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Exact solution to a new anisotropic dimer model with domain-wall behavior

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The exact solution is given for the thermal behavior of a dimer model that has two kinds of infinite energy excitations that can be described as heavy and light domain walls in a 2×1 adsorbed-atom model. These walls may reverse their direction with respect to the anisotropy axis and, upon meeting, unlike walls may annihilate. In the general case there are three phases and the intermediate phase is an incommensurate phase with a difference in population of the two kinds of walls. A further generalization of the model is given in which like walls may also annihilate.

We have discovered an exactly solvable cooperative model with two independent energies, ε and δ, which has the thermal behavior shown in Fig. 1. For the special case when $\delta=\infty$, Fig. 1(a), the model is closely related to a model first solved by Kasteleyn[1] called the K model.[2] The specific heat of both models is zero in the low-temperature phase followed by a square-root divergence above the transition. The square-root divergence above T_c and a finite, but not necessarily zero, specific heat below T_c has been called a $\frac{3}{2}$-order transition[3] because it involves an extra piece proportional to $(T-T_c)^{3/2}$ added to the free energy above T_c. The same kind of thermodynamic behavior was later found for two-dimensional commensurate-incommensurate (CI) transitions[4] and the connection between the two kinds of problems has been observed.[5,6] For the special case when $\delta=0$ the specific heat of the new model has a square-root divergence on the low-temperature side of the transition and is finite on the high-temperature side. This will be called an inverted $\frac{3}{2}$-order transition. For the general cases $0<\delta<\varepsilon$ and for $\varepsilon<\delta<\infty$ there are two transitions, a $\frac{3}{2}$-order transition at a lower temperature and an inverted $\frac{3}{2}$-order transition at a higher temperature. For the special case when $\delta=\varepsilon$ the model is the ferroelectric stannous chloride dihydrate model,[7] which has a symmetric logarithmic divergence in the specific heat similar to the two-dimensional Ising model. In this context the more usual logarithmic Ising-like transition appears as a multicritical point where the $\frac{3}{2}$-order transition becomes confluent with the inverted $\frac{3}{2}$-order transition.

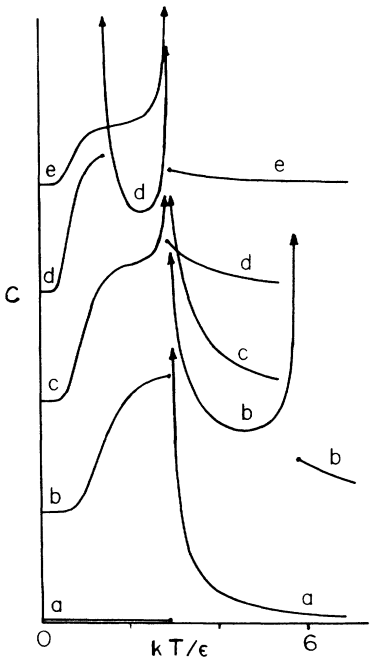

FIG. 1. The specific heat C as a function of K_BT/ε for (a) $r=\delta/\varepsilon=\infty$, (b) $r=2$, (c) $r=1$, (d) $r=\frac{1}{2}$, and (e) $r=0$. Each curve goes to zero at $k_BT/\varepsilon=0$.

The exactly solvable model that has the preceding thermal behavior is a dimer model on the 4-8 lattice shown in Fig. 2. Each lattice site is covered by one end of a dimer which covers a bond and two neighboring lattice sites and with the crucial constraint that no lattice site is covered by two dimers. The energy for each dimer on either vertical

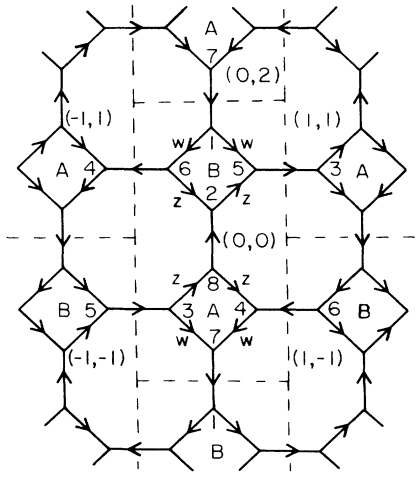

FIG. 2. The 4-8 lattice is shown by the solid lines, and the dashed lines portray the unit cells, indexed by (i,j), of the dimer model which has activities z or w for dimers on bonds around the squares, as indicated, and activity 1 for each dimer on all horizontal and vertical bonds.

