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# A Classical Theory of Hard Squares

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A simple phenomenological theory of the hard-square lattice gas is obtained by analyzing a low-order corner transfer matrix variational approximation. The free energy is of Landau type and expressions are obtained for the order parameter and densities. In this approximation, the model exhibits a critical point at $z_c = 4(3+2\sqrt{3})/9$ with critical exponents given by the classical values: $\alpha = 0_{\rm disc}$, $\beta = 1/2$, $\gamma = 1$, $\delta = 3$.

**KEY WORDS**: Hard squares; corner transfer matrices; variational approximations.

## 1. INTRODUCTION

The hard-square lattice gas is perhaps the simplest model in statistical mechanics to exhibit a solid–fluid phase transition.(1) Unlike its cousin the hard-hexagon model,(2) the hard-square model has not yielded to exact solution. Nevertheless, a great deal is known about hard squares from analytic, series, and numerical work(3) and the model is expected to undergo a second-order phase transition at an activity $z_c \approx 3.7962$ and a density $\rho_c \approx 0.368$ with Ising critical exponents $\alpha = 0_{\log}$, $\beta = 1/8$, $\gamma = 7/4$, $\delta = 15$.

In studying lattice models it is customary to start with mean-field theory. This simple theory typically gives a qualitatively correct and useful description of the thermodynamic behavior. Its phase diagrams generally exhibit single-phase regions, coexistence manifolds, critical manifolds, and so on with the correct topology even though the predicted classical critical exponents are wrong. Mean-field theory, however, is a single-site approximation and cannot correctly incorporate the near-neighbor exclusions of hard-core lattice gases. For these models a viable and much

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improved variational scheme is offered by the corner transfer matrix formalism.[4,5] In fact, corner transfer matrices provide a sequence of variational approximations that converge rapidly to the exact results. So, very good numerical estimates of noncritical thermodynamic properties can be obtained for a wide range of lattice models, including models in more than two dimensions.[6]

In this paper we analyze the hard-square lattice gas in a low-order variational approximation derived from corner transfer matrices. This gives a relatively simple and thermodynamically consistent classical theory of hard squares. In particular, the problems associated with studying this model in a mean-field approximation do not arise. Section 2 describes the hard-square model and the variational approximation. In Sections 3 and 4 the lowest order approximation is solved in the presence and absence of a symmetry-breaking field. The critical behavior is discussed in Section 5. Throughout, the algebra was carried out using the symbolic manipulation program Reduce.

## 2. THE MODEL AND VARIATIONAL EQUATIONS

The hard-square lattice gas is an interaction-round-a-face or IRF model.[7] The Boltzmann weights of allowed configurations around a square face $(i, j, k, l)$ with the sites starting at the bottom left and going anticlockwise, are given by

$$W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) = z^{(\sigma_i + \sigma_j + \sigma_k + \sigma_l)/4} e^{k(\lambda_i\sigma_i + \lambda_j\sigma_j + \lambda_k\sigma_k + \lambda_l\sigma_l)/4} \chi(\sigma_i, \sigma_j, \sigma_k, \sigma_l) \tag{2.1a}$$

Here $\sigma_i = 0, 1$ is the spin or occupation number of lattice site $i$, $z \geqslant 0$ is the activity, $k \geqslant 0$ is the sublattice symmetry-breaking field, and

$$\lambda_i = \begin{cases} +1, & i \in \mathscr{L}_1 \\ -1, & i \in \mathscr{L}_2 \end{cases} \tag{2.1b}$$

where $\mathscr{L}_1$ and $\mathscr{L}_2$ are the two sublattices of the square lattice $\mathscr{L}$. The nearest neighbor exclusion is enforced by the characteristic function

$$\chi(\sigma_i, \sigma_j, \sigma_k, \sigma_l) = (1 - \sigma_i\sigma_j)(1 - \sigma_j\sigma_k)(1 - \sigma_k\sigma_l)(1 - \sigma_l\sigma_i) \tag{2.1c}$$

