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The Effect of a Constant Number of Particles on the Pair Correlation Function and the Density Profile in a One-Dimensional Lattice Gas

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A one-dimensional lattice gas (Ising model) of length L and with nearest-neighbor coupling J is considered in a canonical ensemble with fixed number of particles $N = L/2$. Exact expressions and asymptotic forms for large L are derived for the density–density correlation function, using periodic boundary conditions, and for the density (magnetization) profile, using antisymmetric boundary conditions. The density–density correlation function, g, assumes for temperatures $T > T'$, with $T' = 2J(k_B \ln L)^{-1}$, and for L large, the form

$$g(x) = g^{gc}(x) + BL^{-1} + a(x)\,L^{-1} + O(L^{-2})$$

where x is a distance between considered lattice sites, B is known from earlier work of Lebowitz and Percus,(1b) and $a(x)$ decays exponentially for $x \to \infty$. For $T \leqslant T'$, the correlation function and the density profile behave differently, the latter exhibiting a step in the middle of the interface.

KEY WORDS: One-dimensional lattice gas; canonical ensemble; density profile; correlation function.

1. INTRODUCTION AND RESULTS

In finite systems the correlation functions, calculated in the canonical and grand canonical ensembles, differ from each other, especially for large distances.[1] Similar differences may be present for correlation functions and density profiles in nonuniform systems, for example, in an interface between coexisting phases. Dudowicz and Stecki[2] have observed that these differences in the finite two-dimensional lattice gas are very large. Up

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till now exact results in the canonical ensemble are not known, even for a one-dimensional lattice gas.

It is hoped that these results may be related to the problem of a local structure of an interface. A sharp interface of microscopic extent results in a straightforward manner in meanfield theories,[3] whereas in a two-dimensional lattice gas (in the grand canonical ensemble) one finds a vanishing density profile for vanishing macroscopic external field, even if boundary conditions favor the phase separation.[4]

In this paper exact expressions for the correlation function and the density profile in the canonical ensemble are derived for a one-dimensional lattice gas of length L and their asymptotic forms for $L \to \infty$ are established. Two types of boundary conditions are considered: cyclic boundary conditions and the boundary conditions given by

$$\hat{n}_0 = 1, \qquad \hat{n}_{L+1} = 0 \tag{1}$$

where $\hat{n}_x = 0, 1$ is the microscopic variable associated with the site x, and $\hat{n}_x = 0$ corresponds to an empty cell, whereas $\hat{n}_x = 1$ to an occupied one. L is an even integer.

In the first case we derive the correlation function, whereas in the second one we compute the density (magnetization) profile. The asymptotic form of the density–density correlation function, g, in a closed system is known to be[1]

$$g(x) \underset{\substack{N \to \infty \\ x \to \infty}}{\cong} 1 - n\chi k_B T N^{-1} \tag{2}$$

k_B is Boltzmann's constant, n is the average number density, and χ the compressibility. This form is appropriate for a uniform fluid with no long-range correlations, as is explained in Ref. 1b.

For $n = 1/2$ we have found the exact expression for the correlation function $g(x)$ for any x, and its asymptotic form for $L \to \infty$. We have then compared our result with the form (2) as well as with the function $g^{gc}(x)$ found in the open system (grand canonical ensemble). In the second, non-uniform case, we were interested in the density profile in a large system, especially at low temperatures, because for $T = 0$ K the density profiles in the closed and open systems differ qualitatively from each other, and because

$$\lim_{L \to \infty} \lim_{T \to 0} \langle \hat{n}_x \rangle_n \neq \lim_{L \to \infty} \lim_{T \to 0} \langle \hat{n}_x \rangle_n^{gc}$$

The above is due to the degeneracy (with respect to the number of particles) of the ground state in the grand canonical ensemble.

We have derived the expressions for the density profile and the asymptotic form of $\langle \hat{n}_{L/2} \rangle_n$ for $L \to \infty$ for different values of the temperature, as well as for $T \to 0$. The density profiles were calculated numerically for $L = 60$ and they were then compared with the density profiles in the grand canonical ensemble.

