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# SOLUTION TO THE ONE-DIMENSIONAL CLUSTER MODEL

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A one-dimensional lattice gas model is considered, in which interact only particles inside a cluster. Exact recursion relations for the partition function are obtained and solved in the thermodynamic limit. The cluster size distribution function is determined. Conditions for a thermodynamic size cluster to coexist with vapor are found.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

## Решение одномерной кластерной модели

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Рассмотрена одномерная модель решеточного газа, в которой взаимодействуют только частицы внутри одного кластера. Получены точные рекурсивные соотношения для статистической суммы, которые решены в термодинамическом пределе. Определена функция распределения размеров кластера. Найдены условия, при которых кластер термодинамического размера сосуществует с паром.

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Let $\mathcal{L}$ be a $1D$ lattice (ring) of $V$ sites each of which either is vacant or contains a particle. The total number of particles is equal to $N$. By a cluster $C_k$ we mean a set of $k$ particles on $\mathcal{L}$ which constitute a chain of nearest neighbour on $\mathcal{L}$. Let the energy of an arbitrary particle configuration be given by

$$\mathcal{H} = \sum_k \varepsilon(k)\, n(k), \tag{1}$$

where $\varepsilon(k)$ is the energy of a $C_k$, and $n(k)$ is the number of such clusters. This model belongs to the class of Polymer Models (see [1]), the one in which we fix only the total number of particles and not the numbers of clusters of each type. The examples of such models include, in particular, the nearest-neighbour interaction $1D$ lattice gas, and the $1D$

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version of a hole-induced frustration spin model, in which the spin variables can be summed out leading to an effective hole Hamiltonian of the form (1) (see [2]).

It is well known that lattice gas type models rapidly decaying pair interactions cannot have long-range order at non-zero temperatures; the models with the potential $\propto 1/x^2$ exhibit a first order transition in temperature (see [3], and [4], [5]), and for stronger interactions, for instance for the Coulomb potential [6], which is $\propto x$ in one dimension, classical particles condense, or crystallize, at all temperatures. The simple cluster model (1) considered in this paper seems to have to do with both the cases. In particular, for some cluster energies condensation arises even in one dimension.

The partition function of the system with the interaction (1), laid on the $1D$ lattice $\mathcal{L}$ with free boundary conditions, is given by

$$Z_f(V, N) = \sum_{\{n(k)\}}' C(V, N, \{n(k)\})\, \delta\left(N - \sum_{k=1}^{\infty} kn(k)\right) \exp(-\beta \mathcal{H}), \qquad (2)$$

where $C(V, N, \{n(k)\})$ is the number of particle configurations which form a given set $\{n(k)\}$ of the numbers of clusters:

$$C(V, N, \{n(k)\}) = \frac{(V-N+1)!}{\prod_{k=0}^{\infty} n(k)!}, \quad n(0) = V - N + 1 - \sum_{k=1}^{\infty} n(k). \qquad (3)$$

Let us mention that the partition function of the noninteracting Boltzmann gas of $N_B = V - N + 1$ particles with the discreet spectrum $\varepsilon_B(k) = \varepsilon(k)$, $k = 1,\ldots, \varepsilon_B(0) = 0$, differs from (2) only by the $\delta$-factor $\delta\left(N - \sum_{k=1}^{\infty} kn(k)\right)$ which can be considered as some artificial non-ideality of the Boltzmann gas.

Summing the contributions due to configurations in which the first site of the chain belongs to $C_k$, $k = 1,\ldots, N$, or is empty ($k = 0$), we obtain the following recurrence:

$$Z_f(V, N) = \sum_{k=0}^{N} v(k)\, Z_f(V - k - 1, N - k), \quad V > N \geq 0,$$
$$Z_f(V, V) = 1, \quad V \geq 0. \qquad (4)$$

where $v(k) = \exp(-\beta\varepsilon(k))$, $k = 1, 2,\ldots, N$, and we put, formally, $v(0) = 1$.