or horizontal bonds is taken to be zero; the ground state has each of these bonds occupied by a dimer. Each dimer on a tilted bond around the squares has energy ε for those bonds marked by the activity $z=\exp(-\varepsilon/k_BT)$ in Fig. 2 and energy δ for those bonds marked by the activity $w=\exp(-\delta/k_BT)$.

Using the Pfaffian method[1] the exact solution for the free energy per dimer is

$$F/N=-k_BT(1/16\pi^2)\int_0^{2\pi}d\theta\int_0^{2\pi}d\phi\ln|\det M(z,w,\theta,\phi)|\ , \tag{1}$$

with

$$\det M(z,w,\theta,\phi)=-2\cos\theta(vz^2+v^{-1}w^2)+(1+4z^2w^2)\ , \tag{2}$$

where $u=\exp(i\theta)$ and $v=\exp(i\phi)$. The critical behavior of this model is determined by the roots of M, which are shown in Fig. 3. For $z^2=\frac{1}{2}$ or for $w^2=\frac{1}{2}$ one root appears at $\theta=0=\phi$. This root locates the critical points which divide the zw square in Fig. 3 into four regions which will be named (i) the LT (low-temperature) region for $z^2<\frac{1}{2}$ and $w^2<\frac{1}{2}$, (ii) the HT (high-temperature) region for $z^2>\frac{1}{2}$ and $w^2>\frac{1}{2}$, and two intermediate temperature regions, (iii) IT^+ for $z^2>\frac{1}{2}$ and $w^2<\frac{1}{2}$, and (iv) IT^- for $z^2<\frac{1}{2}$ and $w^2>\frac{1}{2}$. For values of z and w in the two off-diagonal regions, IT^+ and IT^-, there are also roots at values of $\pm\Theta$ between 0 and $\pi/3$ and some contours of Θ are shown in Fig. 3.

The density of z dimers minus the density of w dimers is given by

$$\rho_{z-w}=\pm\Theta/\pi\ , \tag{3}$$

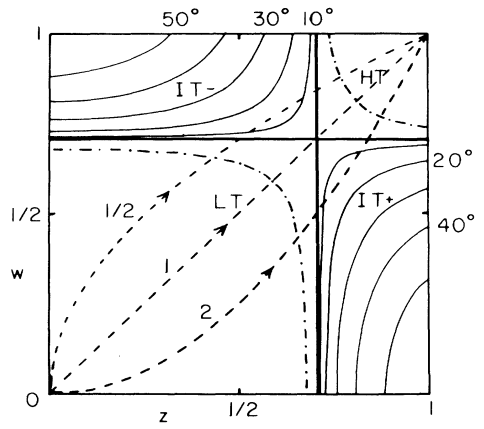

FIG. 3. The zw activity plane for $\varepsilon>0$ and $\delta>0$ with the loci of zeros of det M indicated by solid lines. The dashed lines are the thermal trajectories for $r=\frac{1}{2}$, 1, and 2. The dot-dash lines are the loci of zeros of det M for $x=0.3$ in the generalized model with like-wall dislocations.

where

$$\cos\Theta=(1+4z^2w^2)/2(w^2+z^2)\text{ in }IT^{\pm}$$
$$=1\text{ in LT and HT}\ . \tag{4}$$

