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One-dimensional gas of rods with next-neighbour interaction

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Abstract. We consider the one-dimensional gas of rods with finite range interaction. Using the transfer matrix method we obtain an integral equation that describes the gas of rods. The integral equation has a non-zero solution, if pressure and chemical potential satisfy a condition that is only the equation of state. In particular, we discuss the case of continuum piecewise linear next-neighbour interaction potential for rods.

1. Introduction

In 1941 Takahashi [1] derived the equation of state (connection between chemical potential μ or density ρ and pressure P) for the one-dimensional gas of rods. The range of interaction in his model did not exceed the size of the rod. However, there are a few physical problems, e.g. adsorption on a metal surface [2], where longer range interactions are very important. Therefore, even discussion of one-dimensional physics may be interesting. In our paper we consider a model with an interaction range not exceeding twice the size of the rod.

In the first section we obtain a linear integral equation depending on the parameters P and μ. For a fixed value of μ we look for the maximum pressure P for which the integral equation has a non-trivial solution. Thus, we obtain the equation of state. In this paper we start from a discrete model. This allows us to use the transfer matrix method. The partition function of the discrete model in the thermodynamic limit is expressed by the largest eigenvalue of the transfer matrix. After applying the continuum limit the partially reduced eigenequation for the problem becomes the integral equation. This method was used in [3–5]. Our approach seems to be more elementary than calculation by means of the Laplace method [1, 6]. At the end of the section we give the general results for an arbitrary finite range of the interaction.

In the second section we solve the integral equation for the step-like force. Even in this simplest case the equation of state is very complicated.

2. The integral equation

Suppose that we have a linear lattice with L sites on which we put a number of rods. Each rod covers d lattice sites. We call $U(j)$ the two-rod interaction energy, where j is the number of sites between the rods. The energy equals zero for $2d \leqslant j$.

In order to define a transfer matrix we denote the sites by pairs of numbers. Hereafter we assume a periodic boundary condition. Our construction is the following.

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Let us fix a configuration of the rods, which consists of at least one rod. We say that the rod is a k-rod if there are k empty sites between the rod and its left neighbour. When $k > d$ we put $k = d$.

Further, we construct a sequence of pairs (k, j) in two steps. First, we assign all left ends of the rods, i.e. we fix the label $(k, 1)$ to a site, if the site is covered by the left end of a k-rod. Next, we assign the remaining sites by fixing the label $(k, j+1)$ to a site, if it is on the right side of the site assigned by a pair (k, j), unless $j = 3d$. In this case we choose the label $(k, 3d)$ for the site.

Obviously not all the sequences are images of rod configurations because rods must not cover themselves. Thus, we obtain one-to-one relation between the configurations consisting of at least one rod and their images. In the case of an empty lattice the sequence is not properly defined. Then we choose $j = 3d$ and arbitrary k. This changes the ordinary form of the equation (5).

We can write the partition function by means of a $3d(d-1) \times 3d(d-1)$ matrix with non-zero entries

$$M^{kk}(3d, 3d) = M^{kk}(j, j+1) = 1 \qquad 1 \leqslant j < 3d \tag{1}$$

$$M^{k\,j-d}(j, 1) = zW(j-d)W(j+k) \qquad d \leqslant j < 2d \tag{2}$$

$$M^{kd}(j, 1) = zW(j-d) \qquad 2d \leqslant j \leqslant 3d \tag{3}$$

where

$$W(j) = \exp(-\beta U(j)) \tag{4}$$

and $z = \exp(\beta\mu)$ with $\beta = 1/kT$. Then the partition function of our model is

$$Z_L = \sum_{N=0}^{\infty} z^N \sum_{\text{config N rods}} \exp(-\beta \times \text{energy of config})$$

$$= \operatorname{Tr} M^L - d. \tag{5}$$

For the large L we have

$$Z_L \sim \lambda_{\max}^L \tag{6}$$

where $\lambda_{\max}$ is the largest eigenvalue of M and satisfies the eigenequation

$$\sum_{l=0}^{d} \sum_{i=1}^{3d} M^{kl}(j, i) V^l(i) = \lambda V^k(j) \qquad 0 \leqslant k \leqslant d \qquad 1 \leqslant j \leqslant 3d. \tag{7}$$

