

## Statistical mechanics of a one-dimensional system with exponentially repulsive interactions

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We study the statistical mechanics of a one-dimensional classical system with the purely repulsive interaction  $v(x) = C \exp(-\gamma|x|)$ . Emphasis is laid upon an exact treatment of the long-range character of the interaction. We give explicit analytical expressions for the equation of state as well as for the correlation function. The almost crystalline nature of the system shows up in the low-temperature region.

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### I. INTRODUCTION

In any real fluid the interparticle interaction consists of a short-range repulsive part and a long-range attractive part such as, for example, the Lennard-Jones 6-12 potential. Usually one first considers the system with purely repulsive interaction as a reference system<sup>1</sup> and then includes the attractive part of the potential in some perturbative scheme.

In this work we will treat a one-dimensional classical system with a purely repulsive interaction of the exponential type

$$v(x) = Ce^{-\gamma|x|}, \quad (1.1)$$

where  $C$  and  $\gamma$  are positive parameters and  $x$  denotes the interparticle distance. (The inclusion of an attractive interaction will be discussed in a subsequent paper.) The particular form of this potential has been dictated by mathematical simplicity.

The exponential interaction (1.1) has been studied in the literature before: the dynamics of a linear chain with exponential forces between next neighbors has been constructed by Toda,<sup>2</sup> especially because of the existence of soliton solutions. Toda also gives the thermodynamics of this system, which can be obtained as a special case of our results.

A preliminary investigation of the thermodynamics of a system with the exponential interaction (1.1) is contained in Feynman's book on statistical mechanics.<sup>3</sup> However, Feynman's treatment of the problem is technically incomplete and the equations given by him do not lead to an explicit solution.

The work which is most closely connected to ours is a series of papers by Baxter.<sup>4,5</sup> Baxter derives the basic equations for the thermodynamics and the correlation function using a functional technique. However, no solution is constructed. In Sec. II we rederive these equations using the elementary mathematics of the harmonic oscillator to avoid the rather complicated functional

methods. Thus the treatment becomes very transparent and helps to formulate the perturbative solutions in the high- and in the low-temperature region (Secs. III-V).

In the high-temperature region (Sec. IV) we find that the system behaves like an ideal gas in the dilute regime and like a plasma in the dense regime. In the dilute regime we essentially recover the virial expansion. In the high-density regime the particles are subject only to the short-range part of the potential (1.1), which is proportional to  $|x|$ . This is just the one-dimensional Coulombic interaction. We thus recover essentially the high-temperature equation of state of a one-dimensional electron gas immersed in a positive uniform background.<sup>5</sup> The correlation function in the high-temperature region is also given at the end of Sec. IV.

The low-temperature region is discussed in Sec. V. We give analytical expressions for the equation of state as well as for the correlation function. These equations show that—for low temperatures—the system transforms almost into the crystalline state. As usual in a one-dimensional system a sharp phase transition occurs only in the zero-temperature limit.

The almost crystalline nature for finite but very small temperatures may be seen somewhat indirectly from the equation of state by the appearance of a Grüneisen correction to the zero-point pressure. For high densities the Grüneisen correction is due to plasma oscillations. For low densities the system essentially behaves like a lattice with next-neighbor interaction only.

The correlation function of course gives more direct information about the structure. We show that the correlation function is given by a sum of exponentials. These exponentials oscillate in space and have a damping proportional to the isothermal compressibility. The wavelength of the oscillations is equal to a multiple of the "lattice" constant  $\rho^{-1}$  ( $\rho$  being the particle density). This sum may be rewritten in terms of almost Gaussian functions, which are located at the "lat-

tice" sites. For zero temperature the width of the Gaussian functions vanishes and the crystal structure appears.

Finally the potential (1.1) contains the hard-core interaction as a particular limit of the parameters  $C$  and  $\gamma$ : To this end we set  $C = C_0 e^{\gamma b}$  ( $b > 0$ ) and consider the limit  $\gamma \rightarrow \infty$ ; that is, we pin the interaction at the hard-core radius  $x = b$  and then use the limit of an infinitely fast decrease of the potential over a width  $1/\gamma$ . In this limit we recover very easily the known results of a one-dimensional hard-core system, the equation of state<sup>6</sup> as well as the correlation function<sup>7,8</sup> (Sec. VI).

## II. BASIC EQUATIONS

### A. Partition function

In this section we will derive an expression which is equivalent to the partition function of the classical system with the long-range interaction (1.1).

If the range of the potential is restricted to the next neighbor, the partition function as well as the correlation function are easily calculated by means of a Laplace transform.<sup>6-8</sup> Here our main interest lies in an exact treatment of the long-range character of the interaction potential. To this end we first show that the grand partition function  $Z_G$  of this system may be related to the exponential of a Hamiltonian operator  $\mathcal{H}$  (this method is usually called transfer-matrix method in the literature).

We first recall, that for a one-dimensional system confined to a segment of length  $L$  and interacting through the two-body potential (1.1) the grand partition function is given by

$$Z_G = 1 + \sum_{N=1}^{\infty} z^N \int_0^L dx_N \int_0^{x_N} dx_{N-1} \dots \times \int_0^{x_2} dx_1 \exp\left(-\beta C \sum_{i>j=1}^N e^{-\gamma|x_i-x_j|}\right), \quad (2.1)$$

where  $z$  is the activity

$$z = (2m\pi/\beta h^2)^{1/2} e^{\beta\mu}$$

of a system of particles of mass  $m$  and at a chemical potential  $\mu$ . [ $\beta$  denotes the inverse temperature  $T$ ,  $\beta = (k_B T)^{-1}$ ;  $k_B$ , Boltzmann's constant;  $h$ , Planck's constant.]

Consider now the following Hamiltonian

$$\mathcal{H} = \gamma c^\dagger c - z e^{i\lambda c^\dagger} e^{i\lambda c}.$$

Here  $c$ ,  $c^\dagger$  are two Bose operators, defined by the commutators  $[c, c^\dagger] = 1$ ,  $[c, c] = [c^\dagger, c^\dagger] = 0$ , and  $\lambda$  is

defined by

$$\lambda = (\beta C)^{1/2}.$$

Note that  $\mathcal{H}$  is a non-Hermitian operator.

Splitting  $\mathcal{H}$  into a free part  $\mathcal{H}_0$  and an interaction part  $\mathcal{H}_I$ ,

$$\mathcal{H}_0 = \gamma c^\dagger c, \quad (2.2a)$$

$$\mathcal{H}_I = -z e^{i\lambda c^\dagger} e^{i\lambda c}, \quad (2.2b)$$

one may introduce an interaction picture through

$$O(x) = e^{\mathcal{H}_0 x} O e^{-\mathcal{H}_0 x}$$

for any operator  $O$ . The "time" evolution of the Bose operators is thus

$$c(x) = c e^{-\gamma x}, \quad c^\dagger(x) = c^\dagger e^{+\gamma x}.$$

[Note that  $c^\dagger(x)$  is *not* the Hermitian adjoint of  $c(x)$  unless for  $x = 0$ .] The commutator

$$[c(x), c^\dagger(x')] = e^{-\gamma(x-x')}$$

is essentially the interaction potential (1.1).

