One-particle density matrix of a one-dimensional gas with strong interaction

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The one-particle density matrix in a one-dimensional system of spinless particles (bosons or fermions) with strong repulsion between the particles is found. At zero temperature it oscillates at large distances, and the amplitude of the oscillations decays by a power law. The character of the oscillations and the exponents depend on the statistics. Relations connecting these exponents with the velocity of sound in the system are obtained.

1. In the theory of quantum one-dimensional systems, the problem of finding the various correlation functions is currently very important. In many cases the asymptotic behavior of the correlators at large distances is found to be especially interesting.

In a paper by Efetov and Larkin[1] it was postulated that the asymptotic form of correlation functions of one-dimensional Fermi systems is determined by the long-wavelength gapless excitations. Neglecting all the other excitations, one can find the explicit form of the correlation functions. Another approach to the problem involves linearization of the quadratic spectrum of the fermions and introduction of two kinds of particles, after which the calculations can be performed exactly.[2–4] Recently, Haldane has proposed yet another method of treating one-dimensional quantum Bose and Fermi systems—a method based on conjectures analogous to the hypothesis of Ref. 1 and consisting in the reduction of the system to a certain universal "Luttinger liquid."[5,6] This approach makes it possible to find the correlation functions.

The correlation functions found by means of these approaches qualitatively coincide: Their characteristic feature is a power-law decay at large distances and a continuous dependence of the exponents on the coupling constant. By analogy with the theory of phase transitions, these exponents are sometimes called the critical indices of the corresponding correlators; their determination is one of the problems of the theory.

However, all these approaches are based on assumptions which, though plausible, are difficult to prove. Moreover, in Ref. 7 it was noted that the asymptotic form of the correlation functions may not be connected with excitations of the acoustic type. Nevertheless, it has been shown by Krivnov and Ovchinnikov[7–9] that the qualitative behavior of the correlators does not change, and they postulated that the corresponding exponents are related in a simple way to the velocity of sound in the system. In the case of the density correlator this postulate was proved in Ref. 10 in all orders of perturbation theory in a large coupling constant: The critical exponent was found to be equal to $4\pi\rho c^{-1}$, where ρ is the particle density and c is the velocity of sound. The important point is that this results is valid for a rather arbitrary form of pair-interaction potential. Knowledge of the relationship of the exponents to the velocity of sound greatly facilitates the determination of the asymptotic forms of the correlators, since the problem of calculating c is considerably simpler and for its solution there exist methods that give a good approximation.

In the present paper we shall apply the method developed in Ref. 10 for the determination of the asymptotic behavior of the one-particle density matrix (which, for brevity, we shall sometimes call the Green function) in a one-dimensional system of spinless Bose or Fermi particles with strong pair interaction (repulsion). The Fourier transform of this function is the momentum distribution function of the particles. Only the case of zero temperature will be considered. We shall see that the one-particle density matrix has a more complicated structure than the "density-density" pair correlation function; in particular, its asymptotic form depends on the particle statistics. Nevertheless, even in this case the critical exponents can be expressed in terms of the velocity of sound.

The content of the paper is as follows. In Sec. 2 we define the model to be used, and, following Ref. 10, briefly describe the transformation to the "phonon" Lagrangian that will be used to construct the perturbation theory. In Sec. 3 we obtain a convenient representation of the ground-state wave function in terms of the phonon variables. On the basis of these auxiliary results, the Green function is calculate directly in Sec. 4. Finally, in Sec. 5 we compare our results with certain known results.

2. We consider a one-dimensional system of N spinless particles (bosons or fermions) with the Hamiltonian

$$\hat{H}=-\sum_{i=0}^{N-1}\frac{\partial^2}{\partial x_i^2}+g\sum_{i<j}^{N-1}V(x_i-x_j),\quad \hbar=2m=1. \qquad (1)$$

Here $V(x)$ is the pair-interaction potential, which is assumed to be long-range but sufficiently rapidly decaying with distance (faster than x^{-1})—in other respects, the form of $V(x)$ is arbitrary; g is the coupling constant, and throughout the paper we consider the case of repulsion ($g>0$). We assign boundary conditions by placing the particles on a circle with a large circumference L. Here, strictly speaking, it is necessary to regard the potential $V(x)$ as periodic with period L. We can immediately introduce the periodic potential

$$\tilde{V}(x)=\sum_{n=-\infty}^{\infty}V(x+nL);$$

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in the thermodynamic limit ($L\to\infty$, $N\to\infty$, $L/N=\rho^{-1}$) this will not be reflected in the results.

