

# A Cell Model for Liquids. II. Exact Solution for the Restricted Cell Model for Hard, Parallel Squares

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*Received December 3, 1973*

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A restricted cell model for hard, parallel squares is presented both in a discrete and a continuous version. The model is solved exactly by means of a transfer matrix method and the thermodynamic properties are calculated. Some correlation functions are also obtained, which show that the long range order decays at least as fast as  $1/r^2$ .

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**KEY WORDS:** Theory of fluids; lattice gas; cell model; hard squares; correlation function ; long-range order; transfer matrix.

## 1. INTRODUCTION

The usual cell model description<sup>(1)</sup> of the liquid state has the deficiency of a built-in crystallike structure due to the geometric regularity with which the container of the system is divided into cells. In a previous paper<sup>(2)</sup> a cell model without this crystal structure was introduced. The basic idea is to have the cell of a particle defined by neighboring particles.

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More precisely, the cells of the present model are defined as follows: One starts from a close-packed configuration.<sup>2</sup> This configuration is assumed to have the ordered structure of a lattice, and we can assume that each particle has well-defined nearest neighbors. When the volume increases, the set of nearest neighbors (measured by Euclidean distance) will, in general, depend on the configuration. However, the neighboring particles, which define the cell of a particle, shall always be those that were nearest neighbors in the close-packed configuration; to distinguish, we shall denote these neighbors as topological neighbors (because we, so to speak, use the topology of the regular lattice of the close-packed configuration, rather than the conventional topology induced by the Euclidean measure of distance).

The details of how the cell of a particle is defined by the position of its topological neighbors may depend on the lattice as well as the type of restrictions imposed by the model in which one is interested. In Section 2 we give the details for the case of hard, parallel squares under the restrictions which in Ref. 2 was termed the restricted cell model. In this model the hard core condition is always fulfilled, but the accessible part of phase space is severely restricted. In Section 3 we find the thermodynamic properties in the case of a lattice gas. In Section 4 we proceed to the continuum gas for which the thermodynamic properties were announced in Ref. 2. Finally, in Section 5 we calculate some pair correlation functions which are particularly simple to calculate in the present case. These correlation functions are of rather limited physical significance; however, one can conclude that the long-range correlation will decay at least as fast as  $1/r^2$ . In a subsequent paper more detailed calculations of correlation functions will appear.

## 2. THE MODEL

We consider a system of hard, parallel squares where each particle has four topological neighbors. With a particle and its topological neighbors numbered as shown in Fig. 1 and with  $2d$  for the length of the diagonal of a square, the restrictions on the motion are

$$\begin{aligned}
 x_0 &> x_1 + d; & x_0 &> x_3 + d \\
 x_0 &< x_2 - d; & x_0 &< x_4 - d \\
 y_0 &\geq y_3 + d; & y_0 &\geq y_4 + d \\
 y_0 &\leq y_1 - d; & y_0 &\leq y_2 - d
 \end{aligned}
 \tag{1}$$

where the directions of the coordinate axes for convenience have been chosen parallel to the diagonals of the squares. It is clear from Eq. (1) that the

<sup>2</sup> This assumes the existence of a hard core; the model can be generalized to softer potentials, but this is outside the scope of the present paper.

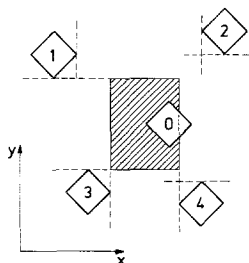


Fig. 1. A hard square and its topological neighbors.

restrictions make the  $x$  coordinates independent of the  $y$  coordinates and visa versa. The two sets of coordinates can therefore be treated separately, and since they are equivalent, it will be sufficient to consider the  $x$  coordinates explicitly. We can thus talk about the topological arrangement of the particles as being in rows parallel to the  $x$  axis. Let there be  $n$  particles in each row and  $2n'$  rows and let the area of the system be  $L \times L = A$ . If one turned the picture  $90^\circ$  and looked at the  $y$  coordinates there would be  $2n$  rows with  $n'$  particles in each. With this ordering the particles are turned  $45^\circ$  compared to the usual convention, and this introduces a minor difference between the odd and even rows as illustrated in Fig. 2, but this is easily taken care of. The  $x$  dependence in the model can now be solved by a transfer matrix method with the transfer in the  $y$  direction. The particles in each row are numbered from 1 to  $n$ . With rigid boundary conditions imposed, all the centers of the particles are restricted between 0 and  $L$ . Let  $x$  stand for a coordinate in an odd-numbered row and  $x'$  for the coordinate in the following even-numbered row (or the preceding even-numbered row); the cell model restrictions will then be

$$\begin{aligned}
 &0 \leq x_1 \leq x_1' - d \leq x_2 - 2d \leq x_2' - 3d \leq \dots \\
 &\leq x_n - (2n - 2)d \leq x_n' - (2n - 1)d \leq L - (2n - 1)d
 \end{aligned}
 \tag{2}$$

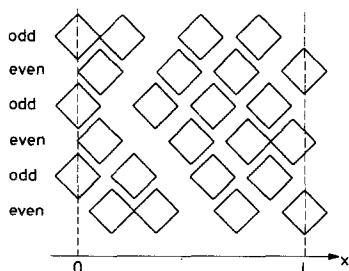


Fig. 2. Six rows with  $n = 4$  particles. For reason of illustrations the particles in a row have the same ordinate.

It is convenient to introduce the following reduced coordinates in Eq. (2):

$$\begin{aligned} u_i &= x_i + (2i - 2)d && \text{for odd rows} \\ v_i &= x_i' - (2i - 1)d && \text{for even rows} \end{aligned} \quad (3)$$

The restrictions (2) for two consecutive rows now read

$$0 \leq u_1 \leq v_1 \leq u_2 \leq v_2 \leq \dots \leq u_n \leq v_n \leq l \quad (4)$$

where

$$l = L - (2n - 1)d \quad (5)$$

is the free length per row.

### 3. THE LATTICE GAS VERSION

#### 3.1. Definitions

An obvious way to impose lattice restrictions on the model is to choose a square lattice with the edges parallel to the diagonals of the squares, since this conserves the independence of the two coordinate directions which is essential for the solubility of the model. The length is measured in units of the lattice constant, which is chosen so that  $d$  is an integer. With this convention, the reduced coordinates  $u_i$  are integer and give the number of uncovered lattice edges up to the  $i$ th particle.

