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Tricriticality of Interacting Hard Squares: Some Exact Results

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Baxter has solved a restricted class of square lattice gas models with nearest-neighbor exclusion (thus "hard squares") and next-nearest-neighbor interactions. Arguments are presented which demonstrate that the subspace spanned by his exact solution contains the line of tricritical points *and* the associated surface of first-order transitions of hard squares with *attractive* next-nearest-neighbor interactions. The tricritical exponents so identified confirm those obtained by Nienhuis for a dilute Ising model.

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Baxter[1,2] has recently solved the hard hexagon model, a triangular lattice gas with nearest-neighbor exclusion. The critical exponents for the specific heat ($\alpha = \alpha' = \frac{1}{3}$), the order parameter ($\beta = \frac{1}{9}$), the correlation length, and the surface tension[3] ($\nu = \nu' = \mu = \frac{5}{6}$) are precisely those conjectured[4,5] or calculated with the help of certain assumptions[6] for a three-state Potts model. Thus, if one accepts the arguments presented,[7,8] on symmetry grounds, that the critical points of the hard hexagon model and the three-state Potts model are in the same universality class, then Baxter's calculation may be regarded as the first exact calculation of the critical exponents of a three-state Potts model.

In solving the hard hexagon model Baxter[1,2] considers a more general class of *square* lattice gas models with nearest-neighbor (nn) exclusion (thus "hard squares"): For each site i of the lattice there is an occupation number $n_i = 0$ or 1. The Boltzmann weight, $W(\underline{n})$, of a configuration, $\underline{n}$, vanishes if any pair of nn sites are simultaneously occupied, reflecting the hard-square condition. Next-nearest-neighbor (nnn) or diagonally connected sites interact, contributing to $W(\underline{n})$ factors of $\exp(Ln_in_k)$ and $\exp(Mn_jn_l)$ for nnn pairs connected by NE-SW and NW-SE diagonals, respectively. The Boltzmann weight also contains a factor z^{n_i} for each site i, where z is the lattice gas activity. Hard hexagons[1] are the limit $L \to 0$, $M \to -\infty$ (or vice versa). This Letter focuses on the case of hard squares with nnn *attractions*, $L, M > 0$.

The anticipated phase diagram for $L = M$ is shown in Fig. 1. The form of this phase diagram should be the same (i.e., universal) for all bounded, positive ratios L/M. At low activity, z, there is a dilute fluid phase, while at high z the system orders, forming a solid phase in which one of the two sublattices is preferentially occupied. When the nnn attraction, L, between hard squares is sufficiently strong the fluid-to-solid phase transition is of first order. On the other hand, if the nnn interactions are less attractive or repulsive the fluid-to-solid transition is continuous[9]; on the basis of symmetry arguments[8] this critical line is expected to be in the Ising universality class. A tricritical point,[10] T in Fig. 1, divides the phase boundary into first-order and critical regimes. The symmetry of the model indicates that this tricritical point should be in the same universality class as the tricritical

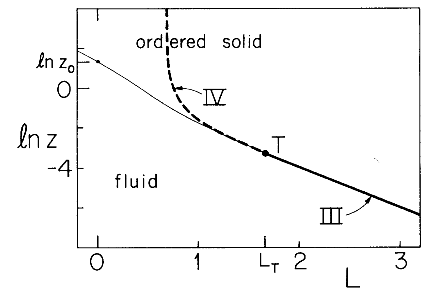

FIG. 1. The phase diagram of a hard square lattice gas with activity z and nnn interactions L. For large L the ordered solid and disordered fluid phases are separated by a first-order phase boundary, marked III, that terminates at a tricritical point, T. The dashed line, IV, represents the balance of Baxter's exactly solvable manifold (see text). The order-disorder transition line, shown schematically, represents a continuous transition for L less than L_T, the tricritical value; the Ising character of this transition has been checked only for the noninteracting case, $L = 0$, where the transition at $z_0 \simeq 3.796$ is indicated (see Ref. 9).

point of a dilute Ising model.