The one-particle density matrix at zero temperature is defined as follows:

$$S(R)=\int\Psi_0^*(x_0,x_1,\ldots,x_{N-1})\times\Psi_0(x_0+R,x_1,\ldots,x_{N-1})\prod_{j=0}^{N-1}dx_j, \qquad (2)$$

where Ψ_0 is the ground-state wave function, appropriately symmetrized.

We shall make use of perturbation theory in the large coupling constant g (Refs. 7, 10). In the case of strong repulsion ($g\to\infty$) a Wigner crystal with lattice constant a is formed, making it possible to regard the system as a gas of interacting phonons, for which the interaction (which vanishes as $g\to\infty$) can be taken into account systematically by means of perturbation theory. In place of the particle coordinates x_n we introduce "phonon" lattice variables φ_n (Ref. 7):

$$\varphi_n=x_n-na,\quad n=0,1,\ldots,N-1.$$

Their Fourier components (normal modes) have the form

$$\varphi_p(t)=N^{-1/2}\sum_{n=0}^{N-1}\varphi_n(t)\exp(-ipn),\quad \varphi_p^+=\varphi_{-p}, \qquad (3)$$

$$\varphi_{p,\omega}=T^{-1/2}\int_{-\infty}^{\infty}dt\,\varphi_p(t)\exp(-i\omega t), \qquad (4)$$

where p is the dimensionless "momentum," which takes quasidiscrete values $2\pi ma/L$; m is an integer; T is a certain large interval of time.

The Hamiltonian (1) corresponds to the following Lagrangian in the new variables[10]:

$$L(\dot\varphi_p,\varphi_p)=\frac{1}{4g}\sum_{p=-\pi}^{\pi}\dot\varphi_p\dot\varphi_{-p}-\frac{1}{4g}\sum_{p=-\pi}^{\pi}\omega_0^2(p)\varphi_p\varphi_{-p}$$
$$-\sum_{n=3}^{\infty}\frac{1}{n!}(gN)^{1-n/2}\sum_{p_l}\Gamma_0^{(n)}(p_1\ldots p_n)\tilde\delta\Big(\sum_{j=1}^{n}p_j\Big)\varphi_{p_1}\ldots\varphi_{p_n}. \qquad (5)$$

Here we have made the dilatation $\varphi_p\to g^{-1/2}\varphi_p$. The frequency $\omega_0(p)$ describes the free-phonon spectrum:

$$\omega_0(p)=\Big[4g\sum_{n=1}^{\infty}V''(na)(1-\cos np)\Big]^{1/2}.$$

The remaining terms of the Lagrangian correspond to the terms after the quadratic term in the expansion of the potential in a Taylor series in the φ_j:

$$\Gamma_0^{(n)}(p_1\ldots p_n)=\sum_{k=1}^{\infty}V^{(n)}(ka)\prod_{m=1}^{n}[\exp(ip_mk)-1].$$

It is important that

$$\Gamma_0^{(n)}(p_1\ldots p_n)\propto\prod_{j=1}^{n}p_j,\quad p_j\to0.$$

Finally, $\tilde\delta(p)$ ensures quasimomentum conservation to within a reciprocal-lattice vector, i.e., to within an integer multiple of 2π.

3. In this section we obtain for the ground-state wave function a representation convenient for calculation of the integral (2). The wave function $\Psi_0(x_0,\ldots,x_{N-1})$ has in the sector $x_0<x_1<\ldots<x_{N-1}$ a maximum at $x_n=na$, i.e., at $\varphi_n=0$. It is found that for large g and R the main contribution to the integral (2) is given by small neighborhoods of similar maxima in different sectors. Taking this into account, we write Ψ_0 in the form

$$\Psi_0(x_0,\ldots,x_{N-1})=\sum_P(\pm1)^P\theta(x_{P(0)}<x_{P(1)}<\ldots<x_{P(N-1)})\times\tilde\psi(x_{P(0)},x_{P(1)},\ldots,x_{P(N-1)}). \qquad (6)$$