Also, the specific heat is given by

$$C/N=(C_1+C_2)/\pi k_BT^2\text{ in regions }IT^{\pm}$$
$$=C_2/\pi k_BT^2\text{ in regions LT and HT}\ , \tag{5}$$

where

$$C_1=\frac{2[\varepsilon z^2(4w^4-1)-\delta w^2(1-4z^4)]^2}{(1+4z^2w^2)|(z^4-w^4)|[(1-4z^4)(4w^4-1)]^{1/2}}\ ,$$

and

$$C_2=8(\varepsilon+\delta)^2(4z^4w^4+z^2w^2)\int_\Theta^{\pi/2}\sin^2\theta[(4z^2w^2+1)^2-16z^2w^2\cos^2\theta]^{-3/2}d\theta\ ,$$

and Θ is given in Eq. (4). The crossover from the pair of $\frac{3}{2}$-order transitions to the Ising-like transition that occurs when $z^2=\frac{1}{2}=w^2$ is fully displayed by Eq. (5) with the C_1 contribution accounting for the $\frac{3}{2}$-order transitions and the C_2 term accounting for the Ising-like transition. By noting that the transition temperature varies with the relevant parameter, $\varepsilon-\delta$, in a linear fashion, one may assign a conventional crossover exponent $\phi=1$.

Some intuitive understanding of the behavior of this model can be obtained by examining a domain-wall isomorphism. In turn, this isomorphic model should be of interest in the study of $p\times l$, domain-wall, commensurate-incommensurate phase transitions in adsorbed monolayers on solid substrates.[6,8-11] The domain-wall isomorphism is illustrated in Fig. 4 in which the heavy lines indicate, for the particular dimer state under consideration, those ground-state bonds that do *not* have dimers and those z and w bonds that *do* have dimers. In the upper left corner is shown, by a heavy octagon, the smallest perturbation, with energy $2(\varepsilon+\delta)$. Starting at the bottom left is a heavy line that wanders through the center of the figure and goes out the top. This will be called a z wall because it must utilize only z bonds when it is going upwards. However, the upwardly directed wandering is reversed in the middle, during which reversal the wall utilizes only w bonds. On the far right of the figure a w wall is shown which utilizes z bonds only when reversals occur, as in the lower right-hand corner.

The domain-wall picture illustrates an important conservation property for the 4-8 lattice. Let n_{z-w} be the number of z bonds minus the number of w bonds for each row of the lattice. The conservation property is that for any dimer state n_{z-w} is the same for every row. For example, in Fig. 4, $n_{z-w}=0$. The addition or deletion of loops does not change n_{z-w}. However, if the w wall in Fig. 4 were deleted, then n_{z-w} would increase to 1. In general, n_{z-w} counts the number of z walls minus the number of w walls, and the corresponding density ρ_{z-w} is proportional to the density of z walls minus the density of w walls. Although this illustrative discussion should suffice to convince most readers, it is also possible to prove this conservation property rigorously.

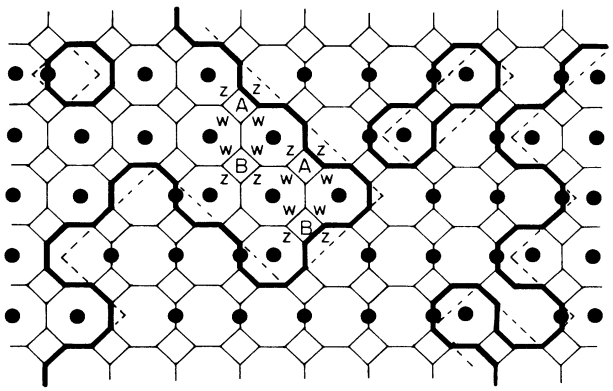

FIG. 4. An illustration of the domain-wall isomorphism and the adsorbed atom state for a particular dimer state of the model.

From the exact result for ρ_{z-w} the density of z walls equals the density of w walls in the low-temperature region in Fig. 3 and it seems very likely that the density of infinitely long walls of both kinds is zero in this low-temperature region. From the exact result for ρ_{z-w} the density of infinitely long z walls is definitely different from the density of infinitely long w walls in the IT$^{\pm}$ regions in Fig. 3. Because ρ_{z-w} becomes zero again in the HT region, it appears that this is the important underlying feature, which stems from the conservation principle elucidated above, that characterizes the intermediate phases IT$^{\pm}$.