The partition function of hard squares is

$$Z_N = \sum_{\sigma} \prod_{(i, j, k, l)} W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) \tag{2.2a}$$

where the sum is over all values of the occupation numbers and the product is over all $N$ faces of the lattice $\mathscr{L}$. The bulk properties of the model are determined in the thermodynamic limit by the partition function per face

$$\kappa = \lim_{N \to \infty} Z_N^{1/N} \tag{2.2b}$$

Variational approximations to $\kappa$, using corner transfer matrices, have been introduced by Baxter *et al.*[4,5] For convenience we summarize their results in this section.

Corner and half-row transfer matrices are defined on a finite lattice relative to a fixed ground-state boundary condition. For hard squares there are two competing ground states, $\sigma_i = (1 + \lambda_i)/2$ for all $i \in \mathscr{L}$ and $\sigma_i = (1 - \lambda_i)/2$ for all $i \in \mathscr{L}$, corresponding to complete occupation of one of the two independent sublattices. We set the boundary spins equal to $\sigma_i = (1 + \lambda_i)/2$ favoring occupation of the sublattice $\mathscr{L}_1$. A corner or quadrant of a square lattice with corner spin $\sigma_1 = \sigma_1'$ and edge spins $\sigma = \{\sigma_1, \sigma_2, ..., \sigma_m\}$ and $\sigma' = \{\sigma_1', \sigma_2', ..., \sigma_m'\}$ can occur with the corner spin on either of the two sublattices, as shown in Fig. 1. If the corner lies on sublattice $\mathscr{L}_1$, a corner transfer matrix **A** is defined by

$$A(\sigma \mid \sigma') = \alpha^{-1} \delta(\sigma_1, \sigma_1') \sum_{\substack{\text{interior} \\ \text{spins}}} \prod_{\text{faces}} W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) \tag{2.3a}$$

where the sum is over the $(m-1)^2$ interior spins and the product is over the $m^2$ faces. The normalizing constant $\alpha$, which cancels out of the

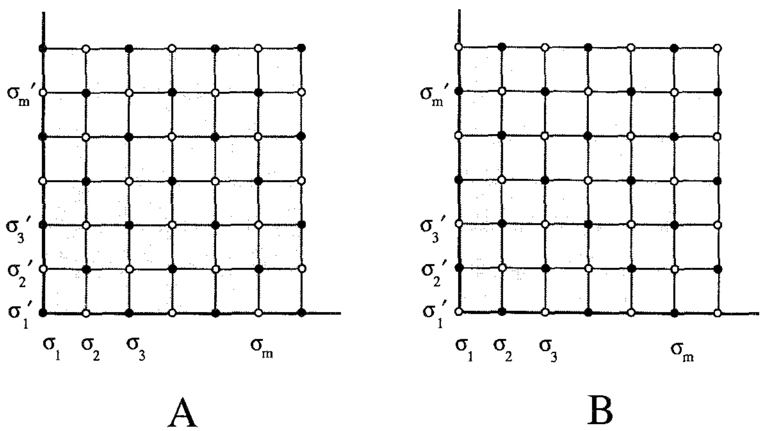


Fig. 1. Lattice quadrants of $m^2$ faces corresponding to the corner transfer matrices **A** and **B**. The boundary spins are set to their ground-state values. The sites of the preferred sublattice $\mathscr{L}_1$ are shown by filled circles.

variational equations, is chosen so that **A** tends to a limiting infinite-dimensional matrix[7] as $m \to \infty$. Similarly, if the corner lies on the sublattice $\mathscr{L}_2$, a corner transfer matrix **B** is defined by

$$B(\sigma \mid \sigma') = \beta^{-1}\delta(\sigma_1, \sigma'_1) \sum_{\substack{\text{interior}\\ \text{spins}}} \prod_{\text{faces}} W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) \tag{2.3b}$$