We can introduce a new set of coordinates constructed in such a way that only odd values are used on odd rows and even values on even rows:

$$\begin{aligned} w_i &= 2u_i + 2i - 2 + 1 && \text{odd rows} \\ w_i &= 2v_i + 2i - 2 && \text{even rows} \end{aligned} \quad (6)$$

Adding  $2i - 2$  ensures that all particles have coordinates that differ by at least two. The condition (4) now reads

$$0 < w_1 < w_1' < w_2 < w_2' < \dots < w_n < w_n' < m \quad (7)$$

with the coordinates on even rows primed;

$$m = 2n + 2l + 1 \quad (8)$$

where  $l$  is the number of uncovered edges, i.e., the free length per row. The number of uncovered edges between the  $i$ th and the  $(i + 1)$ th particle is  $u_{i+1} - u_i = \frac{1}{2}(w_{i+1} - w_i) - 1$  and we can therefore assign the following  $\frac{1}{2}(w_{i+1} - w_i) - 1$  coordinates to these edges:  $w_i + 2, w_i + 4, \dots, w_{i+1} - 2$ . A similar assignment can be used for the uncovered edges before the first particle and after the last.

A configuration of  $n$  particles and  $l$  uncovered edges can therefore be described by either the  $n$  coordinates  $w_i$  of the particles or by the  $l$  coordinates, which we denote  $z_1, \dots, z_l$ , of the uncovered edges. It is advantageous to use the latter description because the transfer condition becomes

$$z_i' = z_i \pm 1 \tag{9}$$

subject to the general constraint

$$0 < z_1 < z_2 < z_3 < \dots < z_l < m \tag{10}$$

valid for all rows, and the solution to this transfer matrix is well known.

### 3.2. Equivalence with Modified KDP Model

The rules given in Eqs. (9) and (10) allow one to make a correspondence between a configuration of the hard square model and a set of self-avoiding walks on a square lattice.

Consider the square lattice of Fig. 3. Each row has  $\frac{1}{2}(m - 1)$  vertices. The vertices are numbered as shown so that a row has either odd or even numbers, and they are seen to be identical to the  $w$  coordinates from the hard square rows. A configuration of hard squares is mapped onto this lattice by marking the vertices numbered  $z_1, \dots, z_l$  for each row. If one now draws lines from row to row through vertices corresponding to the  $i$ th edge, the transfer condition (9) will assure that the result is a walk on the lattice and the condition (10) that the walks do not cross.

It is now easy to identify the model as a transformation of Wu's modified KDP model<sup>(3-5)</sup> except for the fact that the boundary conditions used here differ slightly from the ones used normally in the KDP model, and since the result is sensitive to the boundary condition, we cannot directly use the known solution of Wu's model. It is shown<sup>(6)</sup> that the modified KDP model is equivalent to a dimer covering problem on the hexagonal lattice, and it is well known that dimer covering problems can be solved either by the Pfaffian

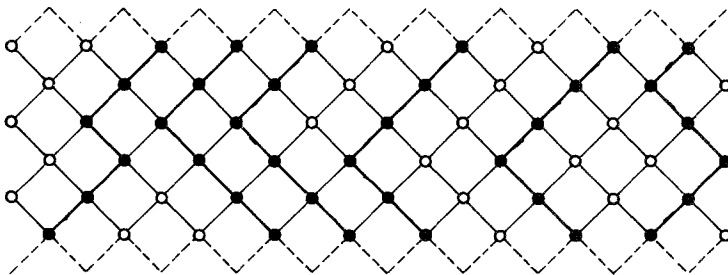


Fig. 3. Square lattice with marked vertices and six walks on the lattice, corresponding to the configuration of hard squares of Fig. 2.

method<sup>(6-8)</sup> or by the transfer matrix method.<sup>(9)</sup> We prefer the latter since it allows us to pass in a straightforward way to the continuum limit.

### 3.3. Diagonalization

The independent particle problem that arises if one considers the transfer of the empty edges (9) under the constraint

$$0 < z_i < m; \quad i = 1, 2, \dots, l \quad (11)$$

has the single particle transfer operator  $\tilde{T}$ , which is an  $(m-1) \times (m-1)$  matrix with the elements

$$\tilde{t}_{i,j} = \begin{cases} 1 & \text{if } |i-j| = 1 \\ 0 & \text{otherwise} \end{cases} \quad (12)$$

The matrix has the eigenvectors

$$\tilde{\psi}_j(z) = (2/m)^{1/2} \sin(j\pi z/m); \quad j = 1, 2, \dots, m-1 \quad (13)$$

and the corresponding eigenvalues

$$\tilde{\lambda}_j = 2 \cos(j\pi/m); \quad j = 1, 2, \dots, m-1 \quad (14)$$

The definition of the coordinates requires, however, that the eigenvectors take values different from zero only on odd or even positions, respectively. To ensure this property, one observes the following properties of the solution:

$$\tilde{\psi}_j(z) = (-1)^{z+1} \tilde{\psi}_{m-j}(z) \quad (15)$$

$$\tilde{\lambda}_j = -\tilde{\lambda}_{m-j} \quad (16)$$

The functions

$$\tilde{\phi}_j^+(z) = \frac{1}{\sqrt{2}} [\psi_j(z) + \psi_{m-j}(z)] = \frac{2}{\sqrt{m}} \left| \sin \frac{\pi z}{2} \right| \sin \frac{j\pi z}{m} \quad (17a)$$

$$\tilde{\phi}_j^-(z) = \frac{1}{\sqrt{2}} [\psi_j(z) - \psi_{m-j}(z)] = \frac{2}{\sqrt{m}} \left| \cos \frac{\pi z}{2} \right| \sin \frac{j\pi z}{m} \quad (17b)$$

$$j = 1, 2, \dots, \frac{1}{2}(m-1)$$

will consequently have the properties

$$\tilde{T}\tilde{\phi}_j^+(z) = \tilde{\lambda}_j\tilde{\phi}_j^-(z); \quad \tilde{T}\tilde{\phi}_j^-(z) = \tilde{\lambda}_j\tilde{\phi}_j^+(z); \quad j = 1, 2, \dots, \frac{1}{2}(m-1) \quad (18)$$

$$\tilde{\phi}_j^+(z) = 0 \quad \text{if } z \text{ is even} \quad (19)$$

$$\tilde{\phi}_j^-(z) = 0 \quad \text{if } z \text{ is odd}$$

which are precisely the desired properties of the single-particle “eigenvectors.”  $\check{\phi}^+$  and  $\check{\phi}^-$  are of course only eigenvectors of  $T^2$ , in agreement with the different description of odd and even rows that the model imposes.

The transfer problem with the constraint (11) is now solved, and the eigenfunction for  $l$  particles is obtained as a direct product of the single-particle eigenfunctions using  $\check{\phi}^+$  on odd rows and  $\check{\phi}^-$  on even rows.

The solution to the transfer problem with the constraint (10) is obtained by constructing the  $l$ -particle eigenfunction as a determinant of the single-particle eigenfunctions, i.e., the  $l$ -particle eigenfunction is (for odd rows)

$$\check{\Phi}^+(j_1, j_2, \dots, j_l; z_1, \dots, z_l) = \det\{\check{\phi}_{j_r}(z_s)\} \tag{20}$$

$$1 \leq j_1 < j_2 < \dots < j_l \leq \frac{1}{2}(m - 1)$$

where  $\{\check{\phi}_{j_r}(z)\}$  is an  $l \times l$  matrix whose element in the  $r$ th row and  $s$ th column is  $\check{\phi}_{j_r}^+(z_s)$ .