In Section 2, the exact results are derived for finite L, whereas Section 3 contains the asymptotic analysis for $L \to \infty$.

2. EXACT EXPRESSIONS FOR FINITE *L*

The lattice gas and the Ising models are equivalent, but it is more convenient for our purposes to use the language of the latter. The variables in the lattice gas and the Ising model are related to each other as follows:

$$\hat{n}_x = \frac{\sigma_x + 1}{2} \tag{3a}$$

where $\sigma_x = \pm 1$ is a spin variable associated with the site x. Thus, we have

$$\langle \hat{n}_x \rangle = \frac{\langle \sigma_x \rangle + 1}{2} \tag{3b}$$

$$g(x) = \frac{\langle \hat{n}_1 \hat{n}_{1+x} \rangle}{\langle \hat{n}_1 \rangle \langle \hat{n}_{1+x} \rangle} = h(x) + 1 \tag{4a}$$

The total correlation function h is equal because of (3a) to the spin–spin distribution function:

$$h(x) = \langle \sigma_1 \sigma_{1+x} \rangle \tag{4b}$$

We fix the number of particles to be $N = L/2$. This implies in the corresponding Ising model the following restriction on configurations:

$$\sum_{i=1}^{L} \sigma_i = 0 \tag{5}$$

As was mentioned in the previous section, two systems will be considered. The first one will be denoted by c (cyclic) whereas the second one by n (nonuniform). The probability distributions are defined by

$$\text{c:} \quad \rho_c((\sigma_i)) = Z_c^{-1} \delta\left(\sum_{i=1}^{L} \sigma_i \right) \exp\left\{ K \left[\sum_{i=1}^{L} \sigma_i \sigma_{i+1} \right] \right\} \tag{6a}$$

$$\text{n:} \quad \rho_n((\sigma_i)) = Z_n^{-1} \delta\left(\sum_{i=1}^{L} \sigma_i \right) \exp\left\{ K \left[\sigma_1 - \sigma_L + \sum_{i=1}^{L} \sigma_i \sigma_{i+1} \right] \right\} \tag{6b}$$

where

$$K=\beta J, \qquad \beta=1/k_B T \tag{7}$$

and $\delta(a)$ denotes the Kronecker symbol.

The following expressions define the quantities of interest:

$$\langle \sigma_i \sigma_{1+x} \rangle_c = \sum_{(\sigma_i)} \sigma_1 \sigma_{1+x} \rho_c(\sigma_i)) \tag{8a}$$

$$\langle \sigma_x \rangle_n = \sum_{(\sigma_i)} \sigma_x \rho_n((\sigma_i)) \tag{8b}$$

By symmetry with respect to the changes

$$\text{c:} \quad x \to L-x \tag{9a}$$

$$\text{n:} \quad x \to L-x-1 \tag{9b}$$

it follows that

$$\text{c:} \quad \langle \sigma_1 \sigma_{1+x} \rangle_c = \langle \sigma_1 \sigma_{1+L-x} \rangle_c \tag{9c}$$

$$\text{n:} \quad \langle \sigma_x \rangle_n = -\langle \sigma_{L-x-1} \rangle_n \tag{9d}$$

Thus we shall restrict ourselves to the case $x \leqslant L/2$.

Applying the identity

$$\delta(a) = \frac{1}{2\pi} \int_0^{2\pi} dk\, e^{ika}$$

and using standard transfer matrix notations, we have

$$Z_c = \frac{1}{2\pi} \int_0^{2\pi} dk \operatorname{Tr} T_k^L \tag{10a}$$

$$\langle \sigma_1 \sigma_{1+x} \rangle_c = \frac{1}{2\pi Z_c} \int_0^{2\pi} dk \sum_{\sigma_1, \sigma_{1+x}} \sigma_1 \sigma_{1+x} T_k^x(\sigma_1, \sigma_{1+x})\, T_k^{L-x}(\sigma_{1+x}, \sigma_1) \tag{10b}$$