We now expand the operator  $\exp(-L\mathcal{H})$  in the interaction picture representation

$$e^{-L\mathcal{H}} = e^{-L\mathcal{H}_0} \left( 1 + \sum_{N=1}^{\infty} (-1)^N \int_0^L dx_N \int_0^{x_N} dx_{N-1} \dots \times \int_0^{x_2} dx_1 \mathcal{H}_I(x_N) \mathcal{H}_I(x_{N-1}) \dots \mathcal{H}_I(x_1) \right), \quad (2.3)$$

where

$$\mathcal{H}_I(x) = -z e^{i\lambda c^\dagger(x)} e^{i\lambda c(x)}.$$

Formula (2.3) is already similar in structure to the basic expression (2.1). Using the identity

$$e^{i\lambda c(x_N)} e^{i\lambda c^\dagger(x_{N-1})} e^{i\lambda c(x_{N-1})} \dots e^{i\lambda c^\dagger(x_2)} e^{i\lambda c(x_2)} e^{i\lambda c^\dagger(x_1)} \\ = e^{i\lambda c^\dagger(x_{N-1})} e^{i\lambda c^\dagger(x_{N-2})} \dots e^{i\lambda c^\dagger(x_1)} e^{i\lambda c(x_N)} \dots e^{i\lambda c(x_2)}$$

$$\otimes \exp\left(-\lambda^2 \sum_{i>j=1}^N [c(x_i), c^\dagger(x_j)]\right) \text{ for } N=2, 3, \dots$$

one may convert the time order in (2.3) into a normal order in  $(c^\dagger, c)$ . If one finally takes the expectation value in the unperturbed vacuum state  $|\text{vac}\rangle$  ( $c|\text{vac}\rangle = 0$ ,  $\langle\text{vac}|c\rangle = 1$ ) one arrives at the identity

$$\langle\text{vac}|e^{-L\mathcal{H}}|\text{vac}\rangle = Z_G, \quad (2.4)$$

which is the basic connection between the grand partition function  $Z_G$  and the Hamiltonian  $\mathcal{H}$ . A formula like (2.4) may also be given for higher dimensions, the definition of  $\mathcal{H}$  of course being

modified. This is shown in the Appendix A.

We assume that there exists a complete set of (discrete) eigenstates of  $\mathcal{H}$ . This assumption may be difficult to justify rigorously, but the results of the calculations presented in this work seem to substantiate this hypothesis. We may then expand the vacuum  $|\text{vac}\rangle$  in this basis. In the thermodynamic limit  $L \rightarrow \infty$  we get the proportionality

$$Z_G \propto e^{-L\epsilon_0}, \quad (2.5)$$

where  $\epsilon_0$  is the ground-state eigenvalue. (As  $\mathcal{H}$  is a non-Hermitian operator, in general, complex eigenvalues will occur, which one may order with increasing real part.)

Recalling the identities  $Z_G = \exp(-\beta\Omega)$  and  $\Omega = -pL$  where  $\Omega(T, L, \mu)$  is the thermodynamic potential and  $p$  the pressure we get from (2.5)

$$\beta p = -\epsilon_0. \quad (2.6a)$$

The particle density  $\rho$  is then obtained from

$$\rho = -z \frac{\partial}{\partial z} \epsilon_0, \quad (2.6b)$$

where use has been made of the thermodynamic relation  $\rho = \beta z \partial p / \partial z$ . The elimination of  $z$  between (2.6a) and (2.6b) yields the equation of state.

From Eq. (2.6a) we see that, for thermodynamic reasons, the ground-state eigenvalue has to be real and negative.

### B. Correlation function

The two-particle correlation function  $g(x_1, x_2)$  is defined by

$$g(x_1, x_2) = \frac{1}{\rho^2} \frac{1}{Z_G} \sum_{N=2}^{\infty} z^N \frac{1}{(N-2)!} \int_0^L dx_3 \int_0^L dx_4 \dots \\ \times \int_0^L dx_N \exp\left(-\beta \sum_{i>j=1}^N v(x_i - x_j)\right).$$

Applying the same procedure that yields the relation (2.4) one may show that  $g(x_1, x_2)$  can be expressed as

$$g(x_1, x_2) = \frac{1}{\rho^2} \frac{1}{\langle \text{vac} | e^{-L\mathcal{H}} | \text{vac} \rangle} \\ \times \langle \text{vac} | e^{-(L-x_2)\mathcal{H}} \mathcal{H} e^{-(x_2-x_1)\mathcal{H}} \mathcal{H} e^{-x_1\mathcal{H}} | \text{vac} \rangle,$$

where  $x_2 > x_1$  is assumed.

Expanding again the vacuum state in terms of a complete set of eigenstates of  $\mathcal{H}$  one gets in the limit  $L \rightarrow \infty$  (thermodynamic limit) and  $x_1 \rightarrow \infty$ ,  $L - x_2 \rightarrow \infty$  (exclusion of boundary effects) the following formula:

$$g(x_1, x_2) = \frac{1}{\rho^2} \frac{1}{\langle g_0 | f_0 \rangle} \langle g_0 | \mathcal{H} e^{-(x_2-x_1)\mathcal{H}} \mathcal{H} | f_0 \rangle \\ \times e^{(x_2-x_1)\epsilon_0}. \quad (2.7)$$

$|f_0\rangle$  and  $|g_0\rangle$  denote the "right" and "left" eigenstates with ground-state eigenvalue  $\epsilon_0$ . The distinction between left and right eigenstates is necessary as  $\mathcal{H}$  is a non-Hermitian operator<sup>9</sup>:

We call a "right" eigenstate  $|f_n\rangle$  an eigenstate with the property

$$\mathcal{H} |f_n\rangle = \epsilon_n |f_n\rangle \quad (2.8a)$$

whereas for a "left" eigenstate we have

$$\langle g_n | \mathcal{H} = \epsilon_n \langle g_n |. \quad (2.8b)$$

Inserting a complete set of states into the matrix element of (2.7) we get

$$g(r) = \frac{1}{\rho^2} \sum_n \frac{\langle g_0 | \mathcal{H} |f_n\rangle \langle g_n | \mathcal{H} |f_0\rangle}{\langle g_0 | f_0 \rangle \langle g_n | f_n \rangle} e^{-(\epsilon_n - \epsilon_0)r} \quad (2.9)$$

where  $r = x_2 - x_1$ . This formula becomes particularly useful for large distances  $r$  since one may then truncate the series after the first excited states.

The first term in (2.9) is equal to unity as one may see from the identity

$$\rho = -z \frac{\partial}{\partial z} \epsilon_0 = -\frac{\langle g_0 | \mathcal{H} |f_0\rangle}{\langle g_0 | f_0 \rangle}, \quad (2.10)$$

which follows from (2.8a).

### III. FORMULATION OF THE EIGENVALUE PROBLEM

In the preceding section we established the connection between the grand partition function  $Z_G$  and the Hamiltonian operator  $\mathcal{H}$ , which was expressed by two Bose operators  $c$  and  $c^\dagger$ . In the usual harmonic-oscillator representation the operators  $c$  and  $c^\dagger$  are represented as

$$c = \frac{1}{\sqrt{2}} \left( y + \frac{d}{dy} \right), \quad c^\dagger = \frac{1}{\sqrt{2}} \left( y - \frac{d}{dy} \right),$$

and the vacuum state is

$$|\text{vac}\rangle = \frac{1}{\pi^{1/4}} e^{-y^2/2}.$$

The eigenvalue problem (2.8a) is then written as

$$\left[ \frac{1}{2} \gamma \left( -\frac{d^2}{dy^2} + y^2 - 1 \right) - \zeta \exp[i(2\beta C)^{1/2} y] \right] f(y) = \epsilon f(y), \quad (3.1)$$

where  $\zeta$  is a rescaled activity

$$\zeta = z e^{\beta C/2}.$$

Equation (3.1) is the eigenvalue equation for a har-

monic oscillator with an exponential perturbation. As the perturbation is bounded we impose on  $f(y)$  the usual boundary conditions as for the harmonic oscillator:  $f(y)$  must go to zero sufficiently fast as  $y \rightarrow \pm\infty$ .