The fact that  $\check{\Phi}^+$  as given by (20) actually has the right form can be seen in several ways. One can use the fact that the condition (10) implies that the empty edges move as a Bose gas with an infinite delta function interaction together with the fact that in the linear case such a gas is equivalent with a free Fermi gas.<sup>(10)</sup> One can also note that if we have a configuration of empty edges which fulfills (10) and then make a configuration in the next row in accordance with (9) but in disagreement with (10), the resulting value of  $\check{\Phi}^+$  (or  $\check{\Phi}^-$ ) would be zero.

The number of eigenvectors given by (20) is

$$\binom{\frac{1}{2}(m - 1)}{l}$$

which is just the dimensionality of the vector space for the system of edges since this is the number of configurations of  $l$  edges on  $\frac{1}{2}(m - 1)$  positions, i.e., we have found all the eigenvectors for the  $l$ -particle problem.

The corresponding eigenvalues are

$$\Lambda(j_1, j_2, \dots, j_l) = 2^l \prod_{k=1}^l \cos(j_k \pi / m) \tag{21}$$

### 3.4. Eigenvectors for the Hard Squares

Obviously, it would be more natural to express the eigenvectors in terms of the positions of the hard squares rather than in terms of the positions of the empty edges. Also, if one wants to obtain the results for the continuum version of the model by taking the continuum limit of the lattice version, this is most easily done if the eigenvectors are expressed in terms of the positions of the hard squares.

This set of eigenvectors can be obtained in several ways. One could apply the Bethe ansatz method to the transfer matrix given by Eq. (27). One could also start from the known eigenvectors [Eqs. (20)] expressed in terms of the positions of the empty edges and use the fact that an allowed position in a row is either occupied by a hard square or an empty edge.

The transformation to the new set of eigenvectors is therefore a simple relabeling of the basic states

$$\begin{aligned} \phi_j(w) &= \tilde{\Phi}(j1, \dots, j_l; z_1, \dots, z_l) \\ j &\neq \{j_1, \dots, j_l\}; \quad w \neq \{z_1, \dots, z_l\} \end{aligned} \quad (22)$$

The desired change of variables in Eqs. (20) and (21) could then be performed by appropriate application of formulas for sums of trigonometric functions.

Here we shall instead accomplish the change of variable by a reference to the fermion formalism. This is most easily done by application of creation and annihilation operators; however, since we have no other use for these operators, we shall only state the arguments in words.

The empty edges can as stated in Section 3.3 be considered as free fermions on a lattice. The remark above implies that the hard squares can be considered as holes in the filled Fermi sea of empty edges. This implies that both the single-particle eigenvectors and the  $n$ -particle eigenvectors for the hard squares can be obtained trivially from the corresponding functions for the empty edges. However, slight care has to be taken to get the signs in agreement with the natural choice; this is connected with the fact that the creation and annihilation operators for fermions anticommute, which means that the sign depends on the order of the operators. In fact, if one moves a hard square one position to the right of left, this causes an interchange of an odd number of operators when referred to the standard ordering of the creation operators for empty edges. This change of sign is clearly unwanted in the hard square formulation.

Therefore the correct single-particle eigenvectors for the hard squares become

$$\phi_j^+(w) = \frac{(-1)^{(w-1)/2}}{\sqrt{2}} [\psi_j(w) + \psi_{m-j}(w)] = \frac{2}{\sqrt{m}} \sin \frac{w\pi}{2} \sin \frac{j\pi w}{m} \quad (23a)$$

$$\phi_j^-(w) = \frac{(-1)^{(w-2)/2}}{\sqrt{2}} [\psi_j(w) - \psi_{m-j}(w)] = -\frac{2}{\sqrt{m}} \cos \frac{w\pi}{2} \sin \frac{j\pi w}{m} \quad (23b)$$

$$j = 1, \dots, \frac{1}{2}(m-1)$$

Empty edges and hard square eigenvectors must have the same eigenvalues, which means that the single hard square eigenvalue will have the value

$$\lambda_j = \prod_{i \neq j}^{l+1} \tilde{\lambda}_i \quad (24)$$



Taking the determinant of  $T$  [see Eq. (12)] and using Eq. (14) and (16), one obtains

$$\prod_{j=1}^{l+1} \tilde{\lambda}_j = 1 \tag{25}$$

by means of which the eigenvalues of the single hard square transfer matrix are written

$$\lambda_j = 1/[2 \cos(j\pi/m)]; \quad j = 1, \dots, \frac{1}{2}(m - 1) \tag{26}$$

Note that we obtain the largest eigenvalue for the largest value of  $j$  in this case.

The final proof for the solution (23) and (26) is obtained by inspection of the single hard square transfer problem: Since the particle in an even row always must be to the right of the particle in an odd row [Eq. 7], the elements of the transfer matrix  $T$  are

$$t_{vw} = \begin{cases} 1 & \begin{cases} w > v, & v \text{ odd, } w \text{ even} \\ w < v, & v \text{ even, } w \text{ odd} \end{cases} \\ 0 & \text{otherwise} \end{cases} \tag{27}$$

The  $v$ th element from  $t$  acting on  $\phi_j^+$  is given by

$$\{T\phi_j^+(w)\}_v = \sum_w \frac{2}{\sqrt{m}} \sin \frac{\pi w}{2} \sin \frac{j\pi w}{m} = \lambda_j \phi_j^-(v) \tag{28a}$$

where the sum over  $w$  runs over odd integers from one to  $v$ . Similarly, we have

$$\{T\phi_j^-(w)\}_v = \sum_w \frac{-2}{\sqrt{m}} \cos \frac{\pi w}{2} \sin \frac{j\pi w}{m} = \lambda_j \phi_j^+(v) \tag{28b}$$

where the sum now takes the values  $m - 1, m - 3$ , etc. down to  $v$ . As before,  $\phi_j^+(w)$  and  $\phi_j^-(w)$  are only eigenvectors to  $T^2$ .

The solution to the  $n$ -particle problem given by (7) is generated as for the empty edges by forming determinants of the single-particle eigenfunctions.

