Critical Points for Dimer Models with $\frac{3}{2}$-Order Transitions*

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A new extensive variable A and its conjugate field Π are introduced for the Kasteleyn dimer model on the honeycomb lattice via an isomorphic membrane-polymer chain model. The resultant phase diagram has a first-order phase line, thereby revealing a nonlocal order parameter in this model for the first time. The first-order line terminates in a critical point with critical exponents $\alpha=\alpha'=0$, $\beta=1=\gamma=\gamma'$, and $\delta=2$. The $\frac{3}{2}$-order exponents appear on the line $\Pi=\Pi_{\text{critical}}$.

The Kasteleyn dimer model on the honeycomb lattice,[1] to be called the K model, is one of the few exactly solvable statistical mechanical models of cooperative phenomena. Therefore, it has been disturbing that the phase transition in the K model is highly unusual. In particular, no order parameter which is identically zero in the high-temperature phase has previously been found even though the model is perfectly ordered in the low-temperature phase.

The known behavior of the transition is that the free energy F is a constant for T less than T_c, while above and near T_c the free energy has an extra piece which behaves as $(T-T_c)^{3/2}$ which gives rise to a $(T-T_c)^{-1/2}$ divergence in the specific heat. Because the lowest derivative to be simply or finitely discontinuous is the third derivative with respect to $(T-T_c)^{1/2}$, this transition has been called a $\frac{3}{2}$-order transition.[2]

The K model is the simplest member of a family of dimer models, the relation being that each member has a $\frac{3}{2}$-order transition. Various members of this family have been used to model ferroelectrics,[3] biomembranes,[4] and polymers.[5] The K model itself is isomorphic to the membrane-polymer model when the latter is constrained to maximum density.

The purpose of this Letter is to define two new variables, an area A and a surface pressure Π, suggested by the membrane analog. In terms of these new variables one obtains a phase diagram in which the $\frac{3}{2}$-order transition for the K model appears as a critical point at the end of a first-order transition line along which two phases coexist in equilibrium. The variable A is discontinuous across the first-order transition and the discontinuity goes to zero at the critical point. This kind of behavior is usually described by the critical exponent β and the corresponding variable is usually called the order parameter. Although the variable A is not a local order parameter of the sort which appears in spin models, it seems reasonable to identify it tentatively it as a nonlocal order parameter and assign the exponent β to the discontinuity in A.

The states of the K model consist of nonoverlapping dimers which completely fill the honeycomb lattice, with dimer energies assigned as in Fig. 1. (Actually, Kasteleyn considered a more general version with unequal energies for the two kinds of horizontal dimers, but the symmetrical case exhibits all the properties of interest.) The partition function is

$$Z(x)=\sum\nolimits_n \Omega(n)x^n, \tag{1}$$

where $x=\exp(-\epsilon/kT)$ and $\Omega(n)$ is the number of configurations with n horizontal dimers. With use of the Pfaffian method[6] and a unit cell of four sites the following expression for the logarithm

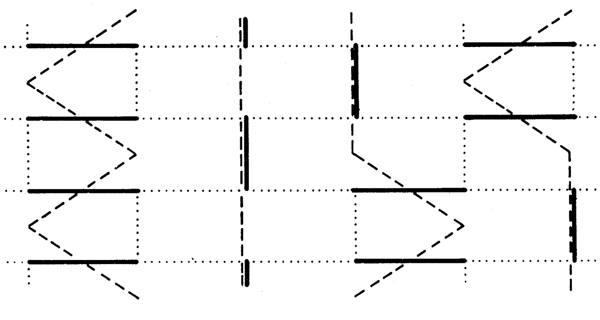

FIG. 1. The brick lattice, which is topologically equivalent to the honeycomb lattice, is shown as dotted and heavy solid lines. The heavy solid lines represent the dimers, of which there are five vertical ones shown or partly shown, each with zero energy, and eight horizontal ones, each with energy ϵ. The isomorphic membrane-polymer chain state with parts of four chains is shown in dashed lines. This finite-lattice state has $\rho_x=\frac{1}{3}$ and $A=1.5$.