The equivalence between the solution of the eigenvalue problem (3.1) and the evaluation of the grand partition function for a classical system with the interaction (1.1) has already been pointed out by Baxter.<sup>4</sup> Baxter used a functional derivative technique, which is particularly well suited for a one-dimensional system. However, his method may not be generalized to higher dimensions, whereas our approach to the problem may also be used in higher dimensions as is discussed in Appendix A.

The harmonic-oscillator representation (3.1) of the eigenvalue problem is most easily solved by perturbative methods in the high-temperature region ( $\beta \rightarrow 0$ ), because then the coupling constant  $\xi$  of the perturbation  $-\xi \exp[i(2\beta C)^{1/2}y]$  is not too large and the exponential oscillates slowly (Sec. IV).

In the physically more interesting low-temperature region ( $\beta \rightarrow \infty$ ) the situation is reversed (large coupling constant and rapid oscillations) and perturbative methods fail to give satisfactory results. In this temperature region the eigenvalue problem may be solved by transforming (3.1) into a linear differential-difference equation. This can be accomplished by a similarity transformation. Define a transformed wave function  $\varphi(y)$  by

$$\varphi(y) = e^{\beta C y^2/2} \int_{-\infty}^{+\infty} dt \exp[i(2\beta C)^{1/2}yt] e^{-t^2/2} f(t) \quad (3.2a)$$

or formally

$$|\varphi\rangle = T|f\rangle. \quad (3.2b)$$

The operators  $c$  and  $c^\dagger$  are then transformed into

$$c \rightarrow \frac{1}{i(\beta C)^{1/2}} \frac{d}{dy}, \quad (3.3a)$$

$$c^\dagger \rightarrow i(\beta C)^{1/2}y, \quad (3.3b)$$

and Eq. (3.1) becomes

$$\gamma y \frac{d}{dy} \varphi(y) - z e^{-\beta C y} \varphi(y+1) = \epsilon \varphi(y). \quad (3.4)$$

The eigenvalue condition is now that  $\varphi(y)$  is a Taylor-expandable function at the origin.<sup>4</sup> This can be seen easily from (3.2), since all derivatives of  $\varphi(y)$  are finite because of the boundary conditions on  $f(t)$ .

#### IV. HIGH-TEMPERATURE REGION

For the solution of the eigenvalue problem in the high-temperature region we adapt a method which was first applied by Götze<sup>10</sup> to the anharmonic-oscillator problem. In this method one expands the resolvent of the Hamiltonian  $\mathcal{H}$  in a continued fraction [where we use the harmonic-oscillator representation for  $\mathcal{H}$ , see Eq. (3.1)]. The only serious work to be done is the calculation of the moments  $C_N = \langle \text{vac} | \mathcal{H}^N | \text{vac} \rangle$  ( $N=0, 1, 2, \dots$ ), which determine the coefficients of the continued fraction. We calculated up to 30 moments, this is equivalent to a [14, 15]-Padé-approximant for the resolvent. The details of the numerical calculations are described in Ref. 11. Satisfactory convergence is obtained in a temperature region down to  $\bar{T} \equiv (\beta C)^{-1} = 0.5$ . The ground-state eigenvalue  $\epsilon_0$  as a function of the activity  $z$  for different temperatures is shown in Fig. 1 (solid curves). For very high temperatures the isotherms approach smoothly the ideal gas limit:  $\epsilon_0 = -z$ .

In order to get analytical insight into the structure of the solution in the high-temperature region it is suggestive to expand the exponential in (3.1) up to terms of second order in  $y$  (harmonic approximation). The eigenvalue equation then becomes

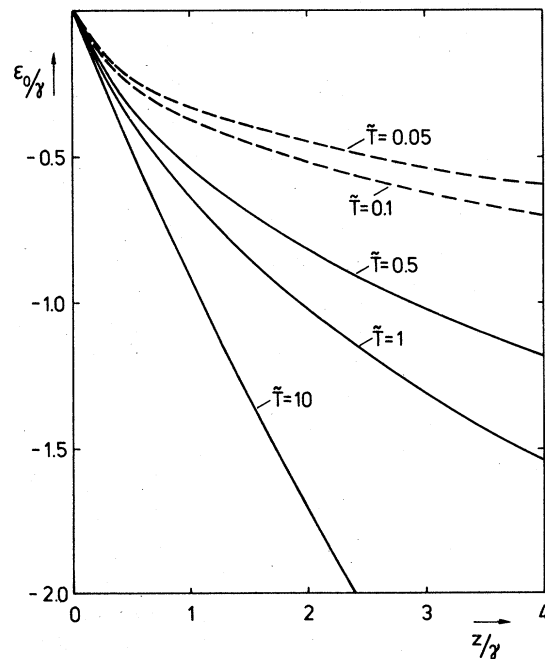


FIG. 1. Ground-state eigenvalue  $\epsilon_0$  as a function of the activity  $z$  for different temperatures  $\bar{T} = (\beta C)^{-1}$ . The broken curves are obtained by numerical integration of the low-temperature formula (5.4). The solid curves were calculated by numerical solution of the eigenvalue equation (3.1) (high-temperature region).

$$\left[ \frac{1}{2} \gamma \left( -\frac{d^2}{dy^2} + (1 + 2\beta C \xi / \gamma) y^2 - i2(2\beta C)^{1/2} \xi / \gamma - 1 \right) - \xi \right] f(y) = \epsilon f(y).$$

After a shift and scaling transformation one readily reads off the harmonic-oscillator spectrum

$$\epsilon_n = \gamma \omega \left( n + \frac{1}{2} \right) - \frac{1}{2} \gamma + \gamma \frac{\beta C}{1 + 2\beta C \xi / \gamma} (\xi / \gamma)^2 - \xi;$$

$$n = 0, 1, 2, \dots$$

where the frequency  $\omega$  is given by

$$\omega = (1 + 2\beta C \xi / \gamma)^{1/2}.$$

In particular for the ground-state energy we get

$$\epsilon_0 = \frac{1}{2} \gamma (1 + 2\beta C \xi / \gamma)^{1/2} - \frac{1}{2} \gamma + \gamma \frac{\beta C}{1 + 2\beta C \xi / \gamma} (\xi / \gamma)^2 - \xi. \quad (4.1)$$

Equation (4.1) is for  $\tilde{T} = 10$  and  $z/\gamma = 3$  up to  $10^{-3}$  in agreement with the numerical result.

We will now discuss the equation of state in the high- and low-density regime, still keeping the temperature at some fixed but high value.

Low densities correspond to small  $\xi$  and we thus expand (4.1) up to terms of second order in  $\xi$

$$\epsilon_0 \approx -\xi \left( 1 - \frac{1}{2} \beta C \right) + \beta C \left( 1 - \frac{1}{4} \beta C \right) \xi^2 / \gamma \quad \text{for } \xi \text{ small}$$

which by the use of (2.6) gives the approximate equation of state

$$\beta p \approx \rho + \frac{\beta C}{\gamma} \frac{1 - \beta C/4}{(1 + \beta C/2)^2} \rho^2. \quad (4.2)$$

In the limit of a very long range but very weak interaction ( $\gamma \rightarrow 0$ ,  $C = \alpha\gamma$ ,  $\alpha > 0$ ) Eq. (4.2) reduces to

$$\beta p = \rho + \beta \alpha \rho^2$$

which is identical to the virial expansion in this limit.<sup>12,13</sup>

If one increases the density of the system, one expects that the particles "experience" mainly the short-range part of the interaction potential

$$v(x - x') = C \exp(-\gamma |x - x'|) = C - C\gamma |x - x'| \pm \dots$$

which is up to a constant just the interaction potential of a one-dimensional system of particles with charges of equal—say negative—sign. The one-dimensional electron gas immersed in a positively charged uniform background has been treated by Baxter<sup>5</sup> and it is interesting to compare his results with ours in the high-density limit (i.e., large values of  $\xi$ ). For  $\xi \rightarrow \infty$  the ground-state eigenvalue (4.1) behaves as

$$\epsilon_0 \approx \frac{1}{2} \gamma (2\beta C \xi / \gamma)^{1/2} - \frac{1}{2} \xi \quad \text{for } \xi \text{ large}$$

which by the use of (2.6) yields

$$\beta p \approx \rho - \frac{1}{2} (\gamma \beta C)^{1/2} \rho^{1/2}, \quad (4.3)$$

where constant terms and terms of the order of  $\rho^{-1/2}$  have been neglected.