The sum is taken over all permutations of the N arguments, and $(-1)^P$ is the parity of the permutation P (here and below, the upper sign refers to bosons, and the lower sign to fermions). The function θ is equal to unity when the inequality indicated in brackets is fulfilled, and equal to zero otherwise. It can be seen from (6) that Ψ_0 possesses the correct symmetry. The function

$$\tilde\psi(x_0,x_1,\ldots,x_{N-1})=\psi(\varphi_0,\varphi_1,\ldots,\varphi_{N-1})=\psi(\varphi)$$

is the wave function in one sector. In Ref. 10 the following representation was obtained for it:

$$|\psi(\varphi)|^2=\int_{-\infty}^{\infty}\prod_p dJ_p\exp\Big\{-\frac12\sum_p J_pD(p)J_{-p}$$
$$+\sum_{n=3}^{\infty}\sum_{p_l}D^{(n)}(p_1\ldots p_n)\tilde\delta\Big(\sum_{k=1}^{n}p_k\Big)\prod_{j=1}^{n}J_{p_j}-ig^{1/2}\sum_pJ_p\varphi_p\Big\}. \qquad (7)$$

The summation over p here, as in (5), is taken over the Brillouin zone form $-\pi$ to π; J_p are auxiliary integration variables; $D(p)$ and $D^{(n)}(p_1\ldots p_n)$ are the exact Green functions $G(p,\omega)$ and $G^{(n)}(p_1,\omega_1;\ldots;p_n,\omega_n)$ of the phonon system with the Lagrangian (5), integrated over the external frequencies with allowance for the conservation laws:

$$D(p)=(2\pi)^{-1}\int_{-\infty}^{\infty}G(p,\omega)\,d\omega,$$

$$D^{(n)}(p_1\ldots p_n)=(2\pi)^{-n+1}\int_{-\infty}^{\infty}\prod_{i=1}^{n}d\omega_i\delta\Big(\sum_{j=1}^{n}\omega_j\Big)G^{(n)}(p_1,\omega_1;\ldots;p_n,\omega_n) \qquad (8)$$

The factor $g^{1/2}$ in the last term in (7) corresponds to the normalization we have used for φ_p.

It can be shown that

$$D(p)=ag(cp)^{-1},\quad p\to0,$$
$$D^{(n)}(p_1,\ldots,p_n)\to\text{const},\quad p_j\to0. \qquad (9)$$

These relations were obtained in Ref. 10. Here c is the exact velocity of sound in the original system with the Hamiltonian (1). It is related to the ground-state energy density ε_0 by the thermodynamic relation

$$c^2=2\rho\partial^2\varepsilon_0/\partial\rho^2.$$

It is convenient to use an abbreviated form of expressions of the type (7), in which we omit the summation symbols and the superscripts and subscripts of $D^{(n)}$ and J_p. In addition, we shall use the path-integration symbol $DJ\equiv\Pi_p\, dJ_p$. The function $\psi(\varphi)$ can be assumed to be real, and therefore (7) can be written in the form

$$\psi^2(\varphi)=\int DJ\exp\left\{-\frac{1}{2}JDJ+\sum_{n=3}^{\infty}D^{(n)}J^n-ig^{1/2}J\varphi\right\}. \qquad (10)$$

However, we shall need not ψ^2 but ψ. The required representation of ψ is most simply obtained from (10) by noting that (9) are the only properties of the coefficient functions D and $D^{(n)}$ that are important for the following. We write ψ in the form

$$\psi(\varphi)=\int DJ\exp\left\{-JDJ+\sum_{n=3}^{\infty}D^{(n)}J^n-ig^{1/2}J\varphi\right\}, \qquad (11)$$

where D and $D^{(n)}$ are certain functions that differ, generally speaking, from the analogous functions in (10) (in order not to encumber the text, we have denoted them by the same symbols). Making use of perturbation theory, we can show in all orders that these new D and $D^{(n)}$ also possess the properties (9) (but, of course, the relations (8) for them are no longer fulfilled).

Thus, (6) and (11) together with (9) are the required representation of the wave function.

4. We now study the calculation of the integral (2). Making use of (6), we can write it entirely in terms of the variables φ_n:

$$S(R)\propto\sum_{k=-N/2}^{N/2}(\pm1)^k\int D\varphi\,\psi(\varphi_0,\varphi_1,\ldots\,\varphi_k,\ldots,\varphi_{N-1})$$
$$\times\psi(\varphi_1+a,\varphi_2+a,\ldots,\varphi_k+a,\varphi_0+R-ka,\varphi_{k+1},\ldots,\varphi_{N-1}). \quad (12)$$