For $\mathcal{L}$ with periodic boundary conditions we have:

$$Z_p(V,N)=\sum_{k=0}^{N}(k+1)\,v(k)\,Z_f(V-k-2,N-k),\quad V\geq N+2. \tag{5}$$

Let $c(k)$ be the average number of clusters $C_k$, $c(k)=\langle n(k)\rangle$. It is not hard to prove that

$$c(k)=Vv(k)\frac{Z_f(V-k-2,N-k)}{Z_p(V,N)},\qquad k=1,\ldots,N. \tag{6}$$

Using the normalization condition $N=\sum_{k=1}^{N}kc(k)$, we get

$$\frac{\sum_{k=0}^{N}kv(k)\,Z_f(V-k-2,N-k)}{\sum_{k=0}^{N}(k+1)\,v(k)\,Z_f(V-k-2,N-k)}=\frac{N}{V}\equiv\rho. \tag{7}$$

Since Eq. (7) holds for any $(V,N)$, for the sequence $S(j)=Z_f(V-N-2+j,j),j=0,\ldots,N$, where $V$ and $N$ are fixed, from Eq. (7) we get the following recurrence:

$$S(j)=\sum_{k=1}^{j}\left((V-N)\frac{k}{j}-1\right)v(k)\,S(j-k),\qquad S(0)=1. \tag{8}$$

Thus, to compute $Z_p(V,N)$ and $c(k)$, $k=1,2,\ldots,N$, it will suffice to use the recurrence (8) only $N$ times, instead of applying Eq. (4) more than $N^2/2$ times.

Suppose that the limit $v=\lim_{k\to\infty}(v(k))^{1/k}$ exists. For any positive $r$, the quantities $c(k)$ are invariant with respect to the transformation

$$v(k)\to v'(k)=v(k)r^k,\qquad Z_f(V,N)\to Z'_f(V,N)=Z_f(V,N)r^N. \tag{9}$$

Thus, choosing $r=v^{-1}$ we reduce the model to the case $v=1$.

Let us start from the case in which only a number of the first terms contribute to the sums in Eq. (7). Then, for sufficiently large $(V,N)$, we have

$$\frac{Z_f(V-k-2,N-k)}{Z_f(V-2,N)}\simeq\exp(k\beta(\mu-p))\equiv\alpha^k, \tag{10}$$

where $p$ and $\mu$ are the pressure and chemical potential in the limit $V \to \infty$, $N/V = \rho$, respectively. If $\alpha < 1/v = 1$, then the contributions to the sums in Eq. (7) decrease exponentially, and in the thermodynamic limit the density $\rho$ as a function of the parameter $\alpha$ is given by

$$\rho = \frac{\sum_{k=0}^{\infty} k v(k) \alpha^k}{\sum_{k=0}^{\infty} (k+1) v(k) \alpha^k}, \tag{11}$$

and the average numbers of clusters decrease exponentially,

$$c(j) = \frac{V v(j) \alpha^j}{\sum_{k=0}^{\infty} (k+1) v(k) \alpha^k}. \tag{12}$$

Denoting $N_B = V - N$, we can rewrite (12) in the form:

$$\frac{c(j)}{N_B} = \frac{v(j) \alpha^j}{\sum_{k=0}^{\infty} v(k) \alpha^k}, \tag{13}$$

which gives exactly the occupation numbers of the noninteracting Boltzmann gas with the chemical potential $\mu_B = \ln \alpha$.

The function $\rho(\alpha)$ (11) is a monotone increasing function of $\alpha$, and $\rho(0) = 0$. If the series $\sum_{k=0}^{\infty} k v(k)$ diverges, then $\rho(1) = 1$ and for any $\rho \in (0, 1)$ Eq. (11) is the equation of state for the cluster model. If, conversely, this series converges, then $\rho_c \equiv \rho(1) < 1$, and at $\rho > \rho_c$ Eq. (11) has no solution. Thus we have obtained the condition under which the delta-factor in (2) makes this model essentially different from the noninteracting Boltzmann gas.

Numerical calculations by the recurrence (8) in the case $\rho_c < 1$ demonstrate that $S(j)$ has a maximum at $j = N_g \propto \kappa(\rho_c)(V - N)$, which gets sharper with the increase of $(V - N)$ (the coefficient $\kappa(\rho_c)$ is independent of $(V, N)$.