The term linear in  $\rho$  reflects, as in (4.2), the ideal-gas behavior, typical for the high-temperature region. Equation (4.3) is essentially Baxter's high-temperature result for the electron gas with uniform background.<sup>5</sup> There is a difference by a factor of 2, which is a consequence of the absence of the positive background in our system.

For the correlation function we have to evaluate the matrix element in (2.7). All quantities (ground-state eigenvalue and wave function) are known explicitly within the high-temperature or harmonic-oscillator approximation. In calculating the matrix element one has to take care of the fact that the "left" eigenfunction  $|g_n\rangle$  is just the complex conjugate of the "right" eigenfunction  $|f_n\rangle$

$$|g_n\rangle = |f_n\rangle^*. \quad (4.4)$$

A straightforward calculation then yields the following expression for the correlation function

$$g(r) = 1 - (z^2/\rho^2) \beta C e^{-rr} \quad (4.5)$$

where  $r = x_2 - x_1$ . Only terms up to linear order in  $\beta$  have been kept.

The relation (4.4) is a consequence of the special symmetry

$$\mathcal{H}^\dagger = \mathcal{H}^*$$

[see Eq. (3.1)]. A further symmetry of  $\mathcal{H}$  under parity transformations  $P$  is

$$\mathcal{H}^* = P\mathcal{H}P^{-1}.$$

Equation (4.5) gives the correct asymptotic behavior  $g(r) \rightarrow 1$  for  $r \rightarrow \infty$ . For very high temperatures  $g(r)$  approaches the ideal-gas limit  $g(r) = 1$  for all  $r$ . By lowering the temperature the effect of the repulsive potential shows up with a finite dip of the correlation function at  $r \approx 0$ . The spatial extent of this dip is given by the range  $\gamma^{-1}$  of the potential as it is physically expected.

## V. LOW-TEMPERATURE REGION

As already pointed out in Sec. III, in the low-temperature region one has to use the differential-difference equation (3.4) as the starting point of the calculation.

For  $y \rightarrow \infty$  the exponential perturbation in (3.4) is negligible and one easily reads off the asymptotic solution as

$$\varphi(y) \approx y^{e/\gamma} \quad \text{for } y \rightarrow \infty \quad (5.1)$$

After a simple algebraic manipulation (3.4) may be written as

$$y^{\epsilon/\gamma+1} \frac{d}{dy} y^{-\epsilon/\gamma} \varphi(y) = (z/\gamma) e^{-\beta C y} \varphi(y+1).$$

Integrating this equation from some finite (positive) value of  $y$  up to infinity one gets

$$\varphi(y) = y^{\epsilon/\gamma} \left( 1 - \frac{z}{\gamma} \int_y^\infty dt e^{-\beta C t} t^{-\epsilon/\gamma-1} \varphi(t+1) \right), \quad (5.2)$$

where the asymptotic form of  $\varphi(y)$  has been used.

Thus  $\varphi(y)$  is determined by the values of  $\varphi(t)$  in the interval  $[y+1, \infty]$ . As the asymptotic form of  $\varphi(t)$  is known, Eq. (5.2) yields a unique wave function  $\varphi(y)$ ,<sup>14</sup> which depends on the parameters  $\epsilon$ ,  $z$ , and  $\beta$ . In general, for  $\epsilon < 0$ , the function  $\varphi(y)$  thus determined will not be a Taylor-expandable function at the origin since the factor  $y^{\epsilon/\gamma}$  in front of (5.2) produces a divergence. This divergence will be suppressed if we demand that the expression in the large parentheses vanishes as  $y \rightarrow 0$ . Hence the eigenvalue condition that  $\varphi(y)$  is a Taylor-expandable function at the origin may be expressed as

$$1 - \frac{z}{\gamma} \int_0^\infty dt e^{-\beta C t} t^{-\epsilon/\gamma-1} \varphi(t+1) = 0. \quad (5.3)$$

Thus for a given  $z$  and  $\beta$  one has to find an  $\epsilon$  such that the wave function  $\varphi(y)$ , given uniquely by (5.2), satisfies the eigenvalue condition (5.3).

So far no use has been made of the fact that we are considering the low-temperature region  $\beta \rightarrow \infty$ . Equations (5.2) and (5.3) are just an alternative way of expressing the eigenvalue problem (3.1). But the eigenvalue condition (5.3) becomes extremely simplified for large values of  $\beta$ .

For very low temperatures ( $\beta \rightarrow \infty$ ) the exponential factor in (3.4) decreases very fast, thus the region around  $y=1$  already belongs to the asymptotic regime and one may replace  $\varphi(t+1)$  in the integrand of (5.3) by its asymptotic form. The eigenvalue condition is then

$$\frac{1}{z/\gamma} = \int_0^\infty dt e^{-\beta C t} t^{-\epsilon/\gamma-1} (1+t)^{\epsilon/\gamma}. \quad (5.4)$$

The definite integral may be expressed by a confluent hypergeometric function—usually denoted by  $U(a, b, x)$ —which is closely related to Whittaker's function [see Ref. 15, Eq. (13.2.5)]

$$1/(z/\gamma) = \Gamma(-\epsilon/\gamma) U(-\epsilon/\gamma, 1, \beta C), \quad (5.5)$$

where  $\Gamma(a)$  is the gamma function.

Although the integral representation that leads from (5.4) to (5.5) holds only for  $\epsilon < 0$ , Eq. (5.5) may be analytically continued such that it holds for all  $\epsilon$ . Equation (5.5) is then a simple trans-

cedental equation, which determines the whole spectrum of the Hamiltonian  $\mathcal{H}$ .

The ground-state eigenvalue  $\epsilon_0$  as a function of  $z$  calculated from (5.4) by numerical integration is shown in Fig. 1 (broken curves).

By means of (2.6) one gets from (5.5) the equation of state

$$\rho/\gamma = -(\psi(a) + \frac{\partial}{\partial a} \ln U(a, 1, \beta C))^{-1}$$

where  $\psi(a)$  is the digamma function and  $a = -\epsilon_0/\gamma$ .

In order to get an idea of the dependence of the right-hand side of (5.5) on  $\epsilon$  we use the asymptotic form of  $U(a, b, x)$  for large argument

$$U(a, b, x) \approx x^{-a} \quad (5.6)$$

[see Ref. 15, Eq. (13.1.8)] which gives

$$1/(z/\gamma) \approx \Gamma(-\epsilon/\gamma) (\beta C)^{\epsilon/\gamma}. \quad (5.7)$$

Equation (5.7) is valid for  $\beta C$  large and  $\epsilon/\gamma$  finite.

As will be seen later, in this approximation only next-neighbor interactions are taken into account.