In the second factor all arguments up to the k th are shifted by the lattice constant a and cyclically permuted. For negative values of k the analogous cycle starts from φ_{N-1} and goes to the left. By substituting (11) into this and taking the integral over φ (φ appears linearly in the exponent), we arrive at the following expression, which is more conveniently written in the "coordinate" representation:

$$S(R)\propto\sum_{k=-N/2}^{N/2}(\pm1)^k$$
$$\times\int DJ\exp\left\{-\sum_{n,m=0}^{N-1}J_n[D_{nm}+(U^+DU)_{nm}]J_m\right.$$
$$+\sum_{l=3}^{\infty}\sum_{n_l}^{N-1}D^{(l)}_{n_1\ldots n_l}\prod_{j=1}^{l}J_{n_j}+\sum_{l=3}^{\infty}\sum_{n_l,m_l}^{N-1}D^{(l)}_{m_1\ldots m_l}\prod_{j=1}^{l}U_{m_j n_j}J_{n_j}$$
$$\left.+iag^{1/2}\sum_{n=0}^{k-1}J_n+ig^{1/2}J_k(R-ka)\right\}. \qquad (13)$$

One must take the limit $N\to\infty$ before calculating the sum over k. In (13) J_n are the Fourier components of J_p (see (3)), and D_{nm} is an $N\times N$ matrix:

$$D_{nm}=D_{n-m}=N^{-1/2}\sum_p D(p)\exp[ip(n-m)];$$

the $D^{(l)}_{n_1\ldots n_l}$ are written analogously. We note that D_n is periodic in n with period N. The matrix U_{mn} is an $N\times N$ unitary matrix, which cyclically permutes the first $k+1$ variables: $U_{mn}=\delta_{m-1,n}$ for $0\leqslant m,n\leqslant k$: $U_{mn}=\delta_{mn}$ for $k+1\leqslant m,n\leqslant N-1$; $U_{mn}=0$ in the remaining cases.

In (13) we shall denote $J_k=\mu$, with the aim of integrating first over all the other variables (the path integral in (13) is understood in the perturbation-theory sense). The quadratic form in (13) is transformed to the form

$$-2\mu^2D_0-2\mu\sum_{n=0}^{N-2}(D_{n+1}-D_{k-n-1})-2\mu\sum_{n=0}^{k-1}(D_{k-n}-D_{k-n-1})$$
$$-2\sum_{n,m=0}^{N-2}J_n\tilde{D}_{nm}J_m-\sum_{n,m=0}^{N-2}J_n\Delta_{nm}J_m. \qquad (14)$$

Here the J_n are now the new, relabelled variables, $N-1$ in number; $\tilde{D}$ is the matrix D without the zeroth row and zeroth column. We note that, in view of (9), the quantities D_n are poorly defined, but only their differences D_n-D_m, which do have meaning, appear in the final answer. The matrix Δ_{mn} has the form

$$\begin{aligned}\Delta_{mn}&=D_{1+m-n}-D_{m-n},\quad k\leqslant m\leqslant N-2,\quad 0\leqslant n\leqslant k-1,\\ \Delta_{mn}&=D_{1+n-m}-D_{n-m},\quad k\leqslant n\leqslant N-2,\quad 0\leqslant m\leqslant k-1,\end{aligned} \qquad (15)$$

with $\Delta_{mn}=0$ in the remaining cases.

Unfortunately, we are not able to diagonalize the quadratic form (14) exactly. Nevertheless, it turns out that the asymptotic behavior of $S(R)$ as $R\to\infty$ is determined entirely by the term with $\tilde{D}$, which, obviously, can be diagonalized. Therefore, we shall proceed as follows: We invert the matrix $\tilde{D}$ exactly, and treat the entire remainder (the term with Δ_{mn} and all terms with higher powers of J_n) as a perturbation. After this it will be possible to verify that the perturbation does indeed have no effect on the asymptotic form.

Let W_{mn} be the inverse of the matrix D_{mn}. It is also diagonal in the momentum representation, and, by virture of (9),

$$W(p)=(ag)^{-1}cp,\quad p\to0.$$

Then the inverse of the matrix $\tilde{D}$ is the matrix

$$\tilde{W}_{mn}=W_{m-n}-W_0^{-1}W_{n+1}W_{m+1}.$$

As we shall see soon, the value of the critical index of $S(R)$ is affected only by the terms with large (of the order of R/a) labels in the sum (13). Therefore, in the calculation of each integral in (13) it is necessary to bear in mind that in the answer the only important terms in the exponent will be those which grow with k (in the present case, as $\ln k$), while those which tend to a constant as $k \to \infty$ can be discarded. Of course, the limit $k \to \infty$ has meaning only after $N \to \infty$. Here it turns out that all the terms that increase with k are obtained as a result of taking the Gaussian integral with the quadratic form (14) (without the last term). As regards all the other contributions, by means of the relations (9) and a diagrammatic technique that is obvious from (13) and (14) it is possible to show in all orders of perturbation theory that they remain bounded as $k \to \infty$.