Because of the Kronecker delta

$$\delta(\sigma_1, \sigma'_1) = \begin{cases} 1, & \sigma_1 = \sigma'_1 \\ 0, & \sigma_1 \neq \sigma'_1 \end{cases} \tag{2.3c}$$

the matrices **A** and **B** are block diagonal with blocks $\mathbf{A}(\sigma_1)$ and $\mathbf{B}(\sigma_1)$

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}(0) & \mathbf{0} \\ \mathbf{0} & \mathbf{A}(1) \end{bmatrix}, \qquad \mathbf{B} = \begin{bmatrix} \mathbf{B}(0) & \mathbf{0} \\ \mathbf{0} & \mathbf{B}(1) \end{bmatrix} \tag{2.4}$$

The half-row transfer matrix **F** is defined by

$$F(\sigma \mid \sigma') = \gamma^{-1} \prod_{i=1}^{m} W(\sigma_i, \sigma_{i+1}, \sigma'_{i+1}, \sigma'_i) \tag{2.5}$$

where $\sigma_{m+1}$ and $\sigma'_{m+1}$ are set to their ground-state values as shown in Fig. 2. The face weights $W$, given by (2.1), are invariant under reflections about the diagonals of the face and are also invariant under rotations through 90° about one of the corners. It follows that all four quadrants with a common corner correspond to the same symmetric corner transfer matrix $\mathbf{A} = \mathbf{A}^T$ or $\mathbf{B} = \mathbf{B}^T$. In general, however, the half-row transfer matrix **F** is a nonsymmetric matrix ($\mathbf{F}^T \neq \mathbf{F}$) with blocks $\mathbf{F}(\sigma_1, \sigma'_1)$ and the block structure

$$\mathbf{F} = \begin{bmatrix} \mathbf{F}(0, 0) & \mathbf{F}(0, 1) \\ \mathbf{F}(1, 0) & \mathbf{0} \end{bmatrix} \tag{2.6}$$

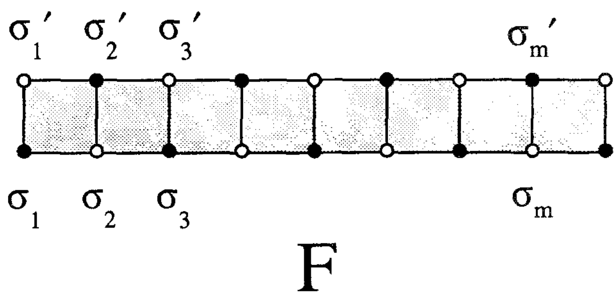


Fig. 2. Half-row of $m$ faces corresponding to the transfer matrix **F**. The boundary spins $\sigma_{m+1}$ and $\sigma'_{m+1}$ are set to their ground-state values. The sites of the preferred sublattice $\mathscr{L}_1$ are shown by filled circles.

The variational expression for the hard-square partition function per face $\kappa$ is

$$\kappa^2 = \max_{\mathbf{A}, \mathbf{B}, \mathbf{F}} \frac{\kappa_1 \kappa_2 \kappa_4^2}{\kappa_3^4} \tag{2.7a}$$

where

$$\kappa_1 = \sum_{\sigma_1} \operatorname{Tr} \mathbf{A}(\sigma_1)^4$$

$$\kappa_2 = \sum_{\sigma_1} \operatorname{Tr} \mathbf{B}(\sigma_1)^4$$

$$\kappa_3 = \sum_{\sigma_1, \sigma_2} \operatorname{Tr} \mathbf{A}(\sigma_1)^2 \mathbf{F}(\sigma_1, \sigma_2) \mathbf{B}(\sigma_2)^2 \mathbf{F}(\sigma_2, \sigma_1)^T$$

