# ICFP M2 Advanced Quantum Mechanics Problem #2: First and second–order spatial correlation functions

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## 1 One–body density matrix

We consider a system of $N$ identical particles (either bosons or fermions) which all share the same spin state. Let $\rho$ be the density operator characterising the system. For instance:

- If the system is in its $N$–particle ground state $|\Psi\rangle$, $\quad \rho = |\Psi\rangle\langle\Psi|$;
- At thermal equilibrium with a fixed number $N$ of particles, $\rho = e^{-\beta H}/\,\mathrm{Tr}(e^{-\beta H})$, where $T = 1/(k_B\beta)$ is the temperature and $H$ is the $N$–particle Hamiltonian.

We introduce the one–body density matrix $\rho^{(1)}$, which is a one–body operator defined as the partial trace of $\rho$ over $N-1$ particles:

$$\langle \boldsymbol{r}|\,\rho^{(1)}\,|\boldsymbol{r}'\rangle = N\,\langle \boldsymbol{r}|\,\mathrm{Tr}_{2,\ldots,N}(\rho)\,|\boldsymbol{r}'\rangle = N\int d^3r_2\ldots d^3r_N\,\langle \boldsymbol{r},\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N|\,\rho\,|\boldsymbol{r}',\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N\rangle\ , \quad (1)$$

and call $g^{(1)}(\boldsymbol{r},\boldsymbol{r}') = \langle \boldsymbol{r}'|\,\rho^{(1)}\,|\boldsymbol{r}\rangle$ the first–order spatial correlation function.

1. Justify that all particles 1, …, $N$ play the same role in Eq. 1.
   Calculate $\mathrm{Tr}(\rho^{(1)})$ and $g^{(1)}(\boldsymbol{r},\boldsymbol{r})$.
2. We consider a one–particle operator $F = \sum_{i=1}^N f^{(i)}$, where $f^{(i)}$ acts on the particle $i$ only. Show that the average value $<F>= \mathrm{Tr}_{1,\ldots,N}(\rho F)$ is given by $<F>= \mathrm{Tr}(\rho^{(1)} f)$.
3. We now choose $F = \sum_{i=1}^N |i:\boldsymbol{r}'\rangle\langle i:\boldsymbol{r}|$. Show that $\langle \boldsymbol{r}|\,\rho^{(1)}\,|\boldsymbol{r}'\rangle = <F>$.
   Hint: For any single–particle operator $A$ and single–particle states $|u\rangle$, $|v\rangle$, $\quad \mathrm{Tr}(A\,|u\rangle\langle v|) = \langle v|\,A\,|u\rangle$.
4. Justify the name given to the function $g^{(1)}(\boldsymbol{r},\boldsymbol{r}')$.
   For a uniform system, justify that $g^{(1)}(|\boldsymbol{r}-\boldsymbol{r}'|)$ depends on the single parameter $|\boldsymbol{r}-\boldsymbol{r}'|$.

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## 2 Two–body density matrix

A natural extension of Eq. (1) is the two–body density matrix $\rho^{(2)}$, which is a two–body operator defined as the partial trace of $\rho$ over $N-2$ particles:

$$\langle \boldsymbol{r}_1, \boldsymbol{r}_2 | \, \rho^{(2)} \, | \boldsymbol{r}'_1, \boldsymbol{r}'_2 \rangle = \langle \boldsymbol{r}_1, \boldsymbol{r}_2 | \, N(N-1) \ \mathrm{Tr}_{3,\ldots,N}(\rho) \, | \boldsymbol{r}'_1, \boldsymbol{r}'_2 \rangle \tag{2}$$

$$= N(N-1) \int d^3r_3 \ldots d^3r_N \ \langle \boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, \ldots, \boldsymbol{r}_N | \, \rho \, | \boldsymbol{r}'_1, \boldsymbol{r}'_2, \boldsymbol{r}_3, \ldots, \boldsymbol{r}_N \rangle \ . \tag{3}$$

The diagonal matrix element $g^{(2)}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \langle \boldsymbol{r}_1, \boldsymbol{r}_2 | \, \rho^{(2)} \, | \boldsymbol{r}_1, \boldsymbol{r}_2 \rangle$ is called the second–order spatial correlation function.