The right-hand side of (5.7) is shown in Fig. 2. As  $z \rightarrow 0$ , the roots of (5.7) are essentially determined by the poles of the gamma function and one recovers the harmonic-oscillator spectrum:  $\epsilon_n = n\gamma$  ( $n=0, 1, 2, \dots$ ). Further one sees that there is always one negative real solution  $\epsilon_0$ , whereas the excited states eventually go into the complex plane, if one increases  $z$ . If we remember that large values of  $z$  correspond to high densities this gives the physically reasonable picture

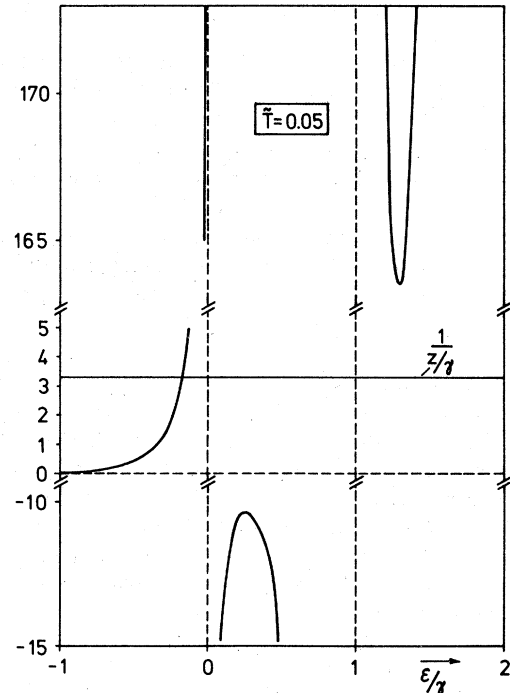


FIG. 2. Function  $\Gamma(-\epsilon/\gamma)(\beta C)^{\epsilon/\gamma}$  for  $\bar{T} \equiv (\beta C)^{-1} = 0.05$ .

that for high densities there occur complex eigenvalues giving rise to oscillations in the correlation function, which are typical for a fluid [see Eq. (2.9)].

#### A. Crystal limit of the equation of state

For  $T \rightarrow 0$  we expect on physical grounds the system to be close to the crystalline state. It is interesting to see whether this limit is contained in our formulas.

Recalling that for the ground state  $\epsilon = \epsilon_0 = -\beta p$  we see that we have to consider the asymptotic form of (5.5), where both  $\beta C$  and  $\epsilon$  are large (of the order  $\beta$ ). We thus go back to the integral representation (5.4) and put it into the form

$$1/(z/\gamma) = I(a),$$

where

$$a = \beta p/\gamma = -\epsilon_0/\gamma$$

and the integral  $I(a)$  is written as

$$I(a) = \int_0^\infty \frac{dt}{t} \exp[-F(t, a)] \quad (5.8)$$

with

$$F(t, a) = \beta C t - a \ln[t/(1+t)].$$

The equation of state is obtained by taking the logarithmic derivative of  $I(a)$  [see Eq. (2.6)],

$$\frac{1}{\rho/\gamma} = -\frac{\partial}{\partial a} \ln I(a). \quad (5.9)$$

Applying the saddle-point method to  $I(a)$  as well as to  $\partial I(a)/\partial a$  and keeping all terms up to  $1/\beta$  we get

$$\frac{1}{\rho/\gamma} = \ln[(1+t_0)/t_0] + \frac{1}{2\beta C} \frac{2t_0 + 4t_0 + 1}{t_0(1+t_0)(2t_0+1)^2}, \quad (5.10)$$

where  $t_0$  is a function of the pressure and to be determined by the positive root of the saddle-point condition  $F'(t_0, a) = 0$ ,

$$a/\beta C = t_0(1+t_0). \quad (5.11)$$

Equations (5.10) and (5.11) give a parametric representation of the equation of state,  $t_0$  being the parameter.

In a zero order approximation we neglect the second term in (5.10) which gives

$$t_0^{(0)} = e^{-\gamma/\rho} / (1 - e^{-\gamma/\rho}). \quad (5.12)$$

Inserting the zero-order value of  $t_0$  in (5.11) one obtains the equation of state

$$p^{(0)}/\gamma = C e^{-\gamma/\rho} / (1 - e^{-\gamma/\rho})^2.$$

This is just the zero-temperature pressure of a

linear chain of particles separated by the lattice constant  $1/\rho$  and interacting via the exponential repulsion (1.1)

In a first approximation—for given density  $\rho$ —we linearize (5.10) and (5.11) at the value  $t_0^{(0)}$  found in the zeroth approximation. We then find

$$p^{(1)}/\gamma = C \frac{e^{-\gamma/\rho}}{(1 - e^{-\gamma/\rho})^2} + \frac{1}{2\beta} \frac{2t_0^{(0)2} + 4t_0^{(0)} + 1}{2t_0^{(0)} + 1}. \quad (5.13)$$

The second term in (5.13) is just the Grüneisen correction<sup>16</sup> to the zero-temperature equation of state. This correction arises as a consequence of the vibrations of the particles about their equilibrium positions in the chain.

For high densities  $t_0^{(0)} \approx \rho/\gamma$ , we thus get

$$p^{(1)}/\gamma \approx C(\rho/\gamma)^2 + (1/2\beta)\rho/\gamma \quad \text{for } \rho \text{ large.} \quad (5.14)$$

The second term coincides with the leading term in Baxter's low-temperature equation of state for the one-dimensional electron gas with a positive uniform background.<sup>5</sup> This is reasonable since for high densities the particles are subject only to the short-range part of the interaction which is like the one-dimensional Coulombic interaction considered by Baxter (see Sec. IV). Thus the second term in (5.14) is due to plasma oscillations. The first term is absent in Baxter's equation because of the uniform background which compensates the pressure due to the repulsion of the electron gas.

For low densities essentially only the next-neighbor interaction is relevant. From (5.12) we have  $t_0^{(0)} \approx e^{-\gamma/\rho}$  and we get

$$p^{(1)}/\gamma = C e^{-\gamma/\rho} + 1/2\beta \quad \text{for } \rho \text{ small.} \quad (5.15)$$

The first term is the zero-point pressure of a linear chain with the interaction (1.1) restricted to next neighbors. The second term is the appropriate Grüneisen correction.

Equation (5.15) could have been obtained directly from (5.7) by using Stirling's formula for the gamma function. This shows that the approximation (5.6) essentially takes only next-neighbor interaction into account.

#### B. Correlation function

In the preceding paragraph we concluded from a discussion of the equation of state that the system behaves almost like a crystal in the limit  $T \rightarrow 0$ . More detailed information about the structure of the system is of course obtained from the correlation function  $g(r)$ . The Laplace transform of  $g(r)$  is defined by

$$\tilde{g}(s) = \int_0^\infty dt e^{-sr} g(r).$$

Then  $\bar{g}(s)$  may be calculated using the same methods already described in this section. The details of the calculation are given in Appendix B. The result is

$$\bar{g}(s) = \frac{1}{\rho\gamma} \frac{\Gamma(-\epsilon_0/\gamma + s/\gamma) U(-\epsilon_0/\gamma + s/\gamma, 1 + s/\gamma, \beta C)}{1 - (z/\gamma) \Gamma(-\epsilon_0/\gamma + s/\gamma) U(-\epsilon_0/\gamma + s/\gamma, 1, \beta C)} \frac{U(-\epsilon_0/\gamma, 1 - s/\gamma, \beta C)}{U(-\epsilon_0/\gamma, 1, \beta C)}. \quad (5.16)$$

Although (5.16) looks a little bit complicated it may be easily discussed for small  $s$ . We note that for  $s=0$  the denominator vanishes as a consequence of the eigenvalue condition (5.5). We write  $-\epsilon_0/\gamma = a$  and expand the denominator up to first order in  $s$

$$1 - (z/\gamma) \Gamma(a + s/\gamma) U(a + s/\gamma, 1, \beta C) \approx -\frac{z}{\gamma} \frac{\partial}{\partial a} I(a) s/\gamma - \dots$$

with

$$I(a) = \Gamma(a) U(a, 1, \beta C).$$

We then get

$$\bar{g}(s) \approx 1/s \text{ for } s \rightarrow 0, \quad (5.17)$$

where use has been made of (5.9). This shows that  $g(r) \approx 1$  for large  $r$ , hence Eq. (5.16) yields the correct asymptotic behavior for  $g(r)$ .

