Pair distribution function of one-dimensional “hard-sphere” Fermi and Bose systems

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Abstract – The pair distributions of one-dimensional “hard-sphere” fermion and boson systems are exactly evaluated by using gap variables.

\[ D(r) = \rho^{-2}\langle \psi^\dagger(r_1)\psi^\dagger(r_2)\psi(r_2)\psi(r_1) \rangle, \]

where \( \rho = N/L \) is the density. \( D(r) \) is an important physical quantity measurable for many liquid systems. In this formula \( \psi(r) \) is the annihilation operator in \( r \) space.

The pair distribution function \( D(r_{12}) \) is also related to the diagonal elements of the reduced density matrix [15]:

\[ D(r_{12}) = \rho^{-2}\text{Tr}[\psi(r_2)\psi(r_1)\rho_N\psi^\dagger(r_1)\psi^\dagger(r_2)], \]

where \( \rho_N = \Psi_0\Psi_0^\dagger \), and \( \Psi_0 \) is the many-body wave function.

The meaning of \( D(r) \) is as follows: given a particle A at one point, the probability of finding another particle B at a distance \( r \) (counterclockwise) is

\[ \rho D(r)\,dr. \]

It is obvious that \( D(r) \to 1 \) as \( r \to \infty \). Also

\[ \int_0^L \rho D(r)\,dr = N - 1. \]

Fermions with \( a = 0 \).

Wave function \( \Psi \) for fermions with \( a = 0 \). In this case, the fermions are free. Their momenta are \( 2\pi k/L \), where \( k = -(N-1)/2 \) to \( (N-1)/2 \). Here we consider the case that the number of fermions in the system is odd, \( N = 2n + 1 \). The normalized many-body wave function \( \Psi(r_1, r_2, \ldots, r_N) \) of the system is of the form [5]

\[ \Psi = \frac{1}{\sqrt{N!}} \det \begin{pmatrix} \epsilon_1^n & \epsilon_2^n & \ldots & \epsilon_{2n+1}^n \\ \epsilon_1^{n-1} & \epsilon_2^{n-1} & \ldots & \epsilon_{2n+1}^{n-1} \\ \epsilon_1^{n-2} & \epsilon_2^{n-2} & \ldots & \epsilon_{2n+1}^{n-2} \\ \vdots & \vdots & \ddots & \vdots \\ \epsilon_1 & \epsilon_2 & \ldots & \epsilon_{2n+1} \\ \end{pmatrix}, \]

where \( \epsilon_j = \exp(i\frac{2\pi}{L}r_j) \). After some calculations, we arrive at a compact form for the wave function,

\[ \Psi = \frac{1}{\sqrt{N!}} \left( \frac{1}{\sqrt{L}} \right)^N 2^{N(N-1)/2} \prod_{1 \leq i < j \leq N} \sin \left[ \frac{\pi}{L} (r_j - r_i) \right]. \]
The pair distribution function $D(r)$ for free fermions can be exactly obtained from this many-body wave function [4],

$$D(r) = 1 - \frac{\sin^2 \left( \frac{N\pi r}{L} \right)}{N^2 \sin^2 \left( \frac{\pi r}{L} \right)}.$$ \hspace{1cm} (7)

**Gap variables for free fermions.** In order to prepare for dealing with the $a \neq 0$ problem, we introduce gap variables in the case $a = 0$. Consider a region of the $N$-body $L \times L \times \cdots \times L$ coordinate system where, modulo $L$,

$$r_1 \leq r_2 \leq \cdots \leq r_N \leq r_1.$$ \hspace{1cm} (8)

We shall designate this region as $R_1$. In this region, we introduce [16] the gap variables \{$g_i$\}:

$$g_i = r_{i+1} - r_i, \quad i = 1, 2, 3, \ldots, 2n + 1.$$ \hspace{1cm} (9)

