effects we do observe seem to be well accounted for by standard finite-size scaling theory for a single critical point: In Fig. 8 we show the standard finite-size scaling plot[30] for $S(\bar{\Delta}_c)$, using data from four different system sizes. The finite-size-scaling behavior of $S(\bar{\Delta}_c)$ is well accounted for by three-state Potts exponents. Thus our data seems to be inconsistent with a floating phase with a width greater than about 1% of T_c. With this conclusion there is an important caveat, howev-

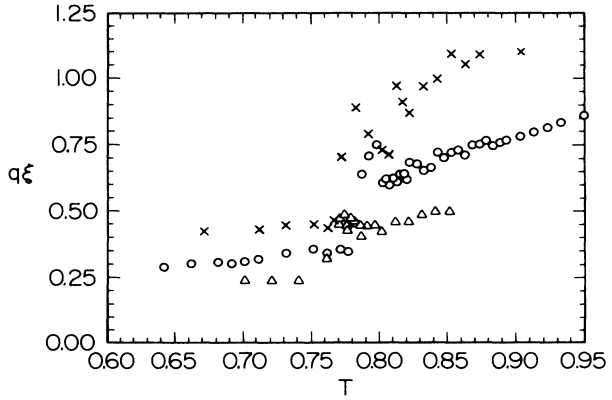

FIG. 7. Temperature dependence of $q\xi_x$ for three activities: $z=4.0$ (×), $z=2.5$ (○), and $z=1.62$ (△).

TABLE I. The dependence of the peak shift q, the inverse correlation length ξ_x^{-1}, $q\xi_x$, and ξ_x/ξ_y on system size at $z=2.5$ and $T=0.855E_2$ ($\approx 8\%$ above T_c).

System size	q	ξ_x^{-1}	$q\xi_x$	ξ_x/ξ_y
12×36	0.0269	0.0501	0.536	0.257
18×54	0.0292	0.0457	0.641	0.252
24×72	0.0305	0.0470	0.648	0.244
30×90	0.0326	0.0458	0.712	0.242
36×108	0.0323	0.0443	0.728	0.248
72×216	0.0320	0.0448	0.715	0.225

er. We cannot preclude the possibility that there is a floating phase over a much larger temperature region because such a phase introduces a new length scale, the average distance between dislocations, which could conceivably be much larger than our system sizes. The scaling behavior we observe could be characteristic of the behavior when the correlation length is much smaller than the system size and dislocation size. This possibility would imply that we (and the experimenter) would need much larger systems to see behavior characteristic of a floating phase, although floating phases have been observed in lattice-gas systems with sizes comparable to ours.[31–33]

Figure 9 shows the temperature dependence of the ratio of correlation lengths ξ_x/ξ_y for $z=2.5$. In a transfer-matrix study of a similar centered-rectangular lattice gas, Kinzel[15] concluded that sufficiently far from the critical point of zero chirality the scaling itself could become anisotropic with the exponent describing the divergence of the ξ_x different from the exponent governing ξ_y. There is no indication of this type of behavior at this activity: If such anisotropy were present one would expect ξ_x/ξ_y to become large or small near the critical point, while Fig. 9 shows little change. The observed behavior is also inconsistent with $\xi_x/\xi_y \propto t^{1/3}$ as observed by Howes[34] near the Lifshitz point of a related model. That the ξ_x/ξ_y above T_c appears to be different from ξ_x/ξ_y below is additional evidence that the scaled structure factors are not Potts-like. For Potts models on anisotropic lattices one expects that a simple change in the units of k_x and k_y will make the structure factors isotropic. (The structure factor of the Ising model with anisotropic interactions has this property.[25]) If this change of units sufficed to make the structure factor isotropic, the ratio ξ_x/ξ_y would be the same above and beneath T_c, contrary to what we observe.

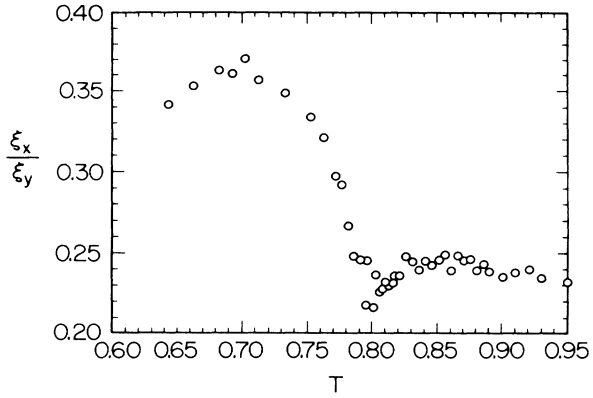

FIG. 9. Temperature dependence of ξ_x/ξ_y at $z=2.5$.