of Z per lattice site N is easily derived:

$$N^{-1}\ln Z=\frac{1}{8\pi^2}\int_0^{2\pi}d\varphi_1\int_0^{2\pi}d\varphi_2\ln|g(\varphi_1,\varphi_2)|^2,$$

where

$$g(\varphi_1,\varphi_2)=2x^2(1-\cos\varphi_1)-\exp(i\varphi_2) \qquad (2)$$

and the density of horizontal dimers ρ_x can be calculated explicitly as

$$\rho_x=\begin{cases}\pi^{-1}\cos^{-1}(1/2x), & x\geq\frac{1}{2},\\ 0, & x\leq\frac{1}{2}.\end{cases} \qquad (3)$$

This demonstrates the $(T-T_c)^{1/2}$ behavior of the energy (which is $\epsilon\rho_x$) at the critical temperature given by $T_c=\epsilon/\ln 2$ where $x_c=\frac{1}{2}$.

The above well-known results are incomplete thermodynamically because there is really only one variable in the problem, call it T or ϵ/T. The customary addition of a field δ imposed on, say, the horizontal dimers only changes the single variable to $(\epsilon+\delta)/T$ without in any way changing the nature of the transition. The obvious trial order parameter is the density ρ_v of vertical dimers which is maximal, namely $\rho_v=\frac{1}{2}$, for $T<T_c$. However, ρ_v is never zero above T_c, nor is any linear combination of ρ_v and ρ_x always zero above T_c, so that these do not behave like ordinary order parameters.

In order to complete the thermodynamic description of the K model let us consider a new variable,

$$A=(1-\rho_x)^{-1}. \qquad (4)$$

If there are M sites on a horizontal row of the lattice, then in the isomorphic membrane-polymer model the number of chains cutting this row is M/A or the mean area per chain is A. (See Fig. 1.) Conservation of chain links demands conservation of the number of lattice sites N, but as ρ_x increases from zero (to a maximum of $\frac{1}{2}$) the number of lattice sites in the horizontal rows increases by a factor of A in order to conserve the number of chains and the number of sites in the vertical direction decreases by a factor of A^{-1} in order to conserve the mean chain length in the vertical direction. These changes in lattice shape are natural for the membrane-polymer model since the conjugate force to A will be a lateral pressure Π operating only in the horizontal direction. In dimer language the parameter A and these changes in lattice shape are not so physically motivated. A more "natural" dimer variable follows from considering the vertical dimers as particles and the horizontal dimers as holes with no change in lattice shape. However, this choice, call it $V=(1-2\rho_x)^{-1}$ and its conjugate field P, leads to a phase diagram with a rather uninteresting line of $\frac{3}{2}$-order transitions, and so we exercise our freedom of choice to consider the variable A. It should be noted that the expansion or contraction of any lattice side is at most by a factor of 2 so that the shape change does not affect the values of ρ_x and $N^{-1}\ln Z$ in Eqs. (2) and (3) in the limit of an infinite lattice, $N\to\infty$.

The statistical mechanics with the new variables A and Π is carried out in a canonical ensemble. In chain language the number of chains N_c is kept fixed and the temperature T and the mean area per chain A are fixed. The latter A constraint is much like the volume constraint imposed in the canonical ensemble calculation for classical gases. Thus, the partition function is

$$Z(T,A)=\sum_{A\text{ states}}\exp(-\epsilon/kT)$$
$$=\Omega(n_A)\exp(-n_A\epsilon/kT), \qquad (5)$$

where n_A is the number of horizontal dimers required by all states with area A and Ω is defined in (1). The unusual feature, which is not shared by spin-type models, is that the total energy $NE=n_A\epsilon$ is completely specified by A and Ω is defined for all states with the same A. This is a consequence of the absence of finite energy interactions between dimers in the model, or the presence of only infinite-excluded-volume interactions. The free energy per lattice site is

$$F(T,A)=-kTN^{-1}\ln Z=\rho_x\epsilon-TS(A), \qquad (6)$$

where $S(A)=-kN^{-1}\ln[\Omega(n_A)]$. Notice that S, like E, is also *not* a function of T but only of A. Computationally, S is obtained from (1)–(3) by using the maximum-term argument,

$$N^{-1}\ln[Z(x)]=\max_n\{N^{-1}[\ln(\Omega(n))+n\ln x]\}$$
$$=k^{-1}S(A)+\rho_x\ln x. \qquad (7)$$

Specifically, given A, ρ_x is determined by (4), x is determined by (3), $\ln Z$ is determined by (2), and $S(A)$ is then determined by (7).