To our knowledge, the inverted $\frac{3}{2}$-order transition has not previously been observed as the exact solution of any model before, although it has been found using the free fermion approximation to the axial next-nearest-neighbor Ising model[12] and a model of adsorbed atoms.[13] In our model this transition is clearly associated with proceeding, as temperature increases, from a phase with nonzero ρ_{z-w} to one with $\rho_{z-w}=0$. However, the description of the high-temperature phase in terms of domain walls is not completely clear. There could be equal nonzero densities of infinitely long z walls and w walls or there could be only finite length walls that occur in loops. Certainly, in either the $T=\infty$ limit or on the isotropic $w=z$ line, the model becomes isotropic in space so there should be no preference for either z or w walls in the upward direction. Perhaps the wall orientation becomes isotropic in the entire HT region, in which case the phase above the inverted $\frac{3}{2}$-order transition is best described as a disordered fluid phase. If so, then this model exhibits the full sequence of a low-temperature commensurate phase, followed by a phase transition into an incommensurate domain-wall phase, followed by another phase transition into a fully fluid phase. Further information for discussing this kind of question will come from a study of the decay of the correlation functions in the two principle directions, like the ones recently performed for the K model.[14]

Starting from the domain-wall picture one may construct states of 2×1 adsorbed atoms in several ways. One way, which is shown in Fig. 4 by the filled circles, places atoms at the centers of the octagons in one of the commensurate phases and at the centers of the vertical bonds in the other commensurate phase, and each domain wall separates unlike phases. The w walls are formed by placing atoms on each vertical wall bond which makes them into heavy walls. The z walls in Fig. 4 are formed by leaving each vertical wall bond vacant, which makes them light walls. (The dashed lines in Fig. 4 join the centers of the pairs of neighboring occupied or unoccupied sites and give a somewhat less wiggly representation of the domain walls.) The energy of each adsorbed atom state is 2ε times the number of pairs of neighboring horizontal sites that are unoccupied plus 2δ times the number of occupied pairs. These are the energies of wall formation. As one proceeds from row to row, the centers of each wall are forced to move by two lattice spacings either way along the x direction. This is different from the more typical picture in which walls can either not move as one proceeds from row to row or can move by two lattice spacings with higher energy, and this difference is reflected in different local energies for the adsorbed atom configurations. Nevertheless, this model should be in the same universality class for phase transitions as models with more realistic local interactions because the nature of critical points is determined not by the details of short-range interactions but by the nature of the long-range correlations. For domain-wall models this means that the important features are the symmetry (striped nature) of the walls which must have a degree of wandering freedom and a mutual repulsion, which in our case is the inability of the walls to touch or cross.

Because of the conservation of n_{z-w} from row to row in the dimer model, the number of adsorbed atoms is conserved in each row in this 2×1 adsorbed atom model. Nevertheless, pairs of unlike walls can be annihilated or created simply by moving one atom by one lattice site in a homogeneous domain, thereby creating either the terminus of a loop or a wall reversal, often called a dislocation point, at which the other phase is inserted. The dislocation points in this model are quite different from the ones present in an exactly solvable dimer model introduced by Bhattacharjee.[15] In terms of the present model, his model with no dislocations is very similar to the special case $w=0$, in which heavy w walls are prohibited. His dislocations are locations where two light z walls annihilate, thereby breaking the mass conservation from row to row. We can also generalize our model to allow dislocations between like walls simply by adding bonds with activity x, corresponding to an energy of like-wall dislocation, between sites 3 and 4 and also between sites 5 and 6 in Fig. 2. The resulting formulas are much more complicated and the details will be presented in a subsequent paper. However, numerical analysis indicates that for each value of $0<x<1$ the IT$^{\pm}$ regions become one region in the zw plane in Fig. 3. The boundary of the new IT region is characterized by two lines of zeros in det M, as is shown by the dot-dash lines in Fig. 3 for $x=0.3$, but there appear to be no zeros within the new IT region. For the special case, $w=0$ and $x\neq0$, there is only one Ising transition, in agreement with Bhattacharjee's result.[15] However, for $w\neq0$ it appears that the generalized model undergoes an Ising-like transition from the LT phase to the IT phase followed by another Ising-like transition from the IT phase to the HT

phase. This suggests that the high-temperature phase in the $w=0$ model with like-wall dislocations may in some sense be more like an incommensurate phase rather than the more disordered phase that is attained at high temperature when $w \neq 0$.

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