Equation (5.17) is the first term of a power series expansion of  $\bar{g}(s)$  at  $s=0$ . Let us see, whether also the constant term after the  $1/s$  singularity is given correctly by (5.16). To this end we recall the general relation between the structure factor  $S(k)$  and the isothermal compressibility  $\chi_T$  (see, for example, Ref. 17)

$$S(k=0) = (\rho/\beta) \chi_T. \quad (5.18)$$

$S(k)$  is defined by

$$S(k) = \rho \int_{-\infty}^{+\infty} d\tau e^{ik\tau} [g(r) - 1] + 1 \quad (5.19)$$

and  $\chi_T$  is given by

$$\chi_T^{-1} = \rho \left( \frac{\partial \rho}{\partial \mu} \right)_T.$$

From (5.19) it follows that

$$S(k) = \rho [g(ik + \eta) + g(-ik + \eta) - 2\pi\delta(k)] + 1; \quad \eta \rightarrow 0^+. \quad (5.20)$$

The  $1/s$  singularity in  $\bar{g}(s)$  is just compensated by the delta function in (5.20). Expanding  $\bar{g}(s)$  up to the constant term and using (5.9) we get

$$S(k=0) = \left( \frac{\rho}{\gamma} \right)^2 \frac{\partial^2}{\partial a^2} \ln I(a).$$

On the other hand, by differentiating (5.9) with respect to  $\rho$ , thereby using  $a = \beta p/\gamma$  and the definition of  $\chi_T$  we get

$$\chi_T = (\beta\rho/\gamma^2) \frac{\partial^2}{\partial a^2} \ln I(a), \quad (5.21)$$

which shows that the general relation (5.18) is satisfied.

The isothermal compressibility may also be calculated explicitly by means of the saddle-point method described above. From (5.21) one gets

$$\chi_T = \frac{\rho}{\gamma^2 C} \frac{1}{t_0(1+t_0)(2t_0+1)},$$

where  $t_0$  is determined by (5.11).

Finally we want to give an expression for  $g(r)$ . By applying the inverse Laplace transform on (5.16) we have to calculate the poles and the residues of  $e^{sr} \bar{g}(s)$ . The poles are given by the roots of

$$1 = (z/\gamma) \Gamma(-\epsilon_0/\gamma + s/\gamma) U(-\epsilon_0/\gamma + s/\gamma, 1, \beta C), \quad (5.22)$$

which is essentially the eigenvalue condition (5.5). Thus the poles  $s_n$  are related to the eigenvalues  $\epsilon_n$  by

$$s_n = -(\epsilon_n - \epsilon_0).$$

Therefore one recovers the general structure of the correlation function as given in (2.9):

$$g(r) = \sum_n e^{-(\epsilon_n - \epsilon_0)r} \text{Res}[\bar{g}(s), s_n]. \quad (5.23)$$

Let us discuss the eigenvalue spectrum determined by the roots of (5.22) in more detail. By taking the logarithm we get

$$-\ln(z/\gamma) + 2\pi in = \ln[\Gamma(-\epsilon_0/\gamma + s/\gamma) U(-\epsilon_0/\gamma + s/\gamma, 1, \beta C)] \quad (n=0, \pm 1, \pm 2, \dots). \quad (5.24)$$

Expansion of the right-hand side with respect to  $s$  yields

$$2\pi in = -(1/\rho)s + (1/2\beta\rho)\chi_T s^2.$$

In the zero-temperature limit the poles are purely imaginary:  $s_n = 2\pi i \rho n$ . For finite but very small values of  $T$  the line of poles bends into the nega-



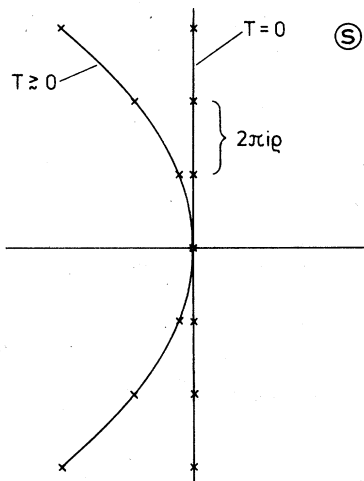


FIG. 3. Eigenvalue spectrum in the low-temperature region.

tive halfplane (see Fig. 3) and the spectrum is approximately given by

$$s_n = 2\pi i \rho n - \frac{2\pi^2 \chi_T \rho^2}{\beta} n^2; \text{ for } n=0, \pm 1, \pm 2, \dots \quad (5.25)$$

Since  $\epsilon_0 = -\beta b$  becomes large as  $\beta \rightarrow \infty$  whereas  $s_n$  is to zero order independent of  $\beta$ , the expansion of (5.24) in powers of  $s$  is justified.

The real part of  $s_n$  gives rise to a damping in the correlation function whereas the imaginary part produces oscillations of wavelength  $1/\rho$  [see Eq. (5.23)]. As  $\chi_T$  is independent of the temperature, the damping becomes negligibly small as  $\beta \rightarrow \infty$ , which shows that the system behaves almost like a crystal in this limit.

The residues of  $\bar{g}(s)$  are in zero-order approximation in  $1/\beta$  all equal to unity, independent of  $s_n$ . Hence

$$g(r) = \sum_n e^{s_n r}.$$

Using the approximate Eq. (5.25) for the  $s_n$  we get

$$g(r) = \sum_{n=0}^{\infty} \epsilon_n \cos(2\pi n \rho r) (e^{-2\pi^2 \delta \rho r} n^2), \quad (5.26)$$

where a dimensionless damping constant

$$\delta = (1/\beta) \chi_T \rho$$

has been introduced ( $\epsilon_n$  are Neuman's symbols  $\epsilon_0 = 1, \epsilon_n = 2$  for  $n = 1, 2, \dots$ ). Equation (5.26) may be expressed by an elliptic theta function<sup>18</sup>

$$g(r) = \vartheta_3(\rho r, 2\pi i \delta \rho r). \quad (5.27)$$

Using the identity<sup>18</sup>

$$\vartheta_3\left(\frac{\zeta}{\tau}, -\frac{1}{\tau}\right) = \left(\frac{\tau}{i}\right)^{1/2} e^{i\pi \zeta^2 / \tau} \vartheta_3(\zeta, \tau)$$

we may write (5.27) in the more convenient form

$$g(r) = \frac{1}{(2\pi \delta \rho r)^{1/2}} e^{-\rho r / 2\delta} \vartheta_3\left(-\frac{i}{2\pi \delta}, \frac{i}{2\pi \delta \rho r}\right)$$

or explicitly

$$g(r) = \frac{1}{(2\pi \delta \rho r)^{1/2}} e^{-\rho r / 2\delta} \sum_{n=0}^{\infty} \epsilon_n \cosh(n/\delta) e^{-n^2 / 2\delta \rho r}.$$

The  $n$ th term in this sum is an almost Gaussian function, which has a maximum approximately at the "lattice" sites  $r_n = n1/\rho$  and a width proportional to  $\delta n$  ( $n = 1, 2, \dots$ ). A similar expression has been obtained by Unger<sup>19</sup> who considered a parabolic interaction restricted to next neighbors.