$$Z_n = \frac{1}{2\pi} \int_0^{2\pi} dk \sum_{\sigma_1, \sigma_L} e^{(K+ik/2)\sigma_1} T_k^{L-1}(\sigma_1, \sigma_L)\, e^{(-K+ik/2)\sigma_L} \tag{10c}$$

and

$$\langle \sigma_x \rangle_n = \frac{1}{2\pi Z_n} \int_0^{2\pi} dk \sum_{\sigma_1, \sigma_x, \sigma_L} e^{(K+ik/2)\sigma_1} T_k^{x-1}(\sigma_1, \sigma_x) \times \sigma_x T_k^{L-x}(\sigma_x, \sigma_L)\, e^{(-K+ik/2)\sigma_L} \tag{10d}$$

where the transfer matrix T_k is defined by

$$T_k(\sigma_1, \sigma_2) = \exp[K\sigma_1\sigma_2 + ik/2\,(\sigma_1 + \sigma_2)] \tag{11}$$

The eigenvalues of T_k are of the form

$$\lambda_{1,2} = e^K f_{1,2}(k) \tag{12a}$$

where

$$f_{1,2}(k) = \cos k \pm (\cos^2 k - b)^{1/2} \tag{12b}$$

and b is given by

$$b = 1 - e^{-4K} \tag{13}$$

After elementary algebraic transformations we get

$$\langle \sigma_1 \sigma_{1+x} \rangle_c = 1 - \frac{\int_0^{2\pi} dk\, G(k)}{\int_0^{2\pi} dk\, R(k)} \tag{14a}$$

and

$$\langle \sigma_x \rangle_n = b^x \frac{\int_0^{2\pi} dk\, W_{L+1-2x}(k)}{\int_0^{2\pi} dk\, Z(k)} \tag{14b}$$

where

$$G(k) = 4e^{-4K} W_x(k)\, W_{L-x}(k) \tag{15a}$$

$$R(k) = R_L(k) \tag{15b}$$

$$Z(k) = \cos k R_{L-1}(k) + (\cos^2 k - b/2)\, W_{L-1}(k) \tag{15c}$$

and

$$R_x(k) = f_1^x(k) + f_2^x(k) \tag{15d}$$

$$W_x(k) = \frac{f_1^x(k) - f_2^x(k)}{f_1(k) - f_2(k)} \tag{15e}$$

3. ASYMPTOTIC ANALYSIS FOR $L \to \infty$

The integrals in (14) have been calculated numerically for $L = 60$ and the results are shown in Figs. 1–3. The density profiles, as calculated in the canonical and the grand canonical ensembles are seen to differ from each other, especially at low temperatures. The density profile in the canonical