### 3.5. Thermodynamics of the Lattice Gas

The largest eigenvalue is

$$\Lambda_0(n, m) = 2^l \prod_{j=1}^l \cos(j\pi/m) \tag{29}$$

In the thermodynamic limit  $n \rightarrow \infty, L/n \rightarrow \sigma'$ , we have the following expressions:

$$l/n \rightarrow \sigma' - 2d \equiv \sigma \quad \text{and} \quad m/n \rightarrow 2\sigma + 2 \tag{30}$$

and the free energy per particle for the  $x$  coordinate is

$$\begin{aligned} f_x &= -\frac{1}{\beta} \lim_{n \rightarrow \infty} \frac{1}{n} \log \Lambda_0(n, m) \\ &= -\frac{1}{\beta} \sigma \log 2 - \frac{1}{\beta} \int_0^\sigma dx \log \cos \frac{x\pi}{2\sigma + 2} \end{aligned} \quad (31)$$

Let the area be  $L \times L$  and let the number of particles in the  $y$  direction be the same as in the  $x$  direction; the total free energy is then  $f = 2f_x$ . In terms of the Lobachevski function

$$L(x) = -\int_0^x \log |\cos t| dt \quad (32)$$

the expression for the free energy becomes

$$f = -\frac{2}{\beta} \left[ \sigma \log 2 - \frac{2\sigma + 2}{\pi} L\left(\frac{\sigma\pi}{2\sigma + 2}\right) \right] \quad (33)$$

For high densities one obtains the expansion (Gradshteyn and Ryzhik,<sup>(11)</sup> 4.224,6)

$$f = -\frac{2\sigma}{\beta} \left[ \log 2 + 2 \sum_{k=1}^{\infty} (-1)^k \frac{(2^{2k} - 1)}{4k(2k + 1)!} B_{2k} \left(\frac{\sigma\pi}{\sigma + 1}\right)^{2k} \right] \quad (34)$$

where the  $B_{2k}$  are the Bernoulli numbers:

$$B_2 = 1/6, \quad B_4 = -1/30, \quad B_6 = 1/42, \dots$$

For low densities the following expansion is valid:

$$f = \frac{2}{\beta} \left[ \log \frac{\pi}{\sigma + 1} - 1 + 2 \sum_{k=1}^{\infty} (-1)^k \frac{B_{2k}}{4k(2k + 1)!} \left(\frac{\pi}{\sigma + 1}\right)^{2k} \right] \quad (35)$$

The pressure is given by

$$p = -\frac{\partial f(\sigma + 2d)}{\partial(\sigma + 2d)^2} = -\frac{1}{2\sigma + 4d} \frac{\partial f(\sigma)}{\partial \sigma}$$

which gives the equation of state

$$\begin{aligned} p(\sigma + 2d)^2 &= \frac{\sigma + 2d}{\beta} \left[ \log 2 - \frac{1}{\pi} L\left(\frac{\sigma\pi}{2\sigma + 2}\right) \right. \\ &\quad \left. + \frac{1}{2\sigma + 2} \log\left(\cos \frac{\sigma\pi}{2\sigma + 2}\right) \right] \end{aligned} \quad (36)$$

A low- and a high-density expansion can be obtained from (34) and (35) by differentiation. An isotherm is shown in Fig. 4. The most remarkable feature is that at close packing ( $\sigma = 0$ ) one has

$$p_{c.p.} = (1/2d\beta) \log 2 \quad (37)$$

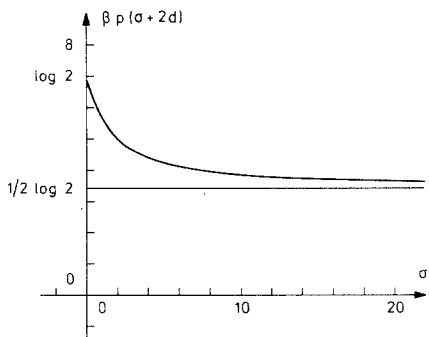


Fig. 4. An isotherm for hard squares on a lattice.

This implies that the system will be in a close-packed configuration if the pressure is higher than  $p_{c.p.}$ , and there is a phase transition of the same type as the one found in the KDP model.<sup>(3)</sup> In the present model it is a rather pathological type of phase transition.

The asymptotic value of the compressibility factor,  $\beta p(\sigma + 2d)^2$ , in the low-density limit is  $\frac{1}{2}(\sigma + 2d) \log 2$ ; this illustrates that the model is a high-density model, which fails to give the ideal gas behavior at low density.

#### 4. THE CONTINUUM MODEL

##### 4.1. Equation of State

In the continuum version of the model the equation of state is obtained by a scaling argument as described in Ref. 2:

$$\frac{pA}{NkT} = \frac{1}{1 - (A_0/A)^{1/2}} = \frac{\sqrt{\tau}}{\sqrt{\tau} - 1} \tag{38}$$

where  $A_0$  is the volume at close packing and  $\tau = A/A_0$ .

##### 4.2. Eigenvectors and Eigenvalues

It is again practical to introduce reduced and this time also scaled coordinates measuring the "free volume" available to the particles. For odd and even rows, respectively, they are

$$\begin{aligned} u_i &= (\pi/l)[x_i - 2(i - 1)d]; & i &= 1, 2, \dots, n \\ v_i &= (\pi/l)[x_i - (2i - 1)d]; & i &= 1, 2, \dots, n \end{aligned} \tag{39}$$

$$l = L - (2n - 1)d \tag{40}$$

The restrictions (2) for two neighboring rows

$$0 \leq u_1 \leq v_1 \leq u_2 \leq v_2 \leq \dots \leq u_n \leq v_n \leq \pi \tag{41}$$

can be expressed in terms of the transfer operators

$$\begin{aligned}
 T(u, v) &= \int_0^{v_1} du_1 \int_{v_1}^{v_2} du_2 \cdots \int_{v_{n-1}}^{v_n} du_n \\
 T'(v, u) &= \int_{u_1}^{u_2} dv_1 \int_{u_2}^{u_3} dv_2 \cdots \int_{u_n}^{\pi} dv_n
 \end{aligned}
 \tag{42}$$

For the independent particle model ( $n = 1$ ) the solution is, by inspection,

$$\phi_j^+ = (2/\pi)^{1/2} \cos[(j + \frac{1}{2})u], \quad \phi_j^- = (2/\pi)^{1/2} \sin[(j + \frac{1}{2})v]
 \tag{43}$$

$$T\phi_j^+ = (j + \frac{1}{2})^{-1}\phi_j^-, \quad T'\phi_j^- = (j + \frac{1}{2})^{-1}\phi_j^+
 \tag{44}$$

This result also obtains from the continuous limit for the single-particle eigenvectors of the lattice gas model. When one substitutes  $j$  for  $\frac{1}{2}(m - 1) - j$  in Eqs. (23a) and (23b) the result is

$$\phi_j^+(w) = (2/\sqrt{m}) \cos[(j + \frac{1}{2})\pi w/m]
 \tag{45}$$

The continuous limit is obtained by letting the lattice constant go to zero while keeping the number of particles and the free volume fixed,

$$l, m \rightarrow \infty, \quad l \times \text{lattice constant} = l$$

and (43) is recovered because  $\lim_{m \rightarrow \infty} (\pi/m)w = u$  for odd rows. The eigenfunctions for the  $n$ -particle problem can again be constructed as determinants made by the independent particle eigenvectors:

$$\begin{aligned}
 \Phi_j^\pm(j_1, j_2, \dots, j_n; u_1, u_2, \dots, u_n) &= \det\{\phi_{j_r}^\pm(u)\} \\
 \mathbf{j} &= \{j_1, j_2, \dots\}
 \end{aligned}
 \tag{46}$$