$$\begin{aligned} \kappa_4 = \sum_{\sigma_1, \sigma_2, \sigma_3, \sigma_4} & W(\sigma_1, \sigma_2, \sigma_3, \sigma_4) \operatorname{Tr} \mathbf{A}(\sigma_1) \mathbf{F}(\sigma_1, \sigma_2) \mathbf{B}(\sigma_2) \\ & \times \mathbf{F}(\sigma_2, \sigma_3)^T \mathbf{A}(\sigma_3) \mathbf{F}(\sigma_3, \sigma_4) \mathbf{B}(\sigma_4) \mathbf{F}(\sigma_4, \sigma_1)^T \end{aligned} \tag{2.7b}$$

and the maximum is taken with respect to variations in the matrices **A**, **B**, and **F**. This variational principle is represented graphically in Fig. 3. From the form of the variational principle it is clear that $\kappa$ is independent of the normalization constants $\alpha$, $\beta$, and $\gamma$. The conditions for $\kappa$ to be stationary are given by the matrix equations

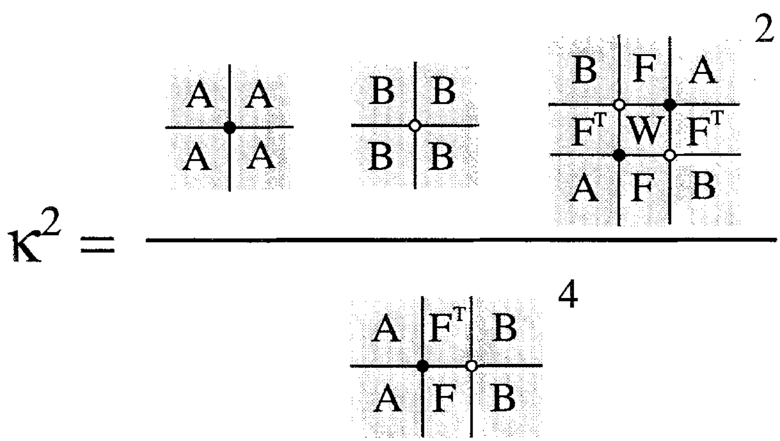


Fig. 3. Graphical representation of the corner transfer matrix variational principle (2.7).

$$\sum_{\sigma_2} \mathbf{F}(\sigma_1, \sigma_2)\mathbf{B}(\sigma_2)^2\,\mathbf{F}(\sigma_2, \sigma_1)^T = \xi\,\mathbf{A}(\sigma_1)^2$$

$$\sum_{\sigma_2} \mathbf{F}(\sigma_1, \sigma_2)^T\,\mathbf{A}(\sigma_2)^2\,\mathbf{F}(\sigma_2, \sigma_1) = \xi'\mathbf{B}(\sigma_1)^2 \tag{2.8}$$

$$\sum_{\sigma_2, \sigma_3} W(\sigma_1, \sigma_2, \sigma_3, \sigma_4)\,\mathbf{F}(\sigma_1, \sigma_2)\,\mathbf{B}(\sigma_2)\,\mathbf{F}(\sigma_2, \sigma_3)^T\,\mathbf{A}(\sigma_3)\,\mathbf{F}(\sigma_3, \sigma_4)$$

$$= \eta\,\mathbf{A}(\sigma_1)\,\mathbf{F}(\sigma_1, \sigma_4)\,\mathbf{B}(\sigma_4)$$

where $\kappa^2 = \eta^2/\xi\xi'$. These self-consistency equations are illustrated graphically in Fig. 4.

The densities of the hard-square model are readily found by differentiating (2.7) and using (2.8). This gives

$$\rho = z\frac{\partial}{\partial z}\ln\kappa = \frac{\rho_1 + \rho_2}{2} \tag{2.9a}$$

$$R = 2\frac{\partial}{\partial k}\ln\kappa = \rho_1 - \rho_2 \tag{2.9b}$$

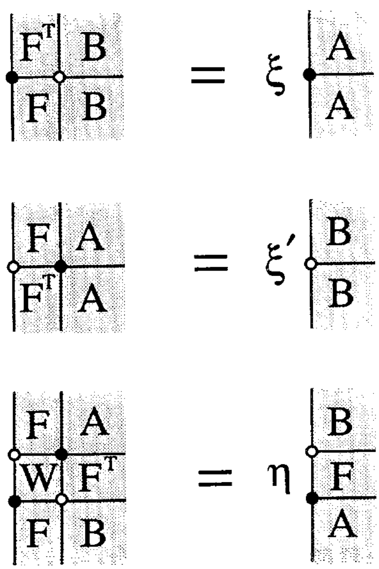


Fig. 4. Graphical representation of the self-consistency equations (2.8).