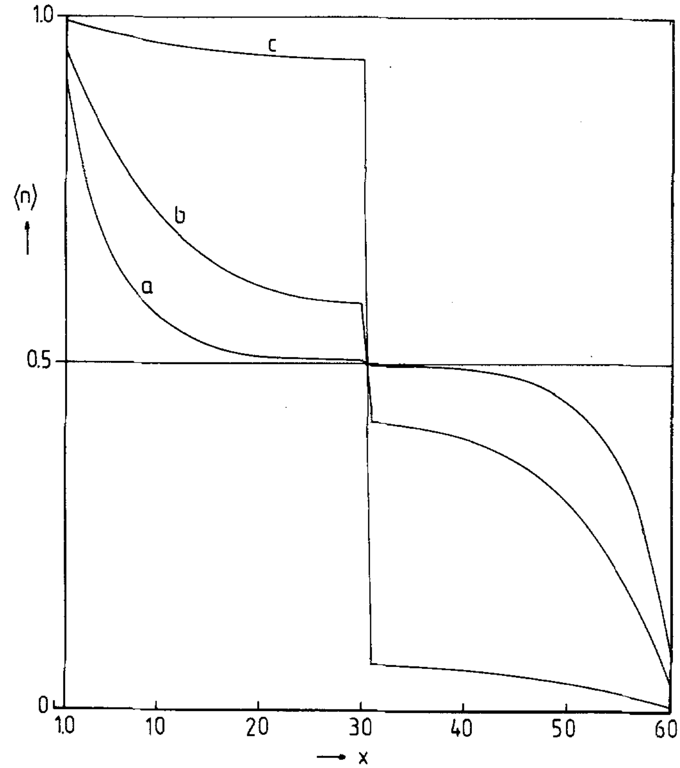

Fig. 1. The density profiles in a system of length $L=60$ as calculated in the canonical ensemble: (a) $K=1.10$; (b) $K=1.47$; (c) $K=2.20$ ($K=J/k_B T$).

ensemble for $K=2 \cdot 2$ looks like the density profile in a system consisting of two different phases separated by an interface of microscopic extent.

In order to study the quantities of interest for large L, we study the asymptotic behavior for $L \to \infty$ of the integrals in (14). If we are interested in a rough qualitative description of the density profile, we may confine ourselves to $x = L/2$ (see Fig. 1c). Eq. (14b) then simplfies to

$$\langle \sigma_{L/2} \rangle_n = 2\pi b^{L/2} \left[4 \int_0^{\pi/2} dk\, Z(k) \right]^{-1} \tag{14c}$$

where the fact that $\langle \sigma_{L/2} \rangle_n \geqslant 0$ follows from the choice of boundary conditions and site labeling.

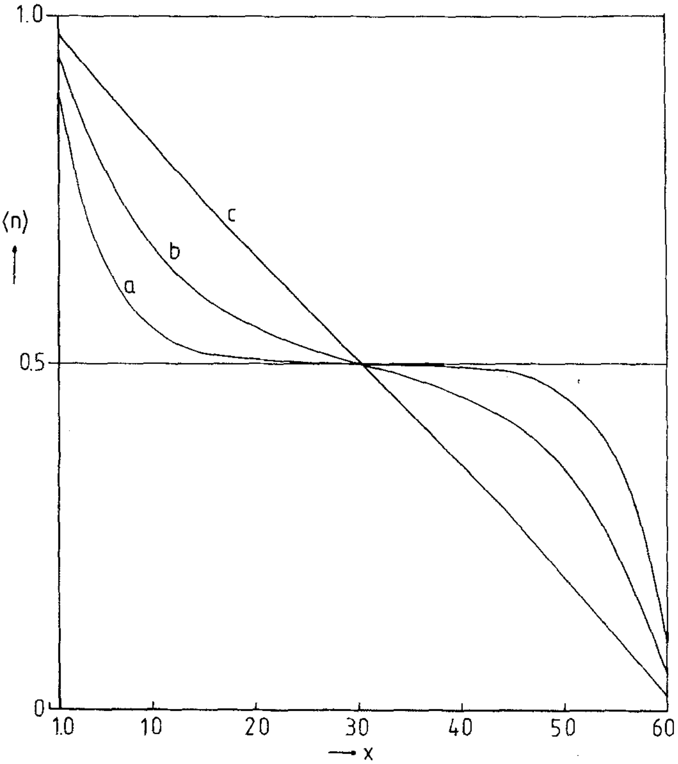

Fig. 2. The density profiles in a system of length $L=60$ as calculated in the grand canonical ensemble: (a) $K=1.10$; (b) $K=1.47$; (c) $K=2.20$ ($K=J/k_BT$).

The explicit forms of the integrands Z, G, R in (14) are

$$Z(k)=\begin{cases} f_1^L(k)\cos k+\dfrac{\cos^2 k-b/2}{\sqrt{\cos^2 k-b}}+f_2^L(k)\cos k-\dfrac{\cos^2 k-b/2}{\sqrt{\cos^2 k-b}} & \text{for} \quad k\leqslant k_1 \\ 2b^{(L-1)/2}\left\{\cos k\cos[(L-1)\varphi]+\dfrac{\cos^2 k-b/2}{\sqrt{\cos^2 k-b}}\sin[(L-1)\varphi]\right\} & \text{for} \quad k\geqslant k_1 \end{cases} \tag{16a}$$