### VI. TONKS-GAS LIMIT

Although we are mainly interested in the effect of the long-range character of the interparticle interaction, it is interesting to see whether we can reproduce known results for a one-dimensional next-neighbor gas within a particular limiting form of the interaction (1.1). To this end we set

$$C = C_0 e^{\gamma b}, \quad b > 0$$

and consider the limit  $\gamma \rightarrow \infty$ , that is we fix the interaction potential at  $x = b$  and then use the limit of an infinitely fast decrease of the exponential function over a width  $1/\gamma$ . In this limit the interaction behaves like a hard-core interaction

$$v(x) = \begin{cases} \infty & \text{for } |x| \leq b \\ 0 & \text{for } |x| > b \end{cases}$$

and we should recover the hard-core equation of state, first derived by Tonks in 1936.<sup>6</sup> (We call this Tonks-gas limit.)

We first note that the parameter  $C$  always appeared in the combination  $\beta C$  in our equations. Thus the limit  $C \rightarrow \infty$  is formally similar to the limit  $\beta C \rightarrow \infty$  and we may use the low-temperature formula (5.7) as a starting point of our discussion. As  $\gamma$  becomes large, whereas  $\epsilon$  remains finite, we may replace  $\Gamma(-\epsilon/\gamma)$  by  $(-\epsilon/\gamma)^{-1}$ . Finally taking the limit  $\gamma \rightarrow \infty$  we get

$$1/z = -(1/\epsilon) \exp \epsilon b,$$

which by means of (2.6) yields the Tonks equation of state

$$\beta p = \rho / (1 - b\rho). \quad (6.1)$$

For the calculation of the correlation function we start with Eq. (5.16) for the Laplace trans-

form  $\bar{g}(s)$ . The functions  $U(a, b, x)$  appearing in (5.16) may be replaced by the simple power dependence (5.6), since  $\beta C$  becomes large

$$\bar{g}(s) = \frac{1}{\rho} \frac{z}{\gamma} \frac{(\beta C)^{\epsilon_0/\gamma - s/\gamma} \Gamma(-\epsilon_0/\gamma + s/\gamma)}{1 - (z/\gamma)(\beta C)^{\epsilon_0/\gamma - s/\gamma} \Gamma(-\epsilon_0/\gamma + s/\gamma)} \quad (6.2)$$

We note that

$$\bar{H}(s) \equiv (1/\gamma)(\beta C)^{\epsilon_0/\gamma - s/\gamma} \Gamma(-\epsilon_0/\gamma + s/\gamma)$$

is just the Laplace transform of

$$g^{(0)}(r) \equiv e^{\epsilon_0 r} \exp(-\beta C e^{-\gamma r})$$

By expanding (6.2) into a geometric series we recover the exact expression for the correlation function of a one-dimensional gas, where the interaction  $v(r) = C e^{-\gamma r}$  is restricted to next neighbors.<sup>7,20</sup>  $g(r)$  may then be written as a sum of convolutions

$$g(r) = \frac{z}{\rho} \left\{ g^{(0)}(r) + z \int_0^r dr' g^{(0)}(r-r') g^{(0)}(r') + \dots \right\} \quad (6.3)$$

Finally taking the Tonks-limit we get

$$g^{(0)}(r) = \vartheta(r-b) e^{\epsilon_0 r} \text{ for } \gamma \rightarrow \infty.$$

[ $\epsilon_0 = -\beta p$  is given for the Tonks gas in (6.1),  $\vartheta(x)$  is the step function.] Equation (6.3) then yields the well-known result for the correlation function of a one-dimensional hard-core system.<sup>7</sup>

## VII. CONCLUSION

In this work we give a complete discussion of the equation of state and the correlation function for a one-dimensional classical system with a long-range interaction. The mathematics is essentially reduced to the solution of a non-Hermitian eigenvalue problem, which we solve analytically in the high- and low-temperature region, respectively. Although the non-Hermiticity of the problem causes some mathematical difficulties the discussion of the correlation function becomes very transparent with the occurrence of complex eigenvalues: the imaginary part of the excited eigenvalues give rise to typical oscillations in the correlation function which are difficult to obtain otherwise.

We show that in the limit of large densities the short distance Coulombic nature of the potential (1.1) essentially determines the thermodynamic behavior of the system. By an appropriate choice of the parameters  $C$  and  $\gamma$  contained in the potential (1.1) we are able to recover all known results for a one-dimensional hard-core gas (Tonks gas). Thus physically quite different systems can be

described by our equations.

In the zero-temperature limit we can study explicitly the appearance of an almost crystalline structure.

## ACKNOWLEDGMENT

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## APPENDIX A

In order to calculate the grand partition function of a two-dimensional classical system one considers the Hamiltonian

$$\mathcal{H}' = \sum_k \omega_k c_k^\dagger c_k - Z \int_0^L dy \exp[i\sqrt{\beta} C^\dagger(y)] \times \exp[i\sqrt{\beta} C(y)],$$

where

$$\omega_k = (k^2 + \gamma^2)^{1/2}$$

and  $C(y)$  is given by

$$C(y) = \left(\frac{2\pi}{L}\right)^{1/2} \sum_k \frac{1}{(2\omega_k)^{1/2}} c_k e^{iky},$$

$$C^\dagger(y) = [C(y)]^\dagger.$$

Periodic boundary conditions are assumed such that

$$k = (2\pi/L)n, \quad n = 0, \pm 1, \pm 2, \dots$$

The operators  $c_k$  and  $c_k^\dagger$  satisfy the usual commutation relation

$$[c_k, c_{k'}^\dagger] = \delta_{k, k'}, \quad [c_k, c_{k'}] = [c_k^\dagger, c_{k'}^\dagger] = 0,$$

where  $\delta_{k, k'}$  is the Kronecker symbol.

Introducing a "time" variable  $x$  via the interaction picture and using the same procedure as in Sec. II one gets

$$\langle \text{vac} | e^{-L\mathcal{H}'} | \text{vac} \rangle = Z_G,$$

where

$$Z_G = \sum_{N=0}^{\infty} \frac{z^N}{N!} \int_0^L dx_N \int_0^L dy_N \dots \int_0^L dx_1 \times \int_0^L dy_1 \exp\left(-\beta \sum_{i>j=1}^N v(\vec{x}_i - \vec{x}_j)\right)$$

is the grand partition function of a two-dimensional system confined to a square of area  $L^2$  and interacting via the repulsive potential

$$v(|\vec{x}|) = K_0 (\gamma(x^2 + y^2)^{1/2}).$$

[ $K_0(\xi)$  is the modified Bessel function of zero order.]

The generalization to three dimensions gives the partition function with a Yukawa interaction potential.

The above stated connections serve as specific examples of the well-known fact<sup>21,22</sup> that an  $n$ -dimensional system in classical statistical mechanics is equivalent to a  $n$ -dimensional Euclidean quantum field theory.

#### APPENDIX B

For the calculation of  $g(r)$  we take the Laplace transform of (2.9)

$$\tilde{g}(s) = \frac{1}{\rho^2} \sum_n \frac{1}{s + \epsilon_n - \epsilon_0} \frac{\langle g_0 | \mathcal{H}_I | f_n \rangle \langle g_n | \mathcal{H}_I | f_0 \rangle}{\langle g_n | f_n \rangle \langle g_0 | f_0 \rangle}. \quad (\text{B1})$$

In order to perform the sum over intermediate states we use a trick originally due to Dalgarno and Lewis.<sup>23,24</sup> To this end we consider the inhomogeneous equation

$$(s + \mathcal{H} - \epsilon_0) |F_s\rangle = \mathcal{H}_I |f_0\rangle \quad (\text{B2})$$

to be solved, where  $|f_0\rangle$  denotes the ground-state eigenfunction of  $\mathcal{H}$ . By formally solving for  $|F_s\rangle$

$$|F_s\rangle = \frac{1}{s + \mathcal{H} - \epsilon_0} \mathcal{H}_I |f_0\rangle$$

we then easily derive form (B1),

$$\tilde{g}(s) = \frac{1}{\rho^2} \langle g_0 | \mathcal{H}_I | F_s \rangle \frac{1}{\langle g_0 | f_0 \rangle}. \quad (\text{B3})$$

Thus, if one knows the solution  $|F_s\rangle$  of the inhomogeneous equation (B2), one has only to calculate the matrix element  $\langle g_0 | \mathcal{H}_I | F_s \rangle$  in order to obtain  $\tilde{g}(s)$ .