where

$$\rho_1 = \frac{\operatorname{Tr} \mathbf{A}(1)^4}{\operatorname{Tr} \mathbf{A}(0)^4 + \operatorname{Tr} \mathbf{A}(1)^4} \tag{2.9c}$$

$$\rho_1 = \frac{\operatorname{Tr} \mathbf{B}(1)^4}{\operatorname{Tr} \mathbf{B}(0)^4 + \operatorname{Tr} \mathbf{B}(1)^4} \tag{2.9d}$$

are the sublattice densities.

## 3. THE LOWEST ORDER APPROXIMATION

In the lowest order approximation the block matrices $\mathbf{A}(\sigma_1)$, $\mathbf{B}(\sigma_1)$, and $\mathbf{F}(\sigma_1, \sigma_2)$ are all scalars. Furthermore, since the variational equations (2.7) and (2.8) are independent of the normalization constants $\alpha$, $\beta$, and $\gamma$, the matrices **A**, **B**, and **F** can be scaled so that

$$\mathbf{A} = \begin{bmatrix} 1 & 0 \\ 0 & a \end{bmatrix}, \qquad \mathbf{B} = \begin{bmatrix} 1 & 0 \\ 0 & b \end{bmatrix}, \qquad \mathbf{F} = \begin{bmatrix} 1 & t \\ s & 0 \end{bmatrix} \tag{3.1}$$

The variational principle then becomes

$$\kappa^2 = \max_{a,b,s,t} \frac{(1+a^4)(1+b^4)[1+2w(vas^2+v^{-1}bt^2)+w^2(v^2a^2s^4+v^{-2}b^2t^4)]^2}{(1+a^2s^2+b^2t^2)^4} \tag{3.2}$$

where $w = z^{1/4}$ and $v = e^{k/4}$. Similarly, the stationary equations (2.8) become

$$\begin{aligned} 1 + b^2t^2 &= \xi \\ s^2 &= \xi a^2 \\ 1 + a^2s^2 &= \xi' \\ t^2 &= \xi' b^2 \\ 1 + w(vas^2 + v^{-1}bt^2) &= \eta \\ wvs + w^2v^2as^3 &= \eta as \\ wv^{-1}t + w^2v^{-2}bt^3 &= \eta bt \end{aligned} \tag{3.3}$$

Eliminating $\xi$, $\xi'$, and $\eta$ now gives

$$\begin{aligned} &1 + b^2t^2 = a^{-2}s^2 \\ &1 + a^2s^2 = b^{-2}t^2 \\ &\frac{st}{ab}\kappa = 1 + w(vas^2 + v^{-1}bt^2) \\ &\qquad = wva^{-1} + w^2v^2s^2 = wv^{-1}b^{-1} + w^2v^{-2}t^2 \end{aligned} \tag{3.4}$$

From (3.4) it follows that

$$s^2 = \frac{w - vb}{wva(v^{-1}a + vb - w)}, \qquad t^2 = \frac{w - v^{-1}a}{wv^{-1}b(v^{-1}a + vb - w)} \tag{3.5}$$