$$G(k)=\begin{cases} \dfrac{e^{-4K}}{\cos^2 k-b}\{f_1^L(k)+f_2^L(k)-b^x[f_1^{L-2x}(k)+f_2^{L-2x}(k)]\} & \text{for} \quad k\leqslant k_1 \\ \dfrac{2e^{-4K}b^{L/2}}{b-\cos^2 k}\{\cos[(L-2x)\varphi]-\cos(L\varphi)\} & \text{for} \quad k\geqslant k_1 \end{cases} \tag{16b}$$

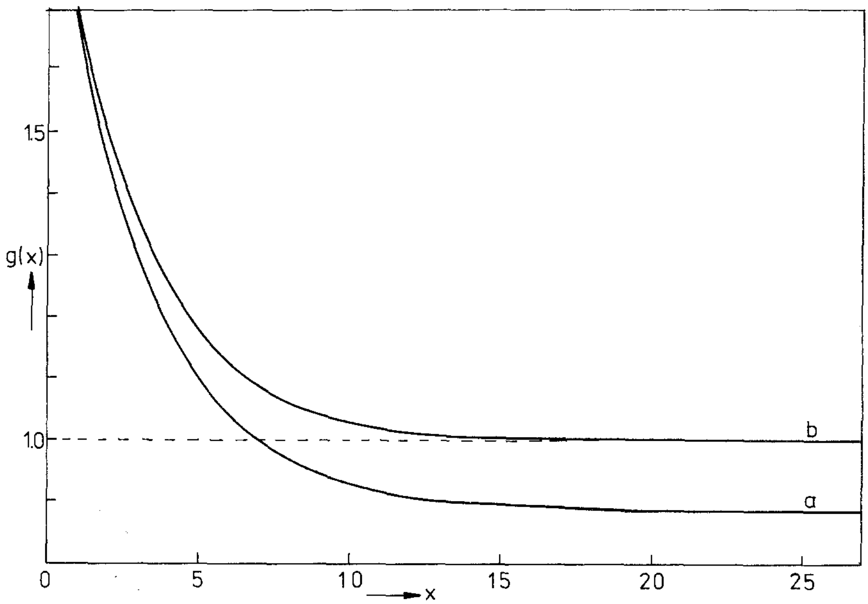

Fig. 3. The correlation function g in a system of length $L=60$ for $K=0.88$: (a) the canonical ensemble; (b) the grand canonical ensemble.

and

$$R(k)=\begin{cases} f_1^L(k)+f_2^L(k) & \text{for} \quad k\leqslant k_1 \\ 2b^{L/2}\cos(L\varphi) & \text{for} \quad k\geqslant k_1 \end{cases} \tag{16c}$$

where

$$tg\varphi=\frac{\sqrt{b-\cos^2 k}}{\cos k} \tag{17}$$

$$\cos^2 k_1=b \tag{18}$$

and $f_{1,2}$ are defined in (12b).

We split the integrals into

$$\int_0^{\pi/2} dk\, F(k)=\int_0^{k_1} dk\, F(k)+\int_{k_1}^{\pi/2} dk\, F(k) \tag{19}$$

where $F=Z$, R or G. The integrands we consider have their global maxima at $k=0$. For $0<k<k_1$ they all decrease monotonically, because their first derivatives are negative. Let us consider the ratios of the values of the

functions Z, R and G for $k=k_1$ to the values of those functions for $k=0$. We get

$$\frac{G(k_1)}{G(0)}=th^{L/2}Ke^{-4K}\frac{L^2-(L-2x)^2}{(1-e^{-4K})(1+th^LK-th^xK-th^{L-x}K)} \tag{20a}$$

$$\frac{R(k_1)}{R(0)}=th^{L/2}K\frac{2}{1+th^LK} \tag{20b}$$

and

$$\frac{Z(k_1)}{Z(0)}=th^{L/2}K\frac{2(L+1)\,e^{-2K}}{(1+e^{-2K})(1-th^{L+1}K)} \tag{20c}$$