This solution fulfills the eigenvalue equations

$$T\Phi_s^+ = \Lambda_s \Phi_s^-, \quad T'\Phi_s^- = \Lambda_s \Phi_s^+
 \tag{47}$$

This is seen when one substitutes (42) and (46) into the left-hand side of (47):

$$\begin{aligned}
 &\int_0^{v_1} du_1 \cdots \int_{v_{n-1}}^{v_n} du_n \det \left[ \left(\frac{2}{\pi}\right)^{1/2} \cos \left[ \left(s1 + \frac{1}{2}\right)u_1 \right]; \right. \\
 &\quad \left. \left(\frac{2}{\pi}\right)^{1/2} \cos \left[ \left(s2 + \frac{1}{2}\right)u_2 \right]; \cdots; \left(\frac{2}{\pi}\right)^{1/2} \left[ \cos \left( sn + \frac{1}{2} \right) u_n \right] \right] \\
 &= \prod_{i=1}^n \left( si + \frac{1}{2} \right)^{-1} \det \left[ \left(\frac{2}{\pi}\right)^{1/2} \sin \left[ \left(s1 + \frac{1}{2}\right)v_1 \right]; \right. \\
 &\quad \left. \left(\frac{2}{\pi}\right)^{1/2} \sin \left[ \left(s2 + \frac{1}{2}\right)v_2 \right] - \left(\frac{2}{\pi}\right)^{1/2} \sin \left[ \left(s2 + \frac{1}{2}\right)v_1 \right]; \right. \\
 &\quad \left. \cdots; \left(\frac{2}{\pi}\right)^{1/2} \sin \left[ \left(sn + \frac{1}{2}\right)v_n \right] - \left(\frac{2}{\pi}\right)^{1/2} \sin \left[ \left(sn + \frac{1}{2}\right)v_{n-1} \right] \right]
 \end{aligned}
 \tag{48}$$

where the diagonal terms are used to specify the determinant. Adding the first row to the second and so forth yields the right-hand side of Eq. (47) with the eigenvalue given as

$$\Lambda_s = \prod_{i=1}^n (si + \frac{1}{2})^{-1} = \prod_{i=1}^n \lambda_{si}^{-1} \quad (49)$$

a result that also is obtained as the continuous limit of (26). The eigenfunctions can be shown to be orthonormal,

$$\begin{aligned} & \int_0^\pi du_n \int_0^{u_n} du_{n-1} \cdots \int_0^u du_1 \Phi_s \Phi_t \\ &= \frac{1}{n!} \sum_{p(s)} \sum_{p(t)} (-1)^{p+p'} \int_0^\pi du_1 \cdots \int_0^\pi du_n \\ & \quad \times [\phi_{s_1}(u_1)\phi_{t_1}(u_1)] \cdots [\phi_{s_n}(u_n)\phi_{t_n}(u_n)] \end{aligned} \quad (50)$$

The single-particle functions  $\phi$  are orthonormal and the  $n$ -fold integral thus equals zero when the sets of indices are different or when the permutations are different. The  $n!$  identical permutations each give the value one for the integral, so the result is

$$\langle \Phi_s | \Phi_t \rangle = \delta_{s,t} \quad (51)$$

### 4.3. The Entropy

The configurational integral for  $h$  rows of  $n$  particles is

$$Z_N = \langle 1 | \overbrace{T \cdots T}^h | 1 \rangle = \sum_{\mathbf{i}} \Lambda_{\mathbf{i}}^h \langle 1 | \Phi_{\mathbf{i}} \rangle^2 \quad (52)$$

where  $|1\rangle$  are the boundary states of the system. In the limit of infinitely many rows the result for the configurational integral for a row is, independent of the boundaries,

$$\lim_{h \rightarrow \infty} Z_N^{1/h} = \Lambda_0 = \prod_{j=0}^{n-1} (j + \frac{1}{2})^{-1} \quad (53)$$

When the “free volume” per row is rescaled from  $\pi$  to  $l$  the result for the entropy per particle in the thermodynamic limit is

$$\frac{s}{k} = 2 \lim_{n \rightarrow \infty} \frac{1}{n} \left( n \log \frac{l}{\pi n} - \sum_{j=0}^{n-1} \log \frac{j + \frac{1}{2}}{n} \right) = 2 \log \frac{\sigma}{\pi} + 2 \quad (54)$$

where  $\sigma$  is defined by

$$\lim_{n \rightarrow \infty} n/l = 1/\sigma \quad (55)$$

The entropy of the rigid, restricted cell model for hard squares is

$$s'/k = 2 \log(\sigma/\sqrt{2}) \quad (56)$$

The difference

$$(s - s')/k = 2 - 2 \log(\pi/\sqrt{2}) = 0.403 \quad (57)$$

is a measure of the degree of disorder introduced by the present model.

Beyerlein *et al.*<sup>(12)</sup> have derived an asymptotic form for the entropy in terms of the deviation from close packing,

$$s_e/k = 2 \log d\sqrt{2} + 2 \log(\tau - 1) - C - 2 \log(\sqrt{\tau} + 1) \quad (58)$$

with

$$\tau = \frac{A}{A_0} = \frac{L^2}{4n^2} = \left( \frac{\sigma + 2d}{2d} \right)^2 \quad (59)$$

When  $\tau$  is substituted into Eq. (54) it is seen that the entropy of the present model is given by the same expression except that the constant  $C + 2 \log 2$  comes out to be  $-0.982$  where the exact value is  $0.260$ <sup>(12)</sup> for the unrestricted hard square model. Part of this discrepancy is explained by the cell restriction which keeps the center of the particles inside the cell defined by the neighbors; in a regular configuration the accessible area will actually be twice the area given by this model adding  $\log 2$  to the entropy (Fig. 5).

## 5. CORRELATION FUNCTIONS

The absence of long-range, crystallike order is illustrated by the following exact calculations of some correlation functions. These calculations are similar to the calculations done by Sutherland for the ferroelectric models.<sup>(13)</sup>

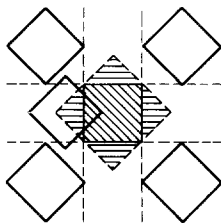


Fig. 5. The total accessible area (shaded) for a hard square in regular surroundings compared to the accessible area of the restricted model (oblique shading).