The lattice gas model described above contains three parameters, z, L, and M, or in terms of the basic Boltzmann factors, z, $x_1 \equiv e^{-L}$, and $x_2 \equiv e^{-M}$. Baxter[1,2] has succeeded in solving this model only on a two-dimensional manifold defined by

$$z = x_1 x_2 (1-x_1)(1-x_2)/(1-x_1-x_2). \tag{1}$$

He divides this exact-solution manifold (call it Baxter's surface) into six regimes: regimes I, II, V, and VI involve $L > 0$ and $M < 0$ or vice versa; these regimes contain the hard hexagon model and will not be discussed here. Regimes III and IV have $x_1 + x_2 < 1$ and so involve attractive nnn interactions along both diagonals. These latter two regimes of his exact solution intersect Fig. 1, where $x_1 = x_2$, in a single curve; call it Baxter's curve. Baxter[2] parametrizes this curve analytically so that $p > 0$ in regime III, where the system is apparently fluid, while $p < 0$ in regime IV, which Baxter finds is in the ordered solid phase. At the point $p = 0$, which divides Baxter's curve into the two regimes, he finds[1,2] that the thermodynamic potential, f (physically the pressure), is singular, with singular part $f_s \sim |p|^{5/2}$, while the singular part of the density varies as $\rho_s \sim |p|^{1/4}$.

A priori, one might not expect Baxter's curve to cross the fluid-to-solid phase boundary at any special point. But the presence of the two quite distinct critical exponents $\frac{5}{2}$ and $\frac{1}{4}$ indicates that Baxter's curve must intersect the phase boundary precisely at the tricritical point, T. As explained in more detail below, this supposition is confirmed by comparing these exponents with those of the corresponding tricritical point of a dilute Ising model, which have been calculated by Nienhuis[6] with the aid of certain plausible assumptions. The thermal exponents at the two tricritical points are identical, as expected by universality. A further surprising feature overlooked by Baxter[1,2] is that regime III of his curve appears to *coincide precisely* with the first-order phase boundary, as indicated in Fig. 1. The remainder of this Letter presents the evidence for these claims, and, allowing $L \neq M$, the more general claim that regime III of Baxter's *surface* (1) coincides with the first-order *surface* of hard squares with anisotropic nnn interactions.

The first, and potentially most compelling, line of evidence can be seen within the context of Baxter's analysis.[2] He uses corner transfer matrices to obtain a series expansion [Eqs. (36) and (37) of Ref. 2] for the sublattice densities. When, in Sec. 5.3 of Ref. 2, he calculates the sublattice densities for regime III he uses the empty or zero-density state as the reference or "ground" state for the expansion. This naturally yields sublattice densities that are equal, indicating a fluid phase. However, the density series for regime III obtained by expanding about the close-packed or full reference state also appears to converge, yielding two different sublattice densities, and thus indicating an ordered solid phase that can coexist with the fluid phase noticed by Baxter. This must be contrasted with each of the other regimes (I, II, and IV–VI), where the series for the sublattice densities clearly do not converge when one attempts to expand about any other reference state.

The surmise that regime III represents a first-order surface has been further tested by calculating standard series expansions for the thermodynamic potential, f, of the lattice gas about (i) the zero-density or *empty* state and (ii) the close-packed or *full* state. With $y \equiv z x_1^{-1} x_2^{-1}$, the low-density expansion to fifth order in (x_1, x_2) is

$$f_l = y x_1 x_2 + y^2 x_1 x_2 (x_1 + x_2) + (y^4 + 4y^3 - 9y^2/2) x_1^2 x_2^2 + y^3 x_1 x_2 (x_1^2 + x_2^2)$$
$$+ (y^6 + 4y^5 + 8y^4 - 14y^3) x_1^2 x_2^2 (x_1 + x_2) + y^4 x_1 x_2 (x_1^3 + x_2^3), \tag{2}$$

while the high-density expansion, to the same order, satisfies

$$2f_h = \ln y + y^{-1}x_1x_2 + y^{-2}x_1x_2(x_1+x_2) + (y^{-4}+4y^{-3} - 5y^{-2}/2)x_1^2x_2^2$$
$$+ y^{-3}x_1x_2(x_1^2+x_2^2) + (y^{-6}+4y^{-5}+8y^{-4} - 8y^{-3})x_1^2x_2^2(x_1+x_2) + y^{-4}x_1x_2(x_1^3+x_2^3). \quad (3)$$