We introduce the new parameter $\delta>0$, defined by

$$e^{2K}=L^{\delta} \tag{21}$$

The asymptotic behaviors of the ratios (20) are the same. Denoting these by η, we have

$$\eta=\begin{cases}O(L^{-M}) \quad M \text{ arbitrary}, & \text{for} \quad \delta<1\\ O(1), & \text{for} \quad \delta\geqslant 1\end{cases} \tag{22}$$

We denote the temperature corresponding to $\delta=1$ by T' and get

$$T'=2J(k_B\ln L)^{-1} \tag{23}$$

3A. Case $T>T'$

Let us consider the case $T>T'$ ($\delta<1$). Because the absolute values of G, R, and Z do not increase for $k>k_1$, we get from (22) that $\int_{k_1}^{\pi/2}dk\,F(k)$ is negligible, where $F=G$, R, or Z. We again split the remaining integrals into two terms:

$$\int_0^{k_1}dk\,F(k)=\int_0^{k_0}dk\,F(k)+\int_{k_0}^{k_1}dk\,F(k) \tag{24}$$

where k_0 is such that satisfies $k_0\ll e^{-2K}$. Expanding about $k=0$ we get for the ratios $F(k_0)/F(0)$ the estimates

$$\frac{F(k_0)}{F(0)}=[1-e^{2K}k_0^2+O(k_0^4e^{2K})]^L[1+O(k_0^2e^{4K})] \tag{25}$$

where $F = G$, R, or Z. The integrands decrease and from the above, we see that the integrals $\int_{k_0}^{k_1} dk\, F(k)$ are negligible for $k_0 = L^{-\alpha}$, where $\alpha < (1+\delta)/2$. Thus the main contribution to the integrals under consideration comes from the interval $(0, k_0)$. For the latter, the Laplace method can be applied, the integrands being of the form

$$F(k) \underset{L \to \infty}{=} w(k)\, e^{-L \cdot h(k)} \tag{26}$$

where

$$h(k) = \ln f_1(k) \tag{27}$$

and

$$w(k) = \begin{cases} \cos k + (\cos^2 k - b/2)(\cos^2 k - b)^{-1/2}, & F = Z \\ 1 & F = R \\ \dfrac{e^{-4K}}{\cos^2 k - b}\left[1 - \left(\dfrac{f_2}{f_1}\right)^x\right], & F = G \end{cases} \tag{28}$$

The functions $w(k)$ are nonsingular for $k < k_0$. The asymptotic series found by the Laplace method is of the form[5]

$$\int_{-\infty}^{\infty} dk\, F(k) \underset{L \to \infty}{\cong} \sum_{\nu=0} d_\nu L^{-1/2-\nu} \tag{29}$$

DENSITY (MAGNETIZATION) AT $x = L/2$

For the density (magnetization) profile, the expansion (29) is truncated at the first term, whereas for the correlation function we keep in (29) the first two terms. As mentioned before, the integrands have their global maxima at $k = 0$. The first two coefficients d_ν are[5]

$$d_0 = h_2 w(0) \tag{30a}$$

and

$$d_1 = h_2^3 w''(0)/4 + 15/8\, h_2^7 w(0)/4!\, h''(0) \tag{30b}$$

where $h_2 = [2\pi/h''(0)]^{1/2}$ and the derivatives of odd order of h and w vanish at $k = 0$.