In the low-temperature region Eq. (B2) is most easily solved after applying the similarity transformation (3.2). Equation (B2) then reads

$$\begin{aligned} \left( s + \gamma y \frac{d}{dy} - \epsilon_0 \right) \phi_s(y) - z e^{-\beta c y} \phi_s(y+1) \\ = -z e^{-\beta c y} \phi_0(y+1), \end{aligned} \quad (\text{B4})$$

where

$$|\phi_s\rangle = T |F_s\rangle, \quad |\phi_0\rangle = T |f_0\rangle.$$

For  $y \rightarrow \infty$  the asymptotic solution of (B4) is given by

$$\phi_s(y) \propto y^{(\epsilon_0 - s)/\gamma}.$$

Therefore  $\phi_s(y)$  is proportional to some power of  $y$  which is essentially the same dependence as in Eq. (5.1) for the asymptotic solution of the homogeneous equation. But as we are dealing here with

the inhomogeneous equation (B2) we may not take the constant of proportionality to be 1 as in (5.1), rather we have to put

$$\phi_s(y) = A(s) y^{(\epsilon_0 - s)/\gamma} \quad (\text{B5})$$

and determine the amplitude  $A(s)$  self-consistently.

Applying the same procedure which leads to (5.3) we get

$$\begin{aligned} \phi_s(y) = y^{(\epsilon_0 - s)/\gamma} \left( A(s) - \frac{z}{\gamma} \int_y^\infty dt e^{-\beta c t} t^{-(\epsilon_0 - s)/\gamma - 1} \right. \\ \left. \times [\phi_s(t+1) - \phi_0(t+1)] \right). \end{aligned} \quad (\text{B6})$$

Again—in the low-temperature region—we may replace  $\phi_s(t+1)$  and  $\phi_0(t+1)$  by their asymptotic forms (B5) and (5.1). Analogous to the argument in Sec. V,  $A(s)$  is then determined by the requirement that the large parentheses in (B6) vanishes for  $y=0$ . This condition yields

$$A(s) = \frac{z}{\gamma} \frac{\Gamma(-\epsilon_0/\gamma + s/\gamma) U(-\epsilon_0/\gamma + s/\gamma, 1 + s/\gamma, \beta C)}{1 - (z/\gamma) \Gamma(-\epsilon_0/\gamma + s/\gamma) U(-\epsilon_0/\gamma + s/\gamma, 1, \beta C)},$$

where all definite integrals have been expressed by the confluent hypergeometric function  $U(a, b, x)$  [see Ref. 15, Eq. (13.2.5)]. Thus the asymptotic solution (B5) is known explicitly.

In order to calculate the matrix element  $\langle g_0 | \mathcal{H}_I | F_s \rangle$  we use only the asymptotic expressions for the wave function. This may, at first sight, look like a crude approximation. But we must remember that the operator  $\mathcal{H}_I$  shifts the arguments of the left and the right wave function by 1 [see Eqs. (2.2b) and (3.3a)]. Hence, as the argument 1 already belongs to the asymptotic regime, it is sufficient to use the asymptotic form of the wave functions.

By means of (3.2) and (3.3b) we get from (B5),

$$|F_s\rangle = \frac{1}{\pi^{1/4}} A(s) \left( \frac{c^\dagger}{i(\beta C)^{1/2}} \right)^{\epsilon_0/\gamma - s/\gamma} |\text{vac}\rangle \quad (\text{B7})$$

and from (5.1) taking into account the relation (4.4),

$$\langle g_0 | = \frac{1}{\pi^{1/4}} \langle \text{vac} | [c/i(\beta C)^{1/2}]^{\epsilon_0/\gamma}. \quad (\text{B8})$$

Equations (B7) and (B8) are not well defined as they stand. This difficulty could have been avoided if we would have used polynomial expressions for the wave functions instead of the asymptotic formulas. For the time being (B7) and (B8) may be looked upon as formal equations, which simplify the calculation. The final result, of course, will be well defined. The matrix element is then

$$\begin{aligned} \langle g_0 | \mathcal{H}_I | F_s \rangle &= -\frac{z}{\sqrt{\pi}} A(s) \langle \text{vac} | \left( \frac{c}{i(\beta C)^{1/2}} \right)^{\epsilon_0/\gamma} \\ &\quad \times \exp[i(\beta C)^{1/2} c^\dagger] \exp[i(\beta C)^{1/2} c] \\ &\quad \times \left( \frac{c^\dagger}{i(\beta C)^{1/2}} \right)^{\epsilon_0/\gamma - s/\gamma} | \text{vac} \rangle \\ &= -\frac{z}{\sqrt{\pi}} A(s) \langle \text{vac} | \left( \frac{c}{i(\beta C)^{1/2}} + 1 \right)^{\epsilon_0/\gamma} \\ &\quad \times \left( \frac{c^\dagger}{i(\beta C)^{1/2}} + 1 \right)^{\epsilon_0/\gamma - s/\gamma} | \text{vac} \rangle. \end{aligned}$$

By formally expanding into a binomial series one gets

$$\begin{aligned} \langle g_0 | \mathcal{H}_I | F_s \rangle &= -\frac{z}{\sqrt{\pi}} A(s) \sum_{n=0}^{\infty} \left( -\frac{1}{\beta C} \right)^n \frac{1}{n!} (-\epsilon_0/\gamma)_n \\ &\quad \times (-\epsilon_0/\gamma + s/\gamma)_n, \end{aligned} \quad (\text{B9})$$

where  $(a)_n \equiv a(a+1)\cdots(a+n-1)$  is Pochhammer's symbol. Equation (B9) represents a divergent series. The series is Borel summable and may again be expressed by the hypergeometric function  $U(a, b, x)$ . One finally gets

$$\begin{aligned} \langle g_0 | \mathcal{H}_I | F_s \rangle &= -(z/\sqrt{\pi}) A(s) (\beta C)^{-\epsilon_0/\gamma + s/\gamma} \\ &\quad \times U(-\epsilon_0/\gamma + s/\gamma, 1 + s/\gamma, \beta C). \end{aligned}$$

[This is most easily seen, if one expands the integral representation for  $U(a, b, x)$ ,

$$U(a, b, x) = \frac{1}{\Gamma(a)} \int_0^\infty dt e^{-xt} t^{a-1} (1+t)^{b-a-1}$$

in a formal series in  $t$ .]

The calculation of the normalization  $\langle g_0 | f_0 \rangle$  in (B3) is achieved by the same methods with the use of (2.10). The resulting expression for  $\tilde{g}(s)$  is then

$$\tilde{g}(s) = \frac{1}{\rho} \frac{z}{\gamma} \frac{\Gamma(-\epsilon_0/\gamma + s/\gamma) U(-\epsilon_0/\gamma + s/\gamma, 1 + s/\gamma, \beta C)}{1 - (Z/\gamma) \Gamma(-\epsilon_0/\gamma + s/\gamma) U(-\epsilon_0/\gamma + s/\gamma, 1, \beta C)} \frac{U(-\epsilon_0/\gamma, 1 - s/\gamma, \beta C)}{U(-\epsilon_0/\gamma, 1, \beta C)}.$$

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