Substituting into (3.2) gives

$$\begin{aligned} \kappa^2 &= \max_{a,b} \frac{(1+a^4)(1+b^4)}{[2z^{-1/4}(e^{-k/4}a + e^{k/4}b) - 2z^{-1/2}ab - 1]^2} \\ &= \max_{x,y} \frac{(1+ze^k x^4)(1+ze^{-k}y^4)}{[2(x+y] - 2xy - 1]^2} \end{aligned} \tag{3.6}$$

where $x = a/wv$, $y = vb/w$, and the maximum is taken over the domain

$$\mathscr{D} = \{(x, y): x \leqslant 1, y \leqslant 1, \text{and } x + y \geqslant 1\} \tag{3.7}$$

to ensure that $s^2$ and $t^2$ are positive. Differentiating (3.6) or using (3.4), we find that the maximum in the required region occurs for $x$ and $y$ satisfying

$$y = \frac{ze^k(x^4 - x^3) - 1}{ze^k(x^4 - 2x^3) - 1} = F(x; z, k) \tag{3.8a}$$

$$x = \frac{ze^{-k}(y^4 - y^3) - 1}{ze^{-k}(y^4 - 2y^3) - 1} = F(y; z, -k) \tag{3.8b}$$

The sublattice densities are given by

$$\rho_1 = \frac{ze^k x^4}{1 + ze^k x^4}, \qquad \rho_2 = \frac{ze^{-k}y^4}{1 + ze^{-k}y^4} \tag{3.9}$$

Differentiating the first form for $\kappa$ in (3.6) gives

$$R = \rho_1 - \rho_2 = \frac{x - y}{2(x+y) - 2xy - 1} \tag{3.10a}$$

$$\rho = \frac{1}{2}(\rho_1 + \rho_2) = \frac{1}{2}\,\frac{x + y - 2xy}{2(x+y) - 2xy - 1} \tag{3.10b}$$

Hence, using (3.8a) to eliminate $y$, we obtain

$$R = \frac{x - 1 - ze^k(x^5 - 3x^4 + x^3)}{1 + ze^k x^4} \tag{3.11a}$$

$$\rho = \frac{1}{2}\,\frac{ze^k(x^5 - x^4 + x^3) - x + 1}{1 + ze^k x^4} \tag{3.11b}$$

If the sublattice symmetry-breaking field is positive ($k > 0$), then Eqs. (3.8) admit a unique solution in the domain $\mathscr{D}$ with $x > y$ and $\rho_1 > \rho_2$. However, in the case of sublattice symmetry ($k = 0$), the solution of (3.8) that maximizes (3.6) at large activities is not unique and leads to spontaneous symmetry breaking ($x \neq y$, $\rho_1 \neq \rho_2$) and a phase transition.

## 4. ZERO-FIELD SOLUTION

In this section we consider the solution of the stationary equations (3.8) in zero symmetry-breaking field ($k = 0$). In this case the stationary equations can be written as

$$x = f(y), \qquad y = f(x) \tag{4.1a}$$

where

$$f(x) = \frac{z(x^4 - x^3) - 1}{z(x^4 - 2x^3) - 1} \tag{4.1b}$$

It follows that $x$ and $y$ are both solutions of the iterated mapping

$$x = f(f(x)) \tag{4.2}$$

which is equivalent to the polynomial equation

$$\begin{aligned}[(1+z)z^2x^8 - (4+z)z^2x^7 + 4z^2x^6 + z^2x^5 - 2z(1+z)x^4 + 4zx^3 - zx + 1] \\ \times (zx^5 - 3zx^4 + zx^3 - x + 1)(zx^4 - 2zx^3 + zx^2 - 1) = 0\end{aligned} \tag{4.3}$$

One solution is the symmetric fixed-point solution $x = y$ with $1/2 \leqslant x \leqslant 1$ and

$$x = f(x) \tag{4.4a}$$

or

$$zx^5 - 3zx^4 + zx^3 - x + 1 = 0 \tag{4.4b}$$

For small activities ($z \leqslant z_c$, where $z_c$ will be given below), this is the unique solution to (4.1) in $\mathscr{D}$ and it yields the maximum in (3.6) with

$$\kappa = \frac{1 + zx^4}{4x - 2x^2 - 1} \tag{4.5a}$$

and

$$\rho = \rho_1 = \rho_2 = \frac{zx^4}{1 + zx^4} \tag{4.5b}$$

This gives the complete solution in the fluid phase.