Equating (2) and (3) yields the small-(x_1, x_2) expansion of the phase boundary, $y = y_\sigma(x_1, x_2)$, which clearly represents a first-order transition. This expansion *coincides identically* with the same expansion of Baxter's surface (1) to the order calculated and yields his value,[1] $f_\sigma = \ln y$, for f on the phase boundary, giving another strong indication that Baxter's regime III *is* the first-order surface. The similarity of the low- and high-density expansions, (2) and (3), and the simplicity of the result for f_σ suggest that a duality relation between the two phases may exist.

A third line of evidence for the above claims is obtained by examining the thermodynamic singularities at the multicritical point, T, which separates Baxter's regimes III and IV. For simplicity, let us consider $L = M$ only, as in Fig. 1. For the singular parts of the thermodynamic potential, $f_s = f - \ln y$, and the density, $\rho = z(\partial f/\partial z) \equiv \rho_c - \Delta\rho$, on his curve Baxter[1,2] finds, in regime III,

$$f_s = 0, \quad \Delta\rho = 5^{-1/2}p^{1/4} + O(p), \quad (4)$$

and in regime IV,

$$f_s = A|p|^{5/2} + O(p^5), \quad \Delta\rho = 5^{1/2}p + O(p^4), \quad (5)$$

where $\rho_c = (5 - \sqrt{5})/10$ is the multicritical density (it is also the critical density of hard hexagons![1]) and A is a constant. One expects f_s to scale[10] near the multicritical point as

$$f_s \approx |t|^{2-\alpha} Y_\pm(g/|t|^\phi), \quad (6)$$

where t and g are nonlinear scaling fields that vanish at T and are related to z and L (and hence to p) by smooth, invertible coordinate transformations; $Y_\pm(w)$ are the (matching) parts of the scaling function for $t \gtrless 0$, respectively. If we assume, without loss of generality, that $t \approx p$ for regime III, the vanishing of f_s implies that the scaling function $Y_+(g/t^\phi) \approx 0$ for $p \to 0$ in regime III. Thus Baxter's curve must take the form $g \approx w_B t^\phi$, where $Y_+(w_B) = 0$. But Baxter's curve is analytic through $t = 0$, and so we conclude that either (i) ϕ is integral, (ii) $1/\phi$ is integral, or (iii) $w_B = 0$. Possibilities (i) and (ii) may be shown to be inconsistent with (4)–(6) so that (iii) must be accepted. Examination of the behavior (5) of f_s in regime IV then reveals $\alpha = -\frac{1}{2}$. Finally, the singular part of the density, ρ_s, in regime III may then be obtained by differentiating (6) as

$$\rho_s \approx |t|^{2-\alpha-\phi} Y_+'(0) z(\partial g/\partial z). \quad (7)$$

Comparison of this to (4) reveals $\phi = 2 - \alpha - \frac{1}{4} = \frac{9}{4}$.

Hard squares with only nnn attractions should not have any multicritical behavior other than a tricritical point; so the multicritical point found by Baxter must be this tricritical point. It is expected, on symmetry grounds,[8] that the tricritical behavior of hard squares is in the Ising universality class. The thermal exponents at the tricritical point of a dilute Ising model have been calculated by Nienhuis[6] by mapping the Ising model, subject to certain plausible assumptions, onto a Gaussian model. The exponents he obtains, $Y_1 = \frac{9}{5}$ and $Y_2 = \frac{4}{5}$ in his renormalization-group notation, correspond *precisely* to those extracted from Baxter's calculation, namely $\alpha = -\frac{1}{2}$ and $\phi = \frac{9}{4}$. Thus, if we assume universality, this interpretation of Baxter's exact results confirms Nienhuis's calculation[6] of the Ising tricritical exponents.[11]