### 5.1. The Density

The probability of finding a particle at  $u = a\pi/l$  is

$$\begin{aligned} \sigma^{-1}g_n^{(1)}(a) &= \frac{\pi}{l} \frac{1}{Z_N} \left\langle 1 \left| T^{h'} \sum_{i=1}^n \delta \left[ u_i - \frac{a\pi}{l} \right] T^h \right| 1 \right\rangle \\ &= \frac{\pi}{l} \left\langle \Phi_0 \left| \sum_{i=1}^n \delta \left[ u_i - \frac{a\pi}{l} \right] \right| \Phi_0 \right\rangle \end{aligned} \tag{60}$$

in the limit  $h, h' \rightarrow \infty$ . The matrix element is calculated in Appendix A; the result for  $g_n^{(1)}$  is

$$g_n^{(1)}(a) = 1 \pm \frac{\sin(2\pi a/\sigma)}{2n \sin(\pi a/\sigma)} \tag{61}$$

for odd and even rows, respectively.

The one-particle correlation along a topological row thus dies out in a damped oscillation.

In the thermodynamic limit the result is

$$g^{(1)}(a) = 1 \pm (\sigma/2\pi a) \sin(2\pi a/\sigma) \tag{62}$$

Far from the boundary,  $a \gg \sigma$ ,  $a/L \rightarrow$  a constant, the particle density is uniform as shown in Fig. 6. The particle distribution in real space cannot be obtained from this result just by substituting the coordinate transformation (39), because there is an unknown distribution of the number of particles to the left of  $a$ .

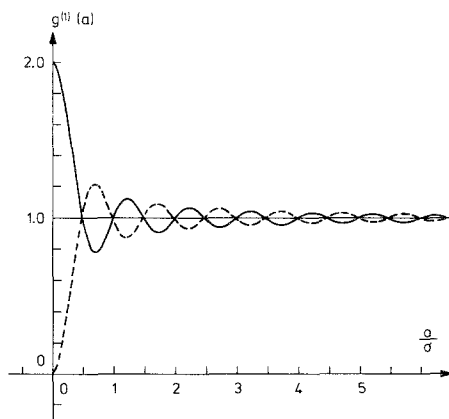


Fig. 6. The hard square density in an odd and an even (dashed) row close to the boundary [Eq. (62)].

### 5.2. The Two-Body Correlation

The probability of finding a particle at  $u = a\pi/l$  and another at  $u = b\pi/l$  on the same row is given by an expression similar to (60),

$$\begin{aligned} &\sigma^{-2}g_n^{(1)}(a)g_n^{(1)}(b)g_n^{(2)}(a, b; 0) \\ &= \left(\frac{\pi}{l}\right)^2 \left\langle \Phi_0 \left| \sum_{s \neq t} \delta\left(u_s - \frac{a\pi}{l}\right) \delta\left(u_t - \frac{b\pi}{l}\right) \right| \Phi_0 \right\rangle \end{aligned} \quad (63)$$

This matrix element is also calculated in Appendix A; the resulting value for the two-body correlation is

$$\begin{aligned} g_n^{(2)}(a, b; 0) &= 1 - \left( \frac{\sin[(a-b)\pi/\sigma]}{\sin[(a-b)\pi/2n\sigma]} \pm \frac{\sin[(a+b)\pi/\sigma]}{\sin[(a+b)\pi/2n\sigma]} \right)^2 \\ &\quad \times [2ng_n^{(1)}(a)g_n^{(1)}(b)]^{-1} \end{aligned} \quad (64)$$

In the thermodynamic limit the result is

$$\begin{aligned} g^{(2)}(a, b; 0) &= 1 - \left[ \frac{\sigma}{\pi(a-b)} \sin\left(\frac{a-b}{\sigma}\pi\right) \pm \frac{\sigma}{\pi(a+b)} \sin\left(\frac{a+b}{\sigma}\pi\right) \right] \\ &\quad \times [g^{(1)}(a)g^{(1)}(b)]^{-1} \end{aligned} \quad (65)$$

Far from the boundary where  $a \gg \sigma$ ,  $b \gg \sigma$ , and  $(a-b)/\sigma$  finite, the two-body correlation takes the following form (see also Fig. 7)

$$g^{(2)}(a-b; 0) = 1 - \left[ \frac{\sigma}{\pi(a-b)} \right]^2 \sin^2\left(\frac{a-b}{\sigma}\pi\right) \quad (66)$$

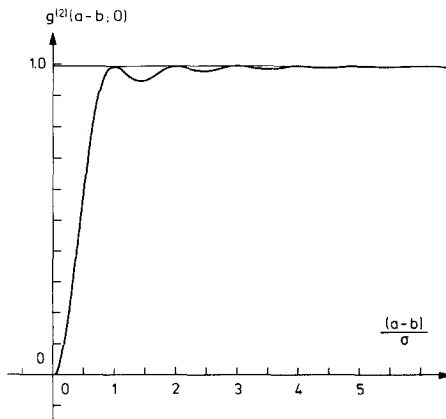


Fig. 7. The two-body correlation in a row far from the boundaries [Eq. (66)].



These results show that there is no crystal-like order in the model, but also that the long-range order decays very slowly.

If we want to consider the two-body distribution for particles in different rows, we are faced with the difficulty that there is no  $y$  coordinate in this description. What we can do is to give the joint distribution of particles at  $u = a\pi/l$  and at  $u = b\pi/l$  in a row numbered  $2z$  higher:

$$\begin{aligned} & \sigma^{-2} g_n^{(1)}(a) g_n^{(1)}(b) g_n^{(2)}(a, b; 2z) \\ &= \left(\frac{\pi}{l}\right)^2 \frac{1}{Z_N} \left\langle 1 \left| T^n \sum_{s=1}^n \delta\left(u_s - \frac{b\pi}{l}\right) T^{2z} \sum_{t=1}^n \delta\left(u_t - \frac{a\pi}{l}\right) T^{n'} \right| 1 \right\rangle \\ &= \left(\frac{\pi}{l}\right)^2 \sum_i \left(\frac{\Lambda_i}{\Lambda_0}\right)^2 \left\langle \Phi_0 \left| \sum_s \delta\left(u_s - \frac{b\pi}{l}\right) \right| \Phi_i \right\rangle \\ & \quad \left\langle \Phi_i \left| \sum_t \delta\left(u_t - \frac{a\pi}{l}\right) \right| \Phi_0 \right\rangle, \end{aligned} \tag{67}$$

in the limit  $h', h \rightarrow \infty$ . The matrix elements are given in Appendix A; there are only contributions from the state  $\Phi_0$  and the states  $\Phi_i$  where one mode is excited, i.e.,

$$\frac{\Lambda_i}{\Lambda_0} = \frac{\lambda_e}{\lambda_g} = \frac{g + \frac{1}{2}}{e + \frac{1}{2}}, \quad i \neq 0 \tag{68}$$

$$\begin{aligned} & g_n^{(1)}(a) g_n^{(1)}(b) g_n^{(2)}(a, b; 2z) \\ &= g_n^{(1)}(a) g_n^{(1)}(b) \\ & \quad + \left[ \frac{1}{n} \sum_{g=0}^{n-1} \left(\frac{g + \frac{1}{2}}{n}\right)^{2z} \left( \cos \frac{(a-b)\pi(g + \frac{1}{2})}{\sigma n} \pm \cos \frac{(a+b)\pi(g + \frac{1}{2})}{\sigma n} \right) \right] \\ & \quad \times \left[ \frac{1}{n} \sum_{e=0}^{n-1} \left(\frac{e + \frac{1}{2}}{n}\right)^{2z} \left( \cos \frac{(a-b)\pi(e + \frac{1}{2})}{\sigma n} \pm \cos \frac{(a+b)\pi(e + \frac{1}{2})}{\sigma n} \right) \right] \end{aligned} \tag{69}$$

for odd and even rows, respectively.