Obviously $\sum g_i = L$. With the gap variables the many-body wave function $\Psi$ is given by

$$\Psi = Q[f(g_1)f(g_2) \cdots f(g_{2n+1})]$$

$$\times [f(g_1 + g_2)f(g_2 + g_3) \cdots f(g_{2n+1} + g_1)]$$

$$\times [f(g_1 + g_2 + g_3) \cdots f(g_{2n+1} + g_1 + g_2)]$$

$$\times \cdots$$

$$\times [f(g_1 + \cdots + g_n) \cdots f(g_{2n+1} + g_1 + \cdots + g_{n-1})],$$ \hspace{1cm} (10)

where $f(g) = \sin(\pi g/L)$, and $Q$ is the normalization factor given by

$$Q = \frac{1}{\sqrt{N!}} \left( \frac{1}{\sqrt{L}} \right)^N \left[ 2^{N(N-1)/2} \right].$$ \hspace{1cm} (11)

$\Psi$ has $(2n+1) \times n$ factors in total.

The probability distributions in $R_1$ is

$$|\Psi|^2 dg_1 dg_2 \cdots dg_N \delta \left( \sum_{i=1}^{N} g_i - L \right).$$ \hspace{1cm} (12)

with all $g_i \geq 0$. Now $R_1$ is only one of the $(N-1)!$ regions of the full coordinate space. In each of these regions we have the same gap distribution as (12). Thus, gap distribution probability $dP$ is

$$dP = (N-1)!L|\Psi|^2 dg_1 dg_2 \cdots dg_N \delta \left( \sum_{i=1}^{N} g_i - L \right).$$ \hspace{1cm} (13)

**Functions $F_i(r)$ for free fermions.** We now evaluate the function $D(r)$ of expression (3) using (13). Going from particle A to B, counterclockwise in the cycle of length $L$, as shown in fig. 1, there may be $i$ other particles, with $i = 0, 1, \cdots, (N-2)$. Thus $D(r)$ becomes a sum of partial terms $F_i$,

$$\rho D(r) = \rho[F_0(r) + F_1(r) + \cdots + F_{N-2}(r)],$$ \hspace{1cm} (14)

where

$$\rho F_i(r)dr = \int \delta \left( \sum_{j=1}^{i+1} g_j - r \right) d\rho dr.$$ \hspace{1cm} (15)

Thus,

$$\rho F_i(r) = (N-1)!L \int |\Psi|^2 \delta \left( \sum_{j=1}^{i+1} g_j - r \right)$$

$$\times \delta \left( \sum_{j=i+2}^{N} g_j - (L-r) \right) dg_1 dg_2 \cdots dg_N,$$ \hspace{1cm} (16)

where all $g_j \geq 0$.

Integrating over $dr$ we get, from (15),

$$\int_0^L \rho F_i(r)dr = \int dP = 1.$$ \hspace{1cm} (17)

Thus by (14), $\int \rho D(r)dr = N-1$, confirming (4). Outside of the interval $(0, L)$ we define $F_i(r)$ by

$$F_i(r) = 0 \quad \text{for} \quad r < 0 \quad \text{and} \quad r > L.$$ \hspace{1cm} (18)

In eq. (14), $D(r)$ is a sum of $N-1$ partial terms. The sum in this case of $a = 0$ of course agrees with expression eq. (7) above. But the partial terms will become the key to the evaluation of $D(r)$ in the case $a \neq 0$. Please see eq. (25) below.

Besides (17), $F_i(r)$ has also the following properties:

i) It is analytic except at $r = 0$ and $r = L$, where $F(r)$ and its first derivative are both zero.

ii) $F_i(r) = F_{N-2-i}(L-r)$.

It is obvious from (16) that $NF_i(r)$ is a function of $N$ and $r/L$. In fig. 2 we plot this function vs. $r/L$ for the case $N = 5$. 

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Fermions with \( a > 0 \). – For fermions with \( a > 0 \), the full cyclic coordinate space is again divided into \((N-1)!\) regions, one of which, \( R_1 \), is defined by the cyclic condition (8) modulo \( L \). We introduce gap variables in \( R_1 \) by equations similar to (9):

\[
g_i = r_{i+1} - r_i - a, \quad i = 1, 2, 3, \ldots, (N-1)
\]

and

\[
g_N = r_1 - r_N + L - a.
\]

Obviously

\[
\sum g = L - Na.
\]