As a final point, note that f_s vanishes *identically* in Baxter's regime III. This might possibly occur via a precise cancellation of all corrections to scaling against the leading scaling form (6). However, it seems more reasonable to assume that both the leading scaling function and the corrections to scaling vanish for regime III. This would imply that Baxter's curve is *precisely* the scaling axis $g = 0$. We know that the first-order line emerging from the tricritical point is also a scaling line,[10] i.e., $g_\sigma = w_\sigma t^\phi$. All other scaling lines should diverge from a phase boundary as one departs from a multicritical point, but we know from our series expansions that Baxter's curve is asymptotic to the first-order line in the large-L limit (away from the tricritical point). This again indicates that Baxter's regime III is *identically* the first-order line. It is interesting to note that in regime IV neither f_s nor ρ exhibit nonanalytic corrections to scaling either, at least to the order calculated. It is thus tempting to speculate that all nonanalytic corrections to scaling vanish for this exact solution, as seems to be the case for the exact solution of the two-dimensional Ising model.[12]

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[11]Baxter also calculates the sublattice order parameter in regime IV, finding $R \sim |p|^{1/4}$. This may be contrasted with the "prediction" of $R \sim |p|^{3/32}$ for the dilute Ising tricritical point, with use of the conjectured leading field exponent, $y_H = \frac{77}{40}$, of Ref. 5. The source of this discrepancy is at present unclear; one possible, if unlikely, explanation is that the order parameter is linked to a dangerous irrelevant variable. Such a dangerous irrelevant variable does play an important role near tricriticality for dimensionalities $d \geq 3$; see S. Sarbach and M. E. Fisher, Phys. Rev. B 18, 2350 (1978).

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Exotic Levels from Topology in the Quantum-Chromodynamic Effective Lagrangian

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Skyrme has shown that the SU ⊗ SU(2) chiral model has nontrivial topological sectors with static solutions for suitable Lagrangians. The baryon number B and strangeness of these sectors have been studied, and the existence of bound states of the nucleon field to the lightest solitons is shown. It is found that there must be long-lived levels with $|B| \gtrsim 6$ and $|s| \gtrsim 6$ and 1.8 GeV $\lesssim m \lesssim$ 5.6 GeV, some having half-integral charge and exotic relation between B and s, that can be pair produced in, say, e^+e^- collisions.

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It is well known that the low-energy behavior of QCD, i.e., pion-nucleon physics, can be well described by the chiral $SU(2)_L \otimes SU(2)_R$ effective Lagrangian,[1]

$$\mathcal{L} = \tfrac{1}{2} f_\pi^2 \,\mathrm{Tr}(\partial_\mu u^\dagger \partial_\mu u) + (32e^2)^{-1}\,\mathrm{Tr}\{[\partial_\mu u u^\dagger, \partial_\nu u u^\dagger]^2\} + \ldots = \mathcal{L}_0 + \mathcal{L}_1 + \ldots, \tag{1}$$

where $f_\pi = 67$ MeV. $u(x)$ is a 2×2 SU(2) matrix. For all finite-energy configurations, $u(x) \to 1$ as $|\vec{x}| \to \infty$.

The term $\mathcal{L}_0$ gives the standard current-algebra results. Terms quartic in the derivatives, like $\mathcal{L}_1$, appear when we include results beyond the soft-pion limit or from renormalization effects.[2]

In this Letter, we discuss some unusual consequences of the Lagrangian (1) associated with soliton solutions. Skyrme[3,4] has shown that this model has nontrivial topological sectors labeled by the integer-valued charge

$$t = (48\pi^2)^{-1} \epsilon_{ijk} \int d^3x \,\mathrm{Tr}(I_i [I_j, I_k]), \tag{2}$$

where $I_i = \partial_i u u^\dagger$. If $e \neq \infty$, the sectors $t \neq 0$ admit