Eliminating $V^k(j)$ from (7) for $0 \leqslant k \leqslant d$ and $1 < j \leqslant 3d$, as in [4, 5], we obtain the following equations:

$$(\lambda - 1)\lambda^{3d-1} V^k(1)$$

$$= z(1 + (\lambda - 1) \sum_{j=d}^{2d-1} W(j)\lambda^{2d-j-1}) V^d(1)$$

$$+ z(\lambda - 1) \sum_{j=0}^{d-1} W(j)W(j+k+d)\lambda^{2d-j-1} V^j(1). \tag{8}$$

It is evident from (5) that the largest eigenvalue of matrix M is larger than 1. For $\lambda > 1$, (8) are equivalent to more compact equations

$$\lambda^d V^k(1) = z \sum_{j=0}^{\infty} W(j)W(j+k+d)\lambda^{-j} V^j(1) \qquad 0 \leqslant k. \tag{9}$$

To see this, we remind the reader of our assumption ($U(j) = 0$ and $W(j) = 1$ for $j \geqslant 2d$) and note that for $k \geqslant d$

$$V^k(1) = V^d(1).$$

The natural unit of length for the model is the length of the rod.Therefore, we change λ to $\lambda^{1/d}$ and z to z/d before taking of the limit $d = \infty$ (continuum limit). In this limit (8) are converted into the integral equation

$$\lambda^3 \ln \lambda \, V_x = z(1 + \ln \lambda \int_1^2 W(y)\lambda^{2-y} \, dy)V_1 + z \ln \lambda \int_0^1 W(y)W(1+x+y)\lambda^{2-y} V_y \, dy \qquad 0 \leqslant x \leqslant 1 \tag{10}$$

where V_x is substituted for discrete $V^k(1)$, and (9) becomes the following:

$$\exp[\beta P]V_x = \exp[\beta\mu] \int_0^{\infty} \exp\{-\beta[U(y) + U(x+y+1) + Py]\}V_y \, dy \tag{11}$$

with $U(x)$ defined by (4) and $\lambda = \exp(\beta P)$ (fulfilled in the thermodynamic limit).

The generalization of (11) for arbitrary finite range of the interaction is

$$\exp[\beta P]V_{x_0,x_1,\ldots,x_{N-1}} = \exp[\beta\mu] \int_0^{\infty} \exp\{-\beta[U(x_N) + U(x_N + x_{N-1} + 1) + \cdots + U(x_N + \cdots + x_0 + N) + Px_N]\}V_{x_1,x_2,\ldots,x_N} \, dx_N. \tag{12}$$

If $U(x) = 0$ for $x > 1$, then the general equation reduces to the well known formula [1, 6]

$$\exp[\beta P] = \exp[\beta\mu] \int_0^{\infty} \exp[-\beta(U(x) + Px)] \, dx. \tag{13}$$

3. The simple example

Equation (10) is difficult to solve even for simple potentials. However, it is possible to solve it for the step-like potential and the continuum piecewise potential. The second potential appears to be better for physical applications. We will restrict ourselves only to this case.

We define $W(x)$ with the help of (4) and the potential

$$\begin{aligned} U(x) &= (2-x)F_2 && 1 \leqslant x \leqslant 2 \\ U(x) &= (1-x)F_1 + F_2 && 0 \leqslant x \leqslant 1 \\ U(x) &= 0 && 2 \leqslant x. \end{aligned} \tag{14}$$

The calculations with different values of forces F_1 and F_2 are the same as in the case when they are equal to each other.

The explicit form of (10) is

$$\begin{aligned} \beta P \exp[3\beta P] V_x = {} & \exp[\beta\mu] \left(\frac{F_2 - P\exp[\beta(P-F_2)]}{F_2 - P} \right) V_1 \\ & + \beta P \exp(\beta(\mu + 2P - F_1 - F_2)) \\ & \times \left(\exp[-\beta F_2(1-x)] \int_0^{1-x} \exp[-\beta(P - F_1 - F_2)y] V_y \, dy \right. \\ & \left. + \int_{1-x}^{1} \exp[-\beta(P-F_1)y] V_y \, dy \right). \end{aligned} \tag{15}$$