The difference between this treatment and all previous treatments, reviewed in Eqs. (1)–(3), is that x in (7) is not determined by $x=\exp(-\epsilon/kT)$. Rather, x is merely a variable related to ρ_x and A whose use enables us to compute $S(A)$. Now, if $x\neq\exp(-\epsilon/kT)$, then some extra force or pressure will be needed to stabilize the homogeneous macrostate described by A and T. This ex-

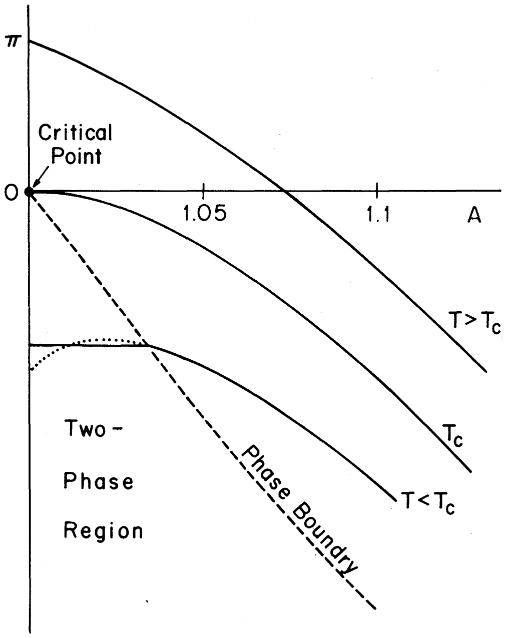

FIG. 2. A schematic sketch of the Π-A isotherms. Each isotherm proceeds to $\Pi = +\infty$ along the line $A=1$.

tra pressure is just Π which is given by

$$\Pi = -(\partial F/\partial A)_T. \qquad (8)$$

Equation (8) is fully equivalent to the combined first and second laws of thermodynamics, namely

$$TdS = dE + \Pi dA.$$

Previous treatments, by requiring $x = \exp(-\epsilon/kT)$, implicitly set $\Pi = 0$.

The Π-A isotherms are plotted in Fig. 2. The isotherms do not end at $A=1$ but continue to $\Pi = +\infty$ at $A=1$, because for a perfectly ordered state of incompressible objects the pressure can increase indefinitely without changing the volume. Isotherms for $T < T_c$ have portions with negative compressibilities, therefore indicating unstable two-phase regions. Although Van der Waals loops are often taken as a sign of an approximate or incomplete calculation, I emphasize that they must appear in this calculation if there are any two-phase regions because the values of S were calculated for a given ρ_x *under the assumption of a homogeneous state.* The unstable and metastable portions of the isotherms are easily eliminated by finding another state with lower Gibbs free energy $G = E - TS + \Pi A$ at the same T and Π; this gives the same result as the Maxwell equal-area construction. There is no difficulty in having low-A and high-A phases coexisting side by side on the same lattice; indeed, the domain-wall energy is zero. The existence of analytic metastable continuations into the two-phase region means that there is no essential singularity on the phase boundary as there is in some models.[7,8] This is reasonable since there is no domain-wall or "dropletlike" free energy because of the lack of finite energy interactions between dimers.

The critical behavior of this model is still somewhat unusual. Close to the critical point at $\Pi = 0$, $A=1$, and $kT_c = \epsilon \ln 2$ the pressure behaves, for $A > 1$, as

$$\Pi \sim \Pi_0(T) - c[A - A_0(T)]^2, \qquad (9)$$

where

$$\Pi_0(T) \sim b(T - T_c) \qquad (10)$$

and

$$A_0(T) \sim 1 + a(T_c - T). \qquad (11)$$

The coexistence curve follows $A_0(T)$ which gives the critical exponent $\beta = 1$ for the nonlocal order parameter, which is the discontinuity in A across the first-order phase line. From (9) the critical isotherm behaves as $\Pi \sim (A-1)^2$ so that $\delta = 2$. Since S is only a function of A, $C_A = 0$ identically and $\alpha = 0 = \alpha'$. Along both the disordered side of the coexistence curve and the line $A=1$, $T > T_c$, the compressibility $K_T = -A^{-1}(\partial A/\partial \Pi)_T$ diverges as $|T - T_c|^{-1}$ so that $\gamma = 1 = \gamma'$. The $\frac{3}{2}$-order exponents appear on the line $\Pi = 0$, where $A - 1 \sim (T - T_c)^{1/2}$ and $C_\Pi \sim (T - T_c)^{-1/2}$.