In the case $F = Z$ we get

$$\int_0^{\pi/2} dk\, Z(k) \underset{L \to \infty}{\cong} \int_0^{k_0} dk\, Z(k)$$

$$\underset{L \to \infty}{=} (2\pi/L)^{1/2}\, e^K (1 + e^{-2K})^{L+1}/4 + O(L^{-3/2}) \tag{31}$$

Hence the magnetization at $x = L/2$ is as follows [see (14c)]

$$\langle \sigma_{L/2} \rangle_n = th^{L/2} K \frac{e^{-K}(2\pi L)^{1/2}}{1 + e^{-2K}} \tag{32}$$

The exact expression for the magnetization at $x = L/2$ calculated in the grand canonical ensemble with the same boundary condition is found, by a straightforward calculation, to be

$$\langle \sigma_{L/2} \rangle_n^{gc} = \frac{2 th^{L/2} K \cdot e^{-2K}}{(1 + e^{-2K})(1 - th^{L+1} K)} \tag{33}$$

Comparing results (32) and (33), we see that $\langle \sigma_{L/2} \rangle_n$ tends to zero for $L \to \infty$, but more slowly than $\langle \sigma_{L/2} \rangle_n^{gc}$.

CORRELATION FUNCTION

Let us consider now the correlation function. Keeping in (29) the first two terms we get

$$\langle \sigma_1 \sigma_{1+x} \rangle_c = 1 - \left[\frac{G_0}{R_0} + \left(G_1 - \frac{G_0 R_1}{R_0} \right) R_0^{-1} L^{-1} \right] + O(L^{-2}) \tag{34}$$

where G_0, G_1 and R_0, R_1 denote the first two coefficients d_0 and d_1 in the expansion (29) for the integrands G and R, respectively. The explicit forms of G_0, G_1, R_0, R_1 are found by straightforward calculations. Substituting them into (34) and making use of the fact that the system c is symmetric with respect to the change $x \to L - x$, we obtain the final form of $h(x)$:

$$h(x) = th^x K + th^{L-x} K - \frac{e^{2K}}{L} + \frac{th^x K(x + e^{2K}) + th^{L-x} K(L - x + e^{2K})}{L} \tag{35}$$

The first two terms of the right-hand side of (35) represent the correlation function $h(x)$ in the grand canonical ensemble.[6] The third term is exactly equal to the correction term in (2), because in the one-dimensional lattice gas for $n = 1/2$ we have

$$n\chi = \frac{1}{2} e^{2K} \frac{1 - th^L K}{1 + th^L K} \beta \xrightarrow[L \to \infty]{} \frac{1}{2} e^{2K} \beta \tag{36}$$

The last term in (35) is a correction which is also of order $O(L^{-1})$ as its preceding term, but unlike the latter, it depends on x.

3B. Case $T \leqslant T'$

Let us consider the case $T \leqslant T'$ ($\delta \geqslant 1$). Because of (22) the two integrals in (19) are now significant and must be taken into account. We shall confine ourselves, in the case of (14a), to $x = L/2$. Thus (15a) simplifies to

$$G(k) = \frac{e^{-4K}}{\cos^2 k - b} [f_1^{L/2}(k) - f_2^{L/2}(k)]^2 \tag{37}$$

Taking into account (22), we approximate the first integral in (19) by

$$\int_0^{L^{-\delta}} dk\, F(k) = F(0)\, L^{-\delta} \tag{38}$$

where $F = Z$, G or R. We obtain the following estimates

$$\int_0^{L^{-\delta}} dk\, Z(k) = L^{1-\delta} + O(L^{2(1-\delta)}) \tag{39a}$$

$$\int_0^{L^{-\delta}} dk\, G(k) = L^{2-3\delta} + o(L^{2-3\delta}) \tag{39b}$$

and

$$\int_0^{L^{-\delta}} dk\, R(k) = [2 + L^{2(1-\delta)} + o(L^{2(1-\delta)})]\, L^{-\delta} \tag{39c}$$

In the interval $(L^{-\delta}, \pi/2)$ we introduce the new integration variable φ defined in (17) and get

$$\int_{L^{-\delta}}^{\pi/2} dk\, Z(k) = b_L b \int_0^{\pi/2} d\varphi \frac{\sin[(L+1)\varphi]}{\cos\varphi (L^{-2\delta} + tg^2\varphi)^{1/2}} \tag{40a}$$

$$\int_{L^{-\delta}}^{\pi/2} dk\, G(k) = b_L L^{-2\delta} \int_0^{\pi/2} d\varphi \frac{1 - \cos(L\varphi)}{\cos\varphi \sin\varphi (L^{-2\delta} + tg^2\varphi)^{1/2}} \tag{40b}$$

and

$$\int_{L^{-\delta}}^{\pi/2} dk\, R(k) = b_L b \int_0^{\pi/2} d\varphi \frac{tg\varphi \cos(L\varphi)}{(L^{-2\delta} + tg^2\varphi)^{1/2}} \tag{40c}$$

where $b_L = 2b^{(L-1)/2}$.