The key point is \( \Psi \) in terms of the gap variables \( \{g\} \) is still given by (10), but with

\[
f(g) = \sin(\pi g/\xi)
\]

and

\[
Q = \frac{1}{\sqrt{N}!} \left( \frac{1}{\sqrt{L - Na}} \right)^N [2^{N(N-1)/2}].
\]

Equation (12) now becomes

\[
|\Psi|^2 d g_1 d g_2 \cdots d g_N \delta \left( \sum_{i=1}^N g_i - (L - Na) \right) L,
\]

and (13) becomes

\[
dP = (N-1)!L|\Psi|^2 d g_1 \cdots d g_N \delta \left( \sum_{i=1}^N g_i - (L - Na) \right).\]

The function \( D(r) \) is again, as in (14), a sum of \((N-1)!F\) functions. To illustrate the reasoning we turn to fig. 3 and fig. 4 for the case \( N = 5 \). We have

\[
D(r) = F_0[(r - a) \xi] + F_1[(r - 2a) \xi] + F_2[(r - 3a) \xi] + F_3[(r - 4a) \xi],
\]

where \( \xi = L/(L - Na) \), and \( F_i(r) \) is defined by (16) and (18).

Since \( F_i(r) \) is nonzero only in the open interval \((0, L)\), for \( N = 5 \),

\[
- F_0[(r - a) \xi] \text{ is nonzero only for } a < r < L - 4a,
- F_1[(r - 2a) \xi] \text{ is nonzero only for } 2a < r < L - 3a,
- F_2[(r - 3a) \xi] \text{ is nonzero only for } 3a < r < L - 2a,
- F_3[(r - 4a) \xi] \text{ is nonzero only for } 4a < r < L - a.
\]

In fig. 4 we indicate the regions where \( F_i[(r - (i + 1)a) \xi] \) is nonzero for \( i = 0 \) to 3.

We present in fig. 5 and fig. 6 the function \( D(r) \) for \( N = 5 \), and for several values of \( L/a \).

Returning now to the general case, we conclude:

In the interval \((0, L)\), \( D(r) \) is analytic everywhere except at \((N-1)!\) open circles at \( r = a, 2a, \ldots, (N-1)a, \) and at \((N-1)!\) full circles at \( r = L - a, L - 2a, \ldots, L - (N-1)a \).
Fig. 5: (Color online) The pair distribution function \( D(r) \) as a function of distance \( r \) for \( N = 5 \). The \( N - 1 = 4 \) open circles and the \( N - 1 = 4 \) closed circles are where \( D(r) \) is singular. For case \( a = L/(5+) \), \( ND(r) \) represents four \( \delta \)-functions (not shown).

The pair distribution function is related to the square of the wave function. Thus, for \( a > 0 \),

\[ D_{BE}(r) = D_{FD}(r). \]  

(26)

Additional remarks. – A) For an even number of particles in a periodic ring, the ground state is doubly degenerate. Any combination of the two is

\[ \Psi = \left[ \alpha \exp \left( \frac{i\pi}{L} \sum_{i=1}^{N} r_i \right) + \beta \exp \left( -\frac{i\pi}{L} \sum_{i=1}^{N} r_i \right) \right] \times \prod_{1 \leq i < j \leq N} \sin \left[ \frac{\pi}{L} (r_i - r_j) \right]. \]  

(27)

Thus, the pair distribution function calculation proceeds exactly as above. We present the case of \( N = 4 \) in fig. 7.

B) How about vanishing boundary conditions at the two ends of the 1D space? We label such problems as \( B \), and periodic boundary problems as \( A \). \( B \) problems do not have translational invariance.

Now a \( B \) problem for \( N \) particles in the 1D space of length \( L - a \) is mathematically the same as an \( A \) problem for \( N + 1 \) particles in a ring of circumference \( L \). For example, take a \( B \) problem with \( N = 4 \). Compare it with the \( A \) problem illustrated in fig. 4 above. If we fix \( r_1 \), the remaining 4 particles move in the 1D space of length \( L - a \) with vanishing boundary conditions at the two ends! Thus, our \( A \) problem for pair distribution also solves a \( B \) problem for single-particle distribution. To solve a pair distribution \( B \) problem requires the solution of a 3-particle distribution \( A \) problem.

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