In the thermodynamic limit the following results obtain:

$$\begin{aligned} g^{(2)}(a, b; 2z) &= 1 + \left[ \int_0^1 dh h^{2z} (\cos \Delta h \pm \cos \Sigma h) \right] \\ & \quad \times \left[ \int_1^\infty dh h^{-2z} (\cos \Delta h \pm \cos \Sigma h) \right] [g^{(1)}(a) g^{(2)}(b)]^{-1} \end{aligned} \tag{70}$$

where  $\Delta \equiv [(a - b)/\sigma]\pi$  and  $\Sigma \equiv [(a + b)/\sigma]\pi$ .

The integrals are calculated in Appendix B; the results are rather lengthy and will not be quoted here.

Far from the boundary  $g^{(2)}$  only depends on  $a - b$ ; choosing  $a + b = l$ , the following simple result is obtained:

$$g^{(2)}(a - b; 2z) = 1 + \left[ \int_0^1 dh h^{2z} \cos \Delta h \right] \left[ \int_1^\infty dh h^{-2z} \cos \Delta h \right] \quad (71)$$

The explicit result for  $z = 1$  is given in Appendix B.

We can finally give the asymptotic behavior of  $g^{(2)}(a - b; 2z)$ . For  $\Delta = [(a - b)/\sigma]\pi \rightarrow \infty$  and eventually  $z \rightarrow \infty$  but  $z/\Delta^4 \rightarrow 0$  the following result is obtained from the expansions in Appendix C:

$$\begin{aligned} g^{(2)}(a - b; 2z) &\simeq 1 + \frac{1}{\Delta^2} \frac{\beta^2 \cos^2 \Delta - \sin^2 \Delta}{(1 + \beta^2)^2} - \frac{1}{\Delta^3} \frac{\beta^2 \sin 2\Delta}{(1 + \beta^2)^3} \\ &+ \frac{1}{\Delta^4} \left[ \frac{\beta^2 \cos^2 \Delta}{(1 + \beta^2)^6} (121\beta^6 - 120\beta^5 + 86\beta^4 - 120\beta^3 + 41\beta^2 - 4) \right. \\ &\left. - \frac{\sin^2 \Delta}{(1 + \beta^2)^8} (5\beta^6 - 54\beta^4 + 21\beta^2) \right] \end{aligned} \quad (72)$$

where  $\beta \equiv 2z/\Delta$ .

For finite  $\Delta$  and  $z \rightarrow 0$  the result (66) is again obtained.

### APPENDIX A. Matrix Elements

$$\begin{aligned} &\left\langle \Phi_0 \left| \sum_{s=1}^n \delta(u_s - \alpha) \right| \Phi_i \right\rangle \\ &= \frac{1}{n!} \int_0^\pi du_1 \dots \int_0^\pi du_n \sum_{p(j)} \sum_{p'(k)} (-1)^{p+p'} \dots [\phi_{j_i}(u_i) \phi_{k_i}(u_i)] \dots \\ &\quad \times \left[ \sum_{s=1}^n \delta(u_s - \alpha) \right] \end{aligned} \quad (A.1)$$

because of the symmetry in  $u_i$ . Exactly one integration is not performed, but the  $u - 1$  others give  $\delta_{j_i, k_i}$ . So the  $u - 1$  indices have to be the same and have the same permutation, too.

For the two remaining indices different ( $e \neq g$ , where  $g$  is in the ground state  $\Phi_0$ ,  $g = 0, \dots, n - 1$ , and  $e$  is in an excited state  $\Phi_i$ ,  $e = n, n + 1, \dots$ ) the result is

$$\left\langle \Phi_0 \left| \sum_{s=1}^n \delta(u_s - \alpha) \right| \Phi_i \right\rangle = \phi_g(\alpha) \phi_e(\alpha); \quad \mathbf{i} \neq \mathbf{0} \quad (A.2)$$

But for all indices equal ( $e = g$ ) there is a contribution from all  $n!$  identity permutations of  $j$  and  $k$ ; so  $g$  can take all values in  $\Phi_0$ ,

$$\sum_{g=0}^{n-1} \phi_g^2(\alpha) = \frac{n}{\pi} \pm \sum_{g=0}^{n-1} \frac{1}{\pi} \cos 2\alpha(g + \frac{1}{2}) \tag{A.3}$$

(the plus sign for odd rows) and

$$\left\langle \Phi_0 \left| \sum_{s=1}^n \delta(u_s - \alpha) \right| \Phi_0 \right\rangle = \frac{n}{\pi} \pm \frac{\sin 2n\alpha}{2 \sin \alpha} \tag{A.4}$$

(Gradshteyn and Ryzhik,<sup>(11)</sup> 1.341). The matrix element

$$\left\langle \Phi_0 \left| \sum_{s \neq t}^n \sum_{t}^n \delta(u_s - \alpha) \delta(u_t - \beta) \right| \Phi_0 \right\rangle$$

can be written analogous to Eq. (A.1). Exactly two integrations are not performed, but the  $n - 2$  others give  $\delta_{ji,ki}$ . So these  $n - 2$  indices have to be equal and have the same permutation, too. For a given permutation of  $ji$  there will be a term

$$\phi_{ji}(\alpha) \phi_{jf}(\beta) \phi_{ki}(\alpha) \phi_{kf}(\beta) \tag{A.5}$$

where

$$\left. \begin{matrix} ji \\ jf \end{matrix} \right\} = 0, 1, \dots, n - 1; \quad ji \neq jf$$

because of the sum over the coordinates. So the sum over permutations of  $ji$  will just give a factor  $n!$  and the permutation of  $k$  will give two terms:

$$\sum_i^{n-1} \sum_f^{n-1} [\phi_i^2(\alpha) \phi_f^2(\beta) - \phi_i(\alpha) \phi_i(\beta) \phi_f(\alpha) \phi_f(\beta)] \tag{A.6}$$

