Advanced quantum mechanics
TD 5 : One-body and Two-body Correlation Functions for an Ideal Gas of Fermions at $T = 0$

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Consider a non-interacting gas of N fermions confined into a D-dimensional box of size L with periodic boundary conditions. We assume the system to be at zero temperature ($T = 0$) and the fermions to be all in the same spin state $|\uparrow\rangle$. Let us denote the N single-particle wave functions of lowest energy by $\varphi_1, \ldots, \varphi_N$.

1 N-particle ground state

1. Write the complete state vector and the wave function of the N fermions in first quantization.
2. How do you write the state in second quantization ?
3. What is the maximal momentum p_F accessible to the fermions in 3D ? And in 1D ?

2 One-body observables

Let $\hat{A}$ be a one-body operator acting on a system of N indistinguishable particles :

$$\hat{A} = \sum_{i=1}^{N} \hat{a}_i \ ,$$

where $\hat{a}_i \equiv \mathbb{1}_1 \otimes \mathbb{1}_2 \otimes \ldots \otimes \mathbb{1}_{i-1} \otimes \hat{a} \otimes \mathbb{1}_{i+1} \otimes \ldots \otimes \mathbb{1}_N$ with $\hat{a}$ acting on the state of the i-th particle (so $\hat{a}$ is defined on the single-particle Hilbert space).

4. Calculate the expectation value $\langle \hat{A} \rangle$ of the operator $\hat{A}$ as a function of $\varphi_1, \ldots, \varphi_N$ (first quantization).
5. Now write the one-body operator in second quantized form using an orthonormal basis $\{\varphi_i\}$, and calculate $\langle \Psi | \hat{A} | \Psi \rangle$.
6. The one-body density matrix [1] $\hat{\rho}^{(1)}$ of an N-particle state can be defined as the operator such that for any one-body operator $\hat{A}$ one has :

   $$\langle \hat{A} \rangle = \mathrm{Tr}_1[\hat{\rho}^{(1)} \hat{a}]$$

   with Tr_1 the trace over states of the single-particle Hilbert space. Starting from this definition, obtain an explicit expression of $\hat{\rho}^{(1)}$ as a function of $\varphi_1, \ldots, \varphi_N$.
7. Consider the one-body operator

   $$\sum_{i=1}^{N} |i : \vec{x}\rangle \langle i : \vec{x}| \ , \tag{1}$$

   where, for simplicity, we omit the unity operators acting on all other particles. What does this operator measure ? Calculate its expectation value. Express the operator in second-quantized form.

1. In practice, the terms density matrix and density operator are often used interchangeably.

8. We define the function $g_1(\vec{r}, \vec{r}')$:

$$g_1(\vec{r}, \vec{r}') = \left\langle \sum_{i=1}^{N} |i : \vec{r}\rangle\langle i : \vec{r}'| \right\rangle ,$$

where we have again omitted the unity operators to simplify the notation. Physically, g_1 is the one-body density matrix in position space ; it measures the spatial coherence of the system.

(a) Use the general expression for a one-body observable in second quantization to express the one-body correlation function $g_1(\vec{r}, \vec{r}')$ in a *general* basis $\{\phi_\alpha\}$ of the single-particle Hilbert space.

(b) Now start from this general expression to write g_1 in the basis of position eigenstates $\{|\vec{r}\rangle\}$.

(c) What is the link between $g_1(\vec{r}, \vec{r}')$ and $\hat{\rho}^{(1)}$?

(d) In the thermodynamic limit, calculate explicitly the single-particle correlation function in 1D and in 3D.

3 Two-body observables

Let the operator $\hat{B}$ be an observable involving only two-body operators [2] :

$$\hat{B} = \sum_{i \neq j}^{N} \hat{b}_{i,j},$$

where $\hat{b}_{i,j}$ acts only on the states of the particles i and j and as the identity operator on the other particles.

9. Calculate the expectation value $\langle \hat{B} \rangle$ as a function of $\varphi_1, \ldots, \varphi_N$ (first quantization).

10. Now write the two-body operator in second quantized form using an orthonormal basis $\{\varphi_i\}$. Calculate $\langle \Psi | \hat{B} | \Psi \rangle$ using Wick's theorem.

11. We define the two-body density matrix $\hat{\rho}^{(1,2)}$ such that for any two-body operator $\hat{B} = \sum_{i \neq j} \hat{b}_{i,j}$ one has :

$$\langle \hat{B} \rangle = \mathrm{Tr}_{1,2}[\hat{\rho}^{(1,2)} \hat{b}_{1,2}] = \mathrm{Tr}_{1,2}[\hat{b}_{1,2} \hat{\rho}^{(1,2)}].$$

Express $\hat{\rho}^{(1,2)}$ as a function of $\varphi_1, \ldots, \varphi_N$.

12. The two-body correlation function $g_2(\vec{r}, \vec{r}')$ gives the probability density (up to a normalization factor) of finding a particle at $\vec{r}$ and another at $\vec{r}'$. In first quantization :

$$g_2(\vec{r}, \vec{r}') = \left\langle \sum_{i \neq j}^{N} \hat{b}_{i,j} \right\rangle$$

with

$$\hat{b}_{i,j} = |i : \vec{r}\rangle\langle i : \vec{r}| \otimes |j : \vec{r}'\rangle\langle j : \vec{r}'|$$

acting on the states of particles i and j.

(a) Use the general expression for a two-body observable in second quantization to express the two-body correlation function $g_2(\vec{r}, \vec{r}')$ in a *general* basis $\{\phi_\alpha\}$ of the single-particle Hilbert space.