That the scaling functions above and below T are no longer Potts-like automatically implies that some amplitude ratios will be different from those of the Potts models. Assuming three-state Potts exponents we find $\xi_+/\xi_-=5.0\pm 1.7$ and $\chi_+/\chi_-=160\pm 80$. The susceptibility amplitude ratio is considerably larger than the value found in I for the three-state Potts model (43 ± 3), while the correlation length ratio is approximately the same (4.1 ± 0.3). Again we note that the large value of χ_+/χ_- will make measurement of critical scattering much more difficult below T_c than above.

Low-resolution LEED instruments, which integrate the structure factor, measure the energy singularity.[35] With this motivation, we present in Fig. 10 the temperature dependence of the energy at $z=2.5$. Fits similar to those of Ref. 35 (not including a linear background term) yield the ratio above and below T_c of the amplitude of the $t^{1-\alpha}$ term as 3.2 ± 1.3 and $\alpha_{\text{eff}}=0.45\pm 0.05$. The effective α is close to what is typically observed for the three-state Potts model.[36] The amplitude ratio is different from the value of unity characteristic of the Potts models and from the values observed for the lattice gases of Ref. 35 (and also Baxter's exact solution[20]). If there were an incommensurate (I) or floating phase between the commensurate (C) and disordered incommensurate (DI) (i.e., with exponential decay of correlations) phases, the C-I transition is expected to be Pokrovsky-Talapov-like,[37,38] and the I-DI transition is expected to be Kosterlitz-Thouless-like.[37] In the C-I transition the specific heat diverges as T_c is approached from above, but remains finite as it is approached from below.[38] In the Kosterlitz-Thouless transition the specific heat peaks above T_{KT} without diverging and does not have a universal shape.[39] Thus if there were two transitions we would not expect to obtain a decent fit of the data with the same type of singularity above and below an effective T_c, as we do, although again we men-

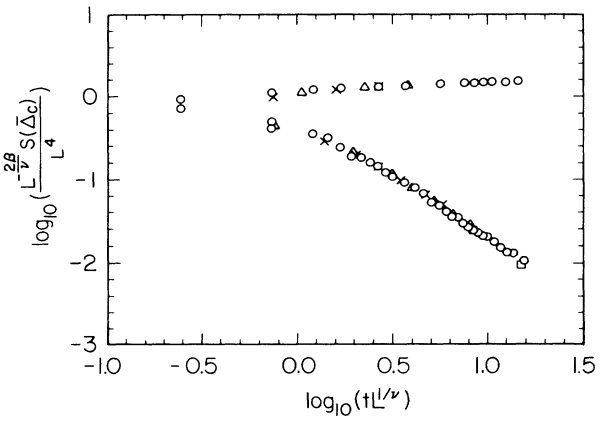

FIG. 8. Finite-size scaling plot of $S(\bar{\Delta}_c)$. The values of β and ν used were those of the three-state Potts model. T_c was taken to be $0.7875E_2$.

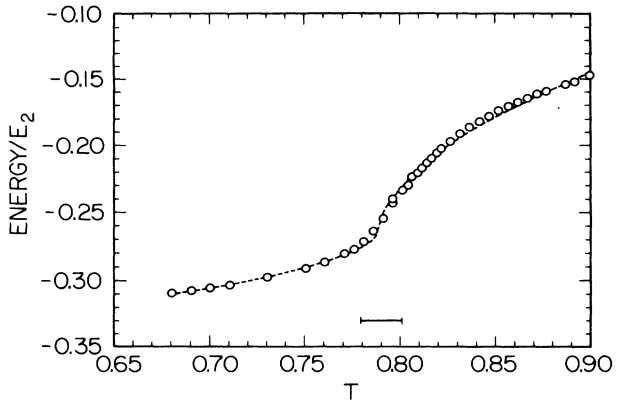

FIG. 10. Temperature dependence of the energy at $z=2.5$. The dashed line gives the best fit to an energylike singularity with $\alpha=\alpha'$ and no linear background term. The thermal range between the bars was excluded in the fit. Notice the evident asymmetry above and below T_c, suggesting that at least the amplitude of the singularity above T_c is not equal to the amplitude below.