Since the last term, which can be written as

$$(1/\pi) \sum_{i=0}^{n-1} \{ \pm \cos[(\alpha + \beta)(i + \frac{1}{2})] + \cos[(\alpha - \beta)(i + \frac{1}{2})] \} \tag{A.7}$$

can be calculated by the same sum formula as above, the matrix element is

$$\begin{aligned} & \left\langle \Phi_0 \left| \sum_{s \neq t}^n \sum_{t}^n \delta(u_s - \alpha) \delta(u_t - \beta) \right| \Phi_0 \right\rangle \\ &= \left[ \frac{n}{\pi} \pm \frac{\sin 2n\alpha}{2\pi \sin \alpha} \right] \left[ \frac{n}{\pi} \pm \frac{\sin 2n\beta}{2\pi \sin \beta} \right] \\ & - \left[ \frac{\sin[(\alpha - \beta)n]}{2\pi \sin \frac{1}{2}(\alpha - \beta)} \pm \frac{\sin[(\alpha + \beta)n]}{2\pi \sin \frac{1}{2}(\alpha + \beta)} \right]^2 \end{aligned} \tag{A.8}$$

**APPENDIX B**

Integrals from  $g^{(2)}(a, b, 2z)$ :

$$\int_0^1 dx x^{2z} \cos ax = \frac{(2z)! (-1)^z}{a^{2z+1}} \sum_{i=0}^{2z} \frac{(-a)^i}{i!} \sin\left(a + \frac{1}{2} \pi i\right) \tag{B.1}$$

(Gradshteyn and Ryzhik, <sup>(11)</sup>2.633,2);

$$\begin{aligned} \int_1^\infty dx x^{-2z} \cos ax \\ = \frac{a^{2z-2} (-1)^{z-1}}{(2z-1)!} \left[ \sum_{j=0}^{2z-2} \frac{j! (-1)^j}{a^j} \cos\left(a + \frac{1}{2} \pi j\right) - a \operatorname{si}(a) \right] \end{aligned} \tag{B.2}$$

(Gradshteyn and Ryzhik, <sup>(11)</sup> 2.639,3). These integrals give the expression for the product in Eq. (70) which in the case  $a + b = l$  reads [Eq. (71)]

$$\begin{aligned} g^{(2)}(a - b; 2z) &= 2z \operatorname{si}(a) \sum_{i=0}^{2z} \frac{(-a)^{i-2}}{i!} \sin\left(a + \frac{1}{2} \pi i\right) \\ &\quad - z \sum_{i=0}^{2z} \sum_{j=0}^{2z-2} (-1)^{i+j} a^{i-j-3} \frac{j!}{i!} \sin\left[2a + \frac{1}{2} (i+j)\pi\right] \\ &\quad + z \sum_{j=0}^{2z-2} (-1)^j j! a^{-2j-2} \sum_{k=E(1/2j)}^{E(j-1/2)+z} \frac{a^{2k}}{(2k-j+1)!} \end{aligned} \tag{B.3}$$

where  $2k + 1 = i + j$ . For  $z = 1$  the result is

$$\begin{aligned} g^{(2)}(a - b; 2) &= 1 + 2 \operatorname{si}(\Delta) \left[ \frac{\sin \Delta}{\Delta^2} - \frac{\cos \Delta}{\Delta} - \frac{1}{2} \sin \Delta \right] - \frac{\sin 2\Delta}{\Delta^3} \\ &\quad + \frac{\cos 2\Delta}{\Delta^3} + \frac{\cos 2\Delta}{\Delta^2} + \frac{\sin 2\Delta}{2\Delta} + \frac{1}{\Delta^2} \end{aligned} \tag{B.4}$$

where  $\Delta \equiv [(a - b)/\sigma]\pi$ .

**APPENDIX C**

Asymptotic expansion of the correlation function Eq. (71):

$$\begin{aligned} \int_1^\infty dh h^{-2z} \cos \Delta h &= \frac{\cos \Delta}{\Delta} \int_0^\infty dx \left(1 + \frac{x}{\Delta}\right)^{-2z} \cos x \\ &\quad - \frac{\sin \Delta}{\Delta} \int_0^\infty dx \left(1 + \frac{x}{\Delta}\right)^{-2z} \sin x \end{aligned} \tag{C.1}$$

Note that we can cut the integrals at  $\Delta$  in the asymptotic expansion, since

$$\frac{1}{\Delta} \int_\Delta^\infty dx \left(1 + \frac{x}{\Delta}\right)^{-2z} \cos x < \frac{1}{\Delta} \int_\Delta^\infty dx \left(1 + \frac{x}{\Delta}\right)^{-2z} = O(e^{-2z}) \tag{C.2}$$

Similarly we find for the other integral

$$\int_0^1 dh h^{-2z} \cos \Delta h = \int_0^1 dx (1-x)^{2z} \cos(\Delta - \Delta x)$$

and the two integrals equal

$$\frac{\cos \Delta}{\Delta} \int_0^\Delta dx \left(1 \pm \frac{x}{\Delta}\right)^{\mp 2z} \cos x \mp \frac{\sin \Delta}{\Delta} \int_0^\Delta dx \left(1 \pm \frac{x}{\Delta}\right)^{\mp 2z} \sin x \quad (C.3)$$

where the upper sign is for the upper integral.

The asymptotic behavior for  $\Delta$  and  $2z \rightarrow \infty$  is found by rewriting and expanding the logarithm and part of the exponent to second order,

$$\begin{aligned} \int_0^\Delta dx \cos x \exp\left[\mp 2z \ln\left(1 \pm \frac{x}{\Delta}\right)\right] & \text{ (and equivalent for sin)} \\ \simeq \int_0^\Delta dx (\cos x) \left(\exp - \frac{2z}{\Delta}x\right) \left(1 \pm \frac{z}{\Delta^2}x^2 - \frac{2z}{3\Delta^3}x^3 + \frac{z^2}{2\Delta^4}x^4 \dots\right) & \quad (C.4) \end{aligned}$$

Since we can extend these integrals to infinity, by the argument from Eq. (C.2), the integrals are given in Ref. 11 (2.663,1-3; 2.667,7-8; 3.944,5-6). We finally find with the notation

$$\begin{aligned} \beta = 2z/\Delta, \quad t = \arctan \beta^{-1}, \quad s = 1 + \beta^2 & \quad (C.5) \\ \cos t = \beta/s^{1/2}, \quad \sin t = 1/s^{1/2} & \end{aligned}$$

that, for example,

$$\int_0^\infty dx (\cos x)x^3 e^{-\beta x} = 3! s^{-2} \cos 4t = 3! s^{-4}(8\beta^4 - 8\beta^2 s + s^2)$$

where  $\cos 4t$  has been rewritten in powers of  $\sin t$  and  $\cos t$ . Collecting terms up to second order gives the expression (72).

**ACKNOWLEDGMENT**

The authors would like to thank E. H. Lieb for valuable discussions.

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