At a critical activity ($z = z_c$), the fixed-point solution bifurcates into a two-cycle as shown in Fig. 5. This bifurcation occurs when

$$\frac{\partial f}{\partial x} = -1 \tag{4.6a}$$

or

$$zx^4 - 4zx^3 + 3zx^2 - 1 = 0 \tag{4.6b}$$

Solving Eqs. (4.4b) and (4.6b) for the critical values of $x$ and $z \geqslant 0$, we find

$$z_c = 4(3 + 2\sqrt{3})/9 \approx 2.8729, \qquad x_c = (3 - \sqrt{3})/2 \approx 0.634 \tag{4.7a}$$

and hence at the critical point

$$\rho_1 = \rho_2 = \rho_c = (3 - \sqrt{3})/4 \approx 0.317, \qquad \kappa_c = 2 \tag{4.7b}$$

Above the critical point ($z > z_c$), the two-cycle maximizes $\kappa$ and the sublattice symmetry is spontaneously broken. In this case both $x$ and $y$ are solutions of

$$(1+z)z^2x^8 - (4+z)z^2x^7 + 4z^2x^6 + z^2x^5 - 2z(1+z)x^4 + 4zx^3 - zx + 1 = 0 \tag{4.8}$$

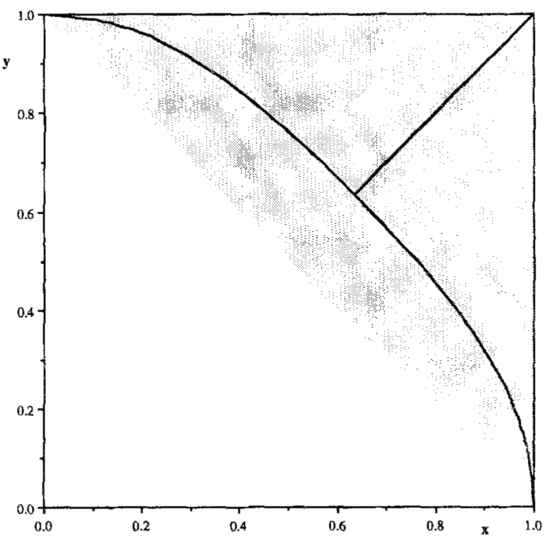


Fig. 5. Zero-field solutions $x$ and $y$ which maximize the partition function per site $\kappa$. The symmetric solution with $x = y$ bifurcates into two asymmetric solutions at the critical point $z = z_c$. The maximum of $\kappa$ is taken over the shaded domain $\mathscr{D}$.

with $x \neq y$ related to each other by (4.1). Since $x$ and $y$ can be freely interchanged, we take $x > y$ so that $\rho_1 > \rho_2$, corresponding to the solid phase with the sublattice $\mathscr{L}_1$ preferentially occupied. In this case the order parameter $R$ and the density $\rho$ are given by (3.11) with $k = 0$.

The value of $z_c$ in (4.7a) is that obtained for the numerical solution of the two-by-two truncation of the corner transfer matrix equations by Baxter *et al.*[5] For higher truncations they give the results 3.4575 (three-by-three) and 3.7066 (five-by-five), indicating the rapid convergence of this sequence of approximations. The most accurate result obtained by series expansions[3] is $z_c = 3.7962$.

## 5. CRITICAL BEHAVIOR

In this section we show that the critical exponents for the lowest order variational approximation to hard squares are given by $\alpha = 0_{\text{disc}}$, $\beta = 1/2$, $\gamma = 1$, $\delta = 3$. These classical values are expected to hold for all variational approximations obtained by finite truncation of the corner transfer matrices.