It is not difficult to see that a solution V_x of the integral equation (15) satisfies the linear differential equation

$$\begin{aligned} & \left\{ \left[\left(V_x' e^{-\beta F_2 x} \right)' \exp(-\beta(P - F_1 - F_2)x) \right]' \exp[\beta F_2 x] \right\}' \exp(\beta(P - F_1 - F_2)x) \\ & \qquad = \beta^2 F_2^2 \exp[-\beta(3P - 2\mu + F_1 + 2F_2)] V_x \end{aligned} \tag{16}$$

where the primes denote derivatives with respect to x. The general solution of the differential equation (16) is

$$V_x = C_1 \exp[\beta\alpha_1 x] + C_2 \exp[\beta\alpha_2 x] + C_3 \exp[\beta\alpha_3 x] + C_4 \exp[\beta\alpha_4 x] \tag{17}$$

where $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ are the zeros of the characteristic polynomial in α

$$\begin{aligned} & \alpha(\alpha - F_2)(\alpha + F_1 - P)(\alpha + F_1 + F_2 - P) \\ & \qquad - (F_2/\beta)^2 \exp[-\beta(3P - 2\mu + F_1 + 2F_2)]. \end{aligned} \tag{18}$$

When the characteristic polynomial (18) has multiple zeros, the general solution of the differential equation (16) differs from (17). We can consider this case as the limit of the case without multiple zeros.

We can number the zeros of the characteristic polynomial (18) such that

$$\begin{aligned}
&\alpha_1 + \alpha_2 = \alpha_3 + \alpha_4 = P - F_1 \\
&\alpha_1\alpha_2 + \alpha_3\alpha_4 = F_2(P - F_1 - F_2) \\
&\alpha_1\alpha_2\alpha_3\alpha_4 + (F_2/\beta)^2 \exp[-\beta(3P - 2\mu + F_1 + 2F_2)] = 0.
\end{aligned} \tag{19}$$

Substituting the solution (17) into the integral equation (15) and comparing coefficients of $\exp[\beta\alpha_1 x], \exp[\beta\alpha_2 x], \exp[\beta\alpha_3 x], \exp[\beta\alpha_4 x], \exp[\beta F_2 x], 1$, we obtain a set of six linear equations for C_1, C_2, C_3, C_4. This set of equations has a non-trivial solution when

$$\begin{aligned}
&\left(\frac{\eta_1 \exp[\beta\alpha_1/2]}{\alpha_1 - F_2} + \frac{\eta_2 \exp[\beta\alpha_2/2]}{\alpha_2 - F_2}\right) \\
&\qquad \times [(P - F_2 \exp[-\beta(P - F_2)])(\eta_3 \exp[\beta\alpha_3/2] + \eta_4 \exp[\beta\alpha_4/2]) \\
&\qquad -(P - F_2)\left(\eta_3 \frac{\exp[-\beta\alpha_3/2]}{\beta\alpha_3} + \eta_4 \frac{\exp[-\beta\alpha_4/2]}{\beta\alpha_4}\right)] \\
&= \left(\frac{\eta_3 \exp[\beta\alpha_3/2]}{\alpha_3 - F_2} + \frac{\eta_4 \mathrm{e}[\beta\alpha_4/2]}{\alpha_4 - F_2}\right) \\
&\qquad \times [(P - F_2 \exp[-\beta(P - F_2)])(\eta_1 \exp[\beta\alpha_1/2] + \eta_2 \exp[\beta\alpha_2/2]) \\
&\qquad -(P - F_2)\left(\eta_1 \frac{\exp[-\beta\alpha_1/2]}{\beta\alpha_1} + \eta_2 \frac{\exp[-\beta\alpha_2/2]}{\beta\alpha_2}\right)]
\end{aligned} \tag{20}$$

where

$$\eta_i = [\alpha_i(\alpha_i - F_2)]^{1/2} \qquad i = 1, 2, 3, 4 \tag{21}$$

and

$$\eta_1\eta_2 = \eta_3\eta_4 = -(F_2/\beta)\exp[\beta(3P - 2\mu + F_1 + 2F_2)/2]. \tag{22}$$

Equation (20) is the equation of state for our model.

For our simple potential (14) we can easily solve the discrete prototype of (10) i.e. (8). However, in the limit $d = \infty$ we obtain the same result as in the continuum case. Equation (20) can be examined numerically. For fixed pressure P and inverse temperature β we can find the chemical potential μ. The technical problem can be the complex zeros of the characteristic polynomial or the complex roots η_i. We can avoid the problem by writing our equation of state using an infinite series. The terms of the series are polynomials in the coefficients of the characteristic polynomials.

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