With allowance for these considerations, and having transformed (as $N \to \infty$) the sums over p into integrals, we can represent the result of the calculation of the integrals over J_n in (13) in the form

$$S(R) \propto \sum_{k=-\infty}^{\infty} (\pm 1)^k \int_{-\infty}^{\infty} d\mu \exp\Big\{ ia\xi\mu + i\mu g^{1/2}(R-ka) - a^2 g (16\pi)^{-1} \int_{-\pi}^{\pi} dp\, D^{-1}(p)(1-\cos kp)(1-\cos p)^{-1} - (2\pi)^{-1}\mu^2 \int_{-\pi}^{\pi} dp\, D(p)(1-\cos kp) + \sum_{l=2} V_l \mu^l \Big\},$$

where ξ and V_l are bounded as $k \to \infty$. Next, the analysis of this expression is carried out as in Ref. 10. Namely, the leading (in k) term of the asymptotic form of the integrals over p (the term proportional to $\ln k$) is determined entirely by the behavior of $D(p)$ and $p \to 0$ (9); it can then be shown that the sum is built up in the vicinity of $k_0 = R/a$, and the terms with higher powers of μ do not make a contribution to the critical index. The constant ξ (the limit of ξ as $k \to \infty$) determines the phase of the oscillating term in the asymptotic form. It is clear that one cannot calculate this phase in the framework of the method under consideration, since the anharmonic terms in (13) contribute to it.

We shall write out the final answer separately for bosons and fermions. In the case of Bose statistics the leading term of the asymptotic form does not contain oscillations; we shall give also the next, oscillating term:

$$S_B(R) = A_1 R^{-\beta_B} + A_2 R^{-\beta_B'} \cos(2\pi\rho R + \varphi_B) \quad R \to \infty. \quad (16)$$

In the case of Fermi statistics the leading term does oscillate, and the frequency is half that for bosons:

$$S_F(R) = A R^{-\beta_F} \cos(\pi\rho R + \varphi_F), \quad R \to \infty. \quad (17)$$

In these expressions, A, A_1, and A_2 are constants that do not depend on R; φ_B and φ_F are phases that are also independent of R $(0 \leqslant \varphi_{B,F} \leqslant 2\pi)$. The values of the critical indices are as follows (c is the exact velocity of sound):

$$\beta_B = (4\pi\rho)^{-1} c, \quad (18)$$

$$\beta_B' = (4\pi\rho)^{-1} c + 4\pi\rho c^{-1}, \quad (19)$$

$$\beta_F = (4\pi\rho)^{-1} c + \pi\rho c^{-1}. \quad (20)$$

We note that $\beta_B = \alpha^{-1}$, where $\alpha = 4\pi\rho c^{-1}$ is the critical index of the "density-density" correlator.[10]

5. In conclusion we shall compare our relations (16)–(20) with certain known results for the one-particle density matrix.

In the case of Fermi statistics the index β_F coincides (in the sense of the dependence (20) on c) with the value obtained in Ref. 8, in which a Fermi gas with weak coupling was considered and a perturbation theory in the small g was constructed. Evidently, this implies that formula (20) has a universal character and is valid for all $g > 0$.

It is interesting to compare (16), (18), and (19) with results for the one-dimensional Bose gas with δ-function interaction. Our method does not work for this model, since the potential is short-range, leading to a number of qualitative difference (in particular, in this model the velocity of sound does not increase without limit as g increases, but remains finite at $g = \infty$). Therefore, generally speaking, we cannot expect any coincidences of critical indices. It is all the more interesting that the result obtained in Ref. 11 for the leading term of the long-wavelength asymptotic form of the one-particle Green function in the one-dimensional Bose gas with δ-function interaction coincides with the first term in (16), the exponent being related to the velocity of sound by the same formula (18). As regards the oscillating term in the asymptotic form of the Green function in this model, here only the result for $g = \infty$ is known[12,13]: $\beta_B' = 5/2$. It is easy to show that the velocity of sound for $g = \infty$ is equal to $2\pi\rho$, i.e., the formula (19) is valid. Thus, here too we find agreement that can hardly be accidental and indicates that the relations obtained for the critical indices of the correlation functions actually have a wider range of applicability.

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