Let $\Delta x = x - x_c$, $\Delta z = z - z_c$, and expand $\kappa$ given by (3.6) to fourth order in $\Delta x$ about the critical point $z = z_c$, $k = 0$, $x = x_c$. Using (3.8a) to eliminate $y$ then leads to the result

$$\ln(\kappa/2) = \max_{\Delta x}[\Psi_0 + \Psi_1\,\Delta x + \Psi_2(\Delta x)^2 + \Psi_3(\Delta x)^3 + \Psi_4(\Delta x)^4] \quad (5.1\text{a})$$

where, to leading orders in $\Delta z$ and $k$, the coefficients are given by

$$\begin{gathered} \Psi_0 \sim (\psi_0 + \psi_0' k + \psi_0''\,\Delta z)\,\Delta z \\ \Psi_1 \sim [\psi_1 k + \psi_1'(\Delta z)^2] \\ \Psi_2 \sim \psi_2\,\Delta z, \qquad \Psi_3 \sim \psi_3\,\Delta z, \qquad \Psi_4 \sim \psi_4 \end{gathered} \quad (5.1\text{b})$$

where $\psi_0$, $\psi_0'$, $\psi_0''$, $\psi_1$, $\psi_1'$, $\psi_2$, $\psi_3$, and $\psi_4$ are nonzero constants.

In particular, differentiating (5.1a) with respect to $x$ gives the cubic stationary condition

$$\psi_1 k + \psi_1'(\Delta z)^2 + 2\psi_2\,\Delta z\,\Delta x + 3\psi_3\,\Delta z(\Delta x)^2 + 4\psi_4(\Delta x)^3 = 0 \quad (5.2)$$

In zero field ($k = 0$), the three roots of this equation to leading order are

$$\Delta x = \begin{cases} (-\psi_1'/2\psi_2)\,\Delta z \\ \pm(-\psi_2/2\psi_4)^{1/2}(\Delta z)^{1/2}, & \Delta z > 0 \end{cases} \quad (5.3)$$

The first root gives the solution in the disordered phase ($\Delta z < 0$); the other two solutions maximize $\kappa$ in the ordered phase ($\Delta z > 0$).

The order parameter $R$ is obtained by differentiating (5.1a) with respect to $k$. Setting $k=0$ thus gives

$$R \sim 2\psi_1\, \Delta x + 2\psi'_0\, \Delta z \tag{5.4}$$

The order parameter $R$ is zero in the disordered phase, since we find $\psi_1 \psi'_1 = 2\psi'_0 \psi_2$ and

$$R \sim (\Delta z)^{1/2} \qquad \text{as} \quad z \to z_c^+ \tag{5.5}$$

so $\beta = 1/2$. Differentiating (5.4) and (5.2) with respect to $k$, we find

$$\left.\frac{\partial R}{\partial k}\right|_{k=0} \sim 2\psi_1 \left.\frac{\partial x}{\partial k}\right|_{k=0} \sim \frac{-2\psi_1^2}{2\psi_2\, \Delta z + 6\psi_3\, \Delta z\, \Delta x + 12\psi_4 (\Delta x)^2}$$
$$= \begin{cases} \dfrac{-2\psi_1^2}{2\psi_2\, \Delta z}, & \Delta z < 0, \\[2ex] \dfrac{-2\psi_1^2}{2(\psi_2 + 6\psi_4)\, \Delta z}, & \Delta z > 0 \end{cases} \tag{5.6}$$

Hence $\gamma = 1$. Similarly, setting $z = z_c$ in (5.4) and (5.2) gives

$$R \sim 2\psi_1\, \Delta x \sim 2\psi_1 \left(\frac{\psi_1 k}{4\psi_4}\right)^{1/3} \tag{5.7}$$

so $\delta = 3$. Finally, substituting (5.3) into (5.1) with $k = 0$, we find that at $z = z_c$ there is a jump discontinuity in

$$C = \frac{\partial^2}{\partial z^2} \ln \kappa \tag{5.8}$$

so that $\alpha = 0_{\text{disc}}$.

The establishes the classical values for the critical exponents.

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