5. We consider a two—particle operator $G = \sum_{i=1}^{N} \sum_{j \neq i} g^{(i,j)}$, where $g^{(i,j)}$ acts on the particles $i$ and $j$ only. Show that $< G >= \mathrm{Tr}_{1,\ldots,N}(\rho G)$ is given by $< G >= \mathrm{Tr}(\rho^{(2)} g)$.

6. We choose $G = \sum_{i=1}^{N} \sum_{j \neq i} |i : \boldsymbol{r}_1, j : \boldsymbol{r}_2\rangle \langle i : \boldsymbol{r}_1, j : \boldsymbol{r}_2|$. Show that $g^{(2)}(\boldsymbol{r}_1, \boldsymbol{r}_2) =< G >$. Justify that $g^{(2)}(\boldsymbol{r}_1, \boldsymbol{r}_2)$ measures the tendency of the atoms to cluster or to stay apart.

## 3 Ideal gases at zero temperature

For Questions 7, 8, and 9, we assume that the gas is ideal, i.e. the identical particles do not interact with each other. Let $h = \boldsymbol{p}^2/(2m) + U(\boldsymbol{r})$ be the single–particle Hamiltonian, and $(|\phi_\alpha\rangle)$ a basis of eigenvectors of $h$, so that $h \, |\phi_\alpha\rangle = \epsilon_\alpha \, |\phi_\alpha\rangle$.

7. Which term in the Hamiltonian pilots the (non)–uniform character of the system? What is its shape for a uniform system? How may one model a non–uniform trapped system? In each of these two cases, what are the basis functions $\phi_\alpha(\boldsymbol{r})$?

8. **For an ideal Bose gas,** what is the ground–state $N$–particle wavefunction?
   Use Eq. (1) to calculate the corresponding one–body density matrix $\rho^{(1)}_{\mathrm{Bose}}$.
   For a uniform gas, show that $\rho^{(1)}_{\mathrm{Bose}} = N/V$, and conclude as to the coherence length.

9. **For an ideal Fermi gas** which is fully polarised (i.e. all particles are in the same spin state), write the ground–state $N$–particle wavefunction as a determinant. Use Eq. (1) to calculate the corresponding one–body density matrix $\rho^{(1)}_{\mathrm{Fermi}}$ in terms of the $(\phi_\alpha(\boldsymbol{r}))$:

$$g^{(1)}_{\mathrm{Fermi}}(\boldsymbol{r}, \boldsymbol{r}') = \sum_{\alpha=1}^{N} \phi^\star_\alpha(\boldsymbol{r}) \phi_\alpha(\boldsymbol{r}') \ . \tag{4}$$

10. For a uniform ideal Fermi gas in 1D at $T = 0$, show that, in the thermodynamic limit:

$$g^{(1)}(x) = (N/L) \ \mathrm{sinc}(k_F x) \ , \tag{5}$$

   with $k_F = \pi \, N/L$ being the Fermi wavevector. What is the coherence length?

11. For a uniform ideal Fermi gas in 3D at $T = 0$, show that, in the thermodynamic limit:

$$g^{(1)}_{\mathrm{Fermi}}(r) = \frac{N}{V} \frac{\sin(k_F r) - k_F r \cos(k_F r)}{(k_F r)^3/3} \ , \tag{6}$$

   with $k_F = (6\pi^2 N/V)^{1/3}$ being the Fermi wavevector. What is the coherence length?

## 4 Second quantisation and calculations at non–zero temperature

The calculation of the operator $\rho^{(1)}$ (or of the function $g^{(1)}(\boldsymbol{r}, \boldsymbol{r'})$) in more general situations is easier if one uses the second quantisation formalism. Hence, we introduce a basis ($|\psi_\alpha\rangle$) of single–particle states, and the corresponding creation and annihilation operators $a^\dagger_\alpha$ and $a_\alpha$.

12. Using Question 3, show that the first–order correlation function reads:

$$g^{(1)}(\boldsymbol{r}, \boldsymbol{r'}) = \langle \boldsymbol{r'} |\, \rho \,| \boldsymbol{r} \rangle \quad = \sum_{\alpha,\beta} < a^\dagger_\beta a_\alpha > \; \psi_\alpha(\boldsymbol{r})\, \psi^*_\beta(\boldsymbol{r'}). \tag{7}$$

13. We introduce the field operator $\Psi(\boldsymbol{r}) = \sum_\alpha \psi_\alpha(\boldsymbol{r})\, a_\alpha$.
Check that Eq. 7 reduces to: $\quad g^{(1)}(\boldsymbol{r}, \boldsymbol{r'}) =< \Psi^\dagger(\boldsymbol{r'})\Psi(\boldsymbol{r}) >$.