The Π-A phase diagram in Fig. 2 is reminiscent of some produced by Fisher and Felderhof[8] for rather different one-dimensional models with many-body interactions. In their case the models did not obey the usual scaling relation $\gamma = \gamma'$ while in the present case $\alpha + 2\beta + \gamma = 3$, not 2.

Although it is clear that the transition in the K model remains an unusual one, at least it now has a phase diagram which can be compared to the more usual ones and a nonlocal order parameter which is the discontinuity in the new variable A across the first-order transition. The unusual features of the transition are reasonable in view of the excluded-volume or "hard" interactions between dimers (or chains) in the model and the lack of finite pairwise or "soft" interactions. This makes the K model an important one for systems in which the excluded-volume effects may dominate the transition. Further work in this direction is being done on other models in the $\frac{3}{2}$-order family including the full membrane-polymer model with variable density, in order to compare to Π-A lipid monolayer experiments.[9]

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Specular Reflection of ^{4}He Atoms from the Surface of Liquid ^{4}He[†]

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Measurements with a pulsed ^{4}He atomic beam incident on the surface of liquid ^{4}He at $T = 0.03$ K show that the probability of specular reflection depends only on the perpendicular momentum of the atom $\hbar k \cos\theta$ and that it varies smoothly from 4×10^{-2} to less than 10^{-4} for $k\cos\theta$ in the range from 0.05 to 0.6 Å^{-1}. The probability of diffuse inelastic scattering is less than 2×10^{-3}. Contrary to theoretical expectations, there is no significant change in the reflection probability at the roton threshold at $k = 0.5$ Å^{-1}.

This Letter describes measurements of the elastic scattering probability of low energy ($0.1\ \mathrm{K} \lesssim \hbar^2k^2/2mk_\mathrm{B} \lesssim 3\ \mathrm{K}$) ^{4}He atoms incident on the free surface of superfluid ^{4}He. The probability of elastic scattering $R(k,\theta)$ was measured as a function of the angle of incidence θ and the momentum $\hbar k$ of the incident atoms. In addition, a search was made for atoms inelastically scattered from the surface which gives an upper limit for the probability of inelastic scattering, $D(k,\theta)$. The liquid-helium surface was varied in temperature between 0.03 and 0.12 K and no temperature dependence in R was observed. The experimental $R(k,\theta)$ is therefore characteristic of the ground state of the liquid and its surface. Our experiment is related to a number of theoretical discussions[1-6] of the process of condensation and evaporation at the surface of superfluid helium. It has been claimed[3,5] that $R(k,\theta)$ is related to the single-particle spectral density function in the liquid and therefore[3] perhaps to the elusive n_0, the fraction of atoms in the condensed state. This claim is based on the application of tunneling theory and supposes that the tunneling Hamiltonian which couples the vacuum states to the liquid is weak, implying that the probability of condensation $f(k,\theta) \equiv 1 - R - D$ is small. Our results, on the contrary, show that, even for large θ and small k, $f(k,\theta) \simeq 1$ with R and D both small. We deduce that "weak" tunneling theory is probably invalid, and note that the effect of the finite thickness of the surface region and the effect of the surface excitations (ripplons) have not been included in any of the published theoretical calculations.

Apart from its possible connection with the condensate fraction, the reflection probability $R(k,\theta)$ is related to $\omega(k)$, the phonon spectrum of the liquid (shown in Fig. 1). As was pointed out by Anderson[2] and Widom and co-workers,[1] a condensing atom with momentum $\hbar k$ transfers an energy $\epsilon = L_0 + \hbar^2k^2/2m$ to the liquid, where $L_0/k_\mathrm{B} = 7.16$ K is the latent heat at absolute zero. If the atom produces a single "roton," i.e., a phonon near the minimum in $\omega(k)$, a minimum kinetic energy $(\Delta - L_0)/k_\mathrm{B} \simeq 1.5$ K is required. It has been predicted[1,2,5] that this will produce a discontinuity in the k dependence of $R(k,\theta)$ at $k = 0.50$ Å^{-1}. The possible detection of this discontinuity was one of the reasons for undertaking