In order to obtain the asymptotical solution to the model with $\rho > \rho_c$, we approximate $S(j)$ in the vicinity of its maximum by the following expression:

$$S(N_g + l) = S(N_g) \exp\left(-\frac{l^2}{2D}\right), \qquad l << N_g. \tag{14}$$

The quantity

$$\Delta(l) = \sum_{k=0}^{N_g} \left((V-N)\frac{k}{N_g + l} - 1\right) v(k) \exp\left(-\frac{(l-k)^2}{2D}\right) \tag{15}$$

is the difference between the l.h.s. and r.h.s. of Eq. (8) at $j = N_g + l$, neglecting the contributions due to $k$ close to $N_g$. Choosing the optimal values of $N_g$ and $D$ from the conditions $\Delta(0) = 0$ and $\Delta'(0) = 0$, we are led to the equations:

$$N_g = (V-N)\frac{\sigma_1}{\sigma_0}; \qquad D = (V-N)\frac{\sigma_2\sigma_0 - (\sigma_1)^2}{(\sigma_0)^2},$$

$$\sigma_\nu \equiv \sigma_\nu(N_g, D) \equiv \sum_{k=0}^{N_g} k^\nu v(k) \exp\left(-\frac{k^2}{2D}\right). \tag{16}$$

If $\rho_c < \rho \le 1$, then, using Eq. (11) at $\alpha = 1$ to find the limit of the quantity $\sigma_1/\sigma_0$, we get the asymptotics of the solution to Eq. (16):

$$\rho_g \equiv \lim_{V\to\infty} \frac{N_g}{V} = \rho_c \frac{1-\rho}{1-\rho_c}, \qquad \lim_{V\to\infty} \frac{\sqrt{D}}{V} = 0. \tag{17}$$

The function (14) is the asymptotically exact solution to Eq. (8) for $|l| < L(V)$, where $L(V)$ is a function of order of magnitude $o(V)$. Now, using (14), we find the asymptotically exact solution to Eq. (8):

$$S(\rho' V) \sim \sqrt{2\pi D} S(N_g)(V-N)\frac{v(\rho' V - N_g)}{\sum_{k=0}^{\infty} v(k)}, \qquad \rho' \in (\rho_c, \rho] \tag{18}$$

(we assume, for simplicity, that $v(k)$ is sufficiently smooth at large $k$).

Let $\rho_V(j)$ be the partial densities. According to (6),

$$\rho_V(j) \equiv \frac{jc(j)}{V} = \frac{jv(j)\,S(N-j)}{N \sum_{k=0} (k+1)\,v(k)\,S(N-k)}. \tag{19}$$

Substituting (14), (17), and (18) into (19), we get the following asymptotics for small clusters and macro-clusters, respectively:

$$\rho_V(j) \sim \frac{N_g}{V} \frac{jv(j)}{\sum_{k=0}^{\infty} kv(k)}, \qquad j << N - N_g, \tag{20}$$

$$\rho_V(N - N_g + l) \sim \frac{N - N_g}{V} \frac{1}{\sqrt{2\pi D}} \exp\left(-\frac{l^2}{2D}\right), \quad l << N - N_g. \tag{21}$$

Clearly, the total density for small clusters is equal to $\rho_g$ (17), that is $N_g$ and $N - N_g$ are the average numbers of particles in the vapor and in the condensate, respectively. The quantity $\sqrt{D}$ describes the fluctuations of these quantities. Taking the sum of $c(k)$ over macro-clusters $k \approx N - N_g$ we see that the condensate consists of exactly one macro-cluster. The density of the vapor in its volume $V - N + N_g$ equals $\rho_c$, that is for $\rho \geq \rho_c$ the vapor is always a critical gas and all «extra»-particles are condenced into the macro-cluster.

As an example, let us consider the model $\varepsilon(k) = \ln(k + 1)$. At high temperatures $0 < \beta < \beta_c = 2$ the system is gaseous at any density. At low temperatures $\beta > \beta_c$ the system is gaseous if $\rho < \rho_c(\beta)$, where

$$\rho_c(\beta) = 1 - \frac{\zeta(\beta)}{\zeta(\beta - 1)}, \qquad \zeta(\beta) = \sum_{k=1}^{\infty} k^{-\beta}, \tag{22}$$

and at $\rho > \rho_c$ an equilibrium coexistence of critical vapor and condensate occurs.

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