14. Using Question 6, show that the second–order correlation function reads:

$$g^{(2)}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \langle \boldsymbol{r}_1, \boldsymbol{r}_2 |\, \rho^{(2)} \,| \boldsymbol{r}_1, \boldsymbol{r}_2 \rangle \sum_{\alpha,\beta,\gamma,\delta} < a^\dagger_\delta a^\dagger_\gamma a_\beta a_\alpha > \; \psi_\alpha(\boldsymbol{r}_1)\psi_\beta(\boldsymbol{r}_2)\psi^*_\gamma(\boldsymbol{r}_2)\psi^*_\delta(\boldsymbol{r}_1)\ . \tag{8}$$

Check that Eq. (8) reduces to: $\quad g^{(2)}(\boldsymbol{r}_1, \boldsymbol{r}_2) =< \Psi^\dagger(\boldsymbol{r}_1)\Psi^\dagger(\boldsymbol{r}_2)\Psi(\boldsymbol{r}_2)\Psi(\boldsymbol{r}_1) >$.

15. **For an ideal gas**, show that, if one chooses the single–particle states to be the eigenstates ($|\phi_\alpha\rangle$) of $h$, the double sum over $\alpha, \beta$ in Eq. 7 reduces to a single sum:

$$g^{(1)}(\boldsymbol{r}, \boldsymbol{r'}) = \sum_\alpha \phi^*_\alpha(\boldsymbol{r'})\phi_\alpha(\boldsymbol{r})\, n_\alpha\ . \tag{9}$$

Express the numbers $n_\alpha$ appearing in the expression for $g^{(1)}$ in terms of averages of creation and annihilation operators. Where does the quantum statistics play a role?

16. **For a uniform ideal gas obeying Boltzmann statistics**,
show that, in the thermodynamic limit:

$$\rho^{(1)}_{\text{classical}}(r) = \frac{N}{V} \exp(-\pi r^2/\Lambda_T^2)\ , \tag{10}$$

where $\Lambda_T = [h^2/(2\pi m k_B T)]^{1/2}$ is the thermal de Broglie wavelength. Conclude as to the coherence length. How does it compare to the mean particle spacing?
Hint: First, show that the occupation numbers are $n_\alpha = N\Lambda_T^3/V\ \exp(-\beta E)$, with $E = \hbar^2 k^2/(2m)$.

17. Using your answers to Questions 8 and 16, explain why Bose–Einstein condensation is also called 'off–diagonal long–range order'.

## 5 Interacting systems

Finally, we relax the ideal–gas hypothesis. The $N$–particle Hamiltonian now reads:

$$H = \sum_{n=1}^{N} \left[ \frac{\boldsymbol{p}_n^2}{2m} + U(\boldsymbol{r}_n) \right] + \sum_{n=1}^{N} \sum_{m=1}^{n-1} V(\boldsymbol{r}_n - \boldsymbol{r}_m)\ . \tag{11}$$

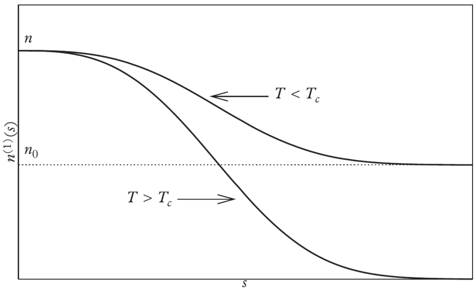


**Figure 1** One–body density matrix $g^{(1)}(s)$ for a uniform Bose gas, as a function of the distance $s = |\boldsymbol{r}_2 - \boldsymbol{r}_1|$. Reproduced from Ref. [1, chap. 2].

18. What does the term $V(\boldsymbol{r}_n - \boldsymbol{r}_m)$ appearing in Eq. 11 represent? Explain the bounds on the double sum over $n$ and $m$. How does $V$ depend on $\boldsymbol{r}$ *(i)* for neutral particles carrying no dipole moment? *(ii)* for neutral dipolar particles? *(iii)* for charged ions?

19. Construct a basis $(\phi_\alpha)$ of single–particle wavefunctions onto which the function $g^{(1)}(\boldsymbol{r}_1, \boldsymbol{r}_2)$ expands as