2. Note that for indistinguishable particles one often adds a factor 1/2 so as not to double count pairs.

(b) Now start from this general expression to write g_2 in the basis of position eigenstates $\{|\vec{r}\rangle\}$.

(c) What is the link between $g_2(\vec{r},\vec{r}')$ and $\hat{\rho}^{(1,2)}$?

(d) Express g_2 as a function of g_1. Note that this is possible because we are dealing with the ideal Fermi gas.

(e) In the thermodynamic limit and considering again the ground-state of the non-interacting system, calculate explicitly $g_2(\vec{r},\vec{r}')$ in 1D then in 3D.

Fig. 1 shows the correlation functions as function of $k_F r$.

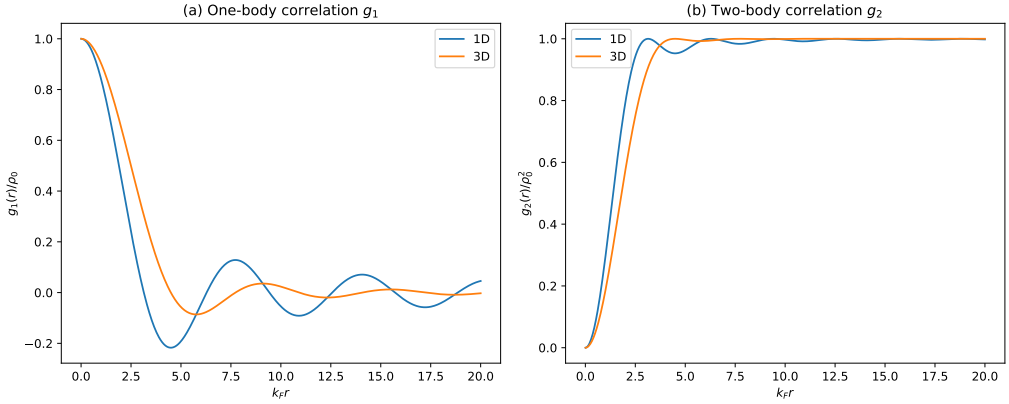


FIGURE 1 – One-body and two-body spatial correlation functions in 1D and 3D for free fermions at $T = 0$.

4 Fluctuation of the number of particles in a spatial interval of length X

Consider a 1D box of length L and a spatial interval of length X along x as represented in Fig. 2. We are interested in the counting statistics of the number of particles in the interval X, which is related to the two-body correlation function $g_2(x)$ calculated above.

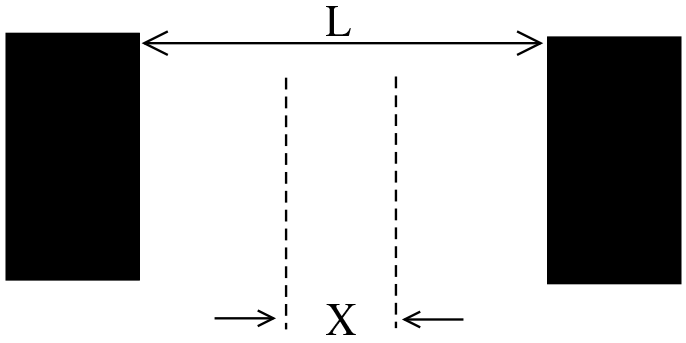


FIGURE 2 – A one-dimensional system (1D) where an interval X is considered.

(a) Let $\hat{N}_X$ be the operator that counts the number of particles inside the interval $[0, X]$. Show that $\left\langle \hat{N}_X^2 \right\rangle = \left\langle \hat{N}_X \right\rangle + \int_0^X dx \int_0^X dx' g_2(x - x')$.

(b) Show that :

$$\int_0^X dx \int_0^X dx' g_2\left(x - x'\right) = 2\left[X \int_0^X dx g_2(x) - \int_0^X dx x g_2(x)\right] \tag{2}$$

To this purpose you can take the derivative of (2) with respect to X.

(c) In the limit where $k_F X \gg 1$ calculate the variance ΔN_X^2, given the following useful relations :

$$\begin{array}{lcll} \int_0^x dt \frac{\sin^2 t}{t^2} & = & \frac{\pi}{2} - \frac{1}{2x} + o\left(\frac{1}{x}\right) & \text{for} \quad x \to \infty \\ \int_0^x dt \frac{\sin^2 t}{t} & \simeq & \frac{1}{2}\ln(2x) + \frac{1}{2}\gamma + o(1) & \text{for} \quad x \to \infty \end{array} \tag{3}$$

where $\gamma = 0.577\ldots$ is Euler's constant. Comment on the result.

(d) (*Bonus*) In the regime of non-zero temperature we have an approximate result for $T \ll T_F$, calculated by Efetov and Larkin (Sov. Phys. JETP 42 (1976), 390) :

$$g_2(x) \simeq n_0^2 - \left(k_F \frac{T}{2T_F} \frac{\sin\left(k_F x\right)}{\sinh\left(\pi T k_F x / 2T_F\right)}\right)^2 \tag{4}$$

Find the condition on T/T_F and on $k_F x$ such that $g_2(x)$ is close to its value at $T = 0$.

(e) (*Bonus*) At $k_F X = 100$, calculate $\left\langle \hat{N}_X \right\rangle, \Delta N_X^2$ and $\Delta N_X^2 / \left\langle \hat{N}_X \right\rangle$.

Evaluate the upper bound of T/T_F such that our equations are valid for this specific value of $k_F X$.