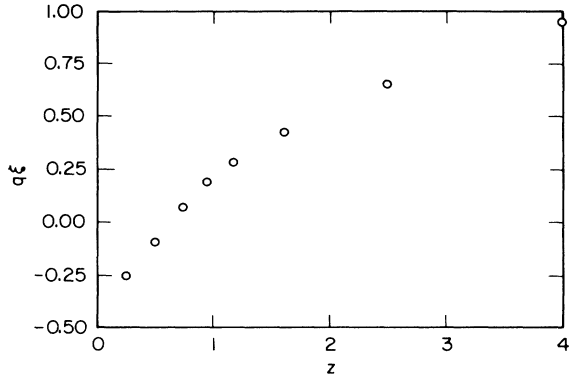

FIG. 11. Activity dependence of $q\xi_x$ 5% above T_c (where T_c was estimated through the use of transfer-matrix scaling).

tion the caveat that our systems might be too small to observe the correct asymptotic behavior.

If $X_+(\mathbf{w})$ is universal and peaks away from $\mathbf{w}=\mathbf{0}$, then $q\xi_x$ in the limit of T approaching $T_c(z)$ from above should be universal[4] and thus independent of z. To test this prediction, we performed extensive simulations at two other activities ($z=1.62$ and 4.0). Plots of $q\xi_x$ versus T at these activities are shown in Fig. 7. If a thermal range 3–10% above T_c is in the asymptotic scaling regime then this figure suggests that the limit of $q\xi_x$ as t approaches zero, and thus the scaled structure factor, is not universal. Figure 11 shows the dependence of $q\xi_x$ on the activity 5% above T_c (as estimated for each z from a standard finite-size scaling study using transfer matrices[40]). Taken at their face value these plots suggest that at least the effective scaling function is not universal. This could occur if the chiral field were a marginal operator away from the line of zero chirality (as is simple lattice anisotropy in the Ising model[41]). The other possibility is that we are observing crossover from the behavior at zero chirality to something else, which would mean that none of our data shows the asymptotically correct behavior. This alternative would leave unexplained why the data evidently scale, in a way different from at zero chirality, for relatively large ranges of t and $\delta\mathbf{k}$.

IV. FINAL COMMENTS

In the finite-sized lattice gas studied here, we observe that the structure factor effectively scales with three-state Potts model exponents but with a non-Potts-like scaling function. Whether this behavior is characteristic of the infinite system asymptotically close to T_c is difficult to know, but it suggests the behavior that one might expect to be encountered in chemisorption-system realizations on imperfect substrates.

The questions raised in this discussion are not unique to the (3×1) phase of course, and any experimental measurement of the temperature dependence of $q\xi$ in a system where q is temperature dependent would be interesting. As an example of a system where an incommensurately disordered system has evidently been observed, we mention O/Ni(111).[42] At coverages slightly above $\frac{1}{4}$ of a monolayer, the $p(2\times2)$ ordered state makes a transition to a state with diffuse diffraction beams peaked at noncommensurate positions. Monte Carlo simulations[43] suggest that the incommensurability is coupled to the occurrence of two types of binding sites. It would be interesting to examine experimentally the transition of the $p(2\times2)$ commensurate state to this disordered state—especially the coverage dependence of the incommensurability. In some systems the breakdown of lattice-gas symmetries causes the disordered phase to be incommensurate.[44,45]

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$$\psi_{\mathbf{k}}=\int d^2r\,\psi(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}},$$

$\langle \mathcal{H}_c \rangle$ becomes

$$2g_c\ \mathrm{Re}\left[\int d^2k k_x \langle \psi_{\mathbf{k}}\psi_{\mathbf{k}}^{*}\rangle\right]=2g_c\int d^2k\, k_x \mathcal{S}(\mathbf{k},g_c,T)\ ,$$

where $\mathcal{S}(\mathbf{k},g_c,T)$ is the structure factor appropriate for the three-state Potts model: For the q-state Potts model the structure factor is defined as $\mathcal{S}(k)=\langle\,|\sum_{\mathbf{r}}\hat{\epsilon}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}|^2\rangle$, where $\hat{\epsilon}(\mathbf{r})$ points to one of the q symmetric directions of a hypertetrahedron in $q-1$ dimensions (here to three corners of an equilateral triangle). Thus the first moment of the structure factor measures the expectation value of the chiral term: The chiral term makes the structure factor anisotropic. Notice that the structure factor has the property that $\mathcal{S}(\mathbf{k},g,T)=\mathcal{S}(-\mathbf{k},-g,T)$ [D. A. Huse, A. M. Szpilka, and M. E. Fisher, Physica **121A**, 363 (1983)]. For $|\mathbf{k}|$'s much smaller than the inverse lattice constant, $\mathcal{S}$ should be proportional to S defined by Eq. (1) evaluated close to the 3×1 superlattice δ-function positions.

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