MAGNETIZATION AT $x=L/2$

The following inequalities hold

$$b_L b \int_0^{\pi/2} d\varphi \sin[\varphi(L+1)] \leqslant \int_{L^{-\delta}}^{\pi/2} dk\, Z(k) \leqslant b_L b \int_0^{\pi/2} d\varphi \frac{\sin[\varphi(L+1)]}{\sin \varphi} \tag{41}$$

from which we get the estimates

$$b_L b(L+1)^{-1} \leqslant \int_{L^{-\delta}}^{\pi/2} dk\, Z(k) \leqslant b_L b \frac{\pi}{2} \tag{42}$$

From the above and from (39a), (21), and (14c), it follows that in the canonical ensemble (closed system) the magnetization at the point nearest to the center is of the form

$$\langle \sigma_{L/2} \rangle_n \underset{L\to\infty}{\cong} 1 - \frac{2}{\pi} L^{1-\delta} + o(L^{1-\delta}) \tag{43}$$

whereas in the corresponding open system we get from (33)

$$\langle \sigma_{L/2} \rangle_n^{\text{gc}} \underset{L\to\infty}{=} L^{-1} - O(L^{1-\delta}) \tag{44}$$

CORRELATION FUNCTION

The integrals (40b) and (40c) are found for $L \to \infty$ to be of the form

$$\int_0^{\pi/2} d\varphi\, \bar{R}(\varphi) \underset{L\to\infty}{\cong} -2L^{-\delta} + L^{1-2\delta} \int_0^{\pi/2L} dx \frac{\sin x}{x} + O(L^{2-3\delta}) \tag{45a}$$

and

$$\int_0^{\pi/2} d\varphi\, \bar{G}(\varphi) \underset{L\to\infty}{\cong} 2L^{1-2\delta} \int_0^{\pi/2L} dx \frac{\sin x}{x} + O(L^{2-3\delta}) \tag{45b}$$

Combining the above and (39) and substituting the resulting integrals into (14a) gives the final expression:

$$\langle \sigma_1 \sigma_{1+L/2} \rangle_c \underset{L\to\infty}{=} -1 + O(L^{2-3\delta}) \tag{46}$$

In the open system (grand canonical ensemble) the correlation function is[6]

$$h(x) = \frac{th^x K + th^{L-x} K}{1 + th^{L+1} K} \underset{L\to\infty}{\cong} 1 - O(L^{2-3\delta}) \tag{47}$$

4. SUMMARY

From the results obtained above it follows that in a closed system (canonical ensemble) of length L there are two temperature regions: above and below $T' = 2Jk_B \ln L^{-1}$ which may be regarded as a critical temperature. In the first region the correlation function, g, is of the form (35) which, using (36), reads

$$g(x) = g^{gc}(x) - n\chi k_B T N^{-1} + \frac{th^x K(x + e^{2K}) + th^{L-x} K(L - x + e^{2K})}{L} \tag{48}$$

For $x \to \infty$ this is exactly the same expression as predicted in Ref. 1.

The qualitative behavior of the density profile is also similar to that in the open system (grand canonical ensemble). This is in agreement with expectation.

Below T', where $T' \to 0$ as $L \to \infty$, the considered functions behave differently. The expression (48) for g is not valid. In the system n appears a localized interface of microscopic extent. Thus in one-dimensional lattice gas the canonical constraint and antisymmetric boundary conditions are sufficient to separate the phases below a critical temperature, appropriate to the system of extension of L. In addition the width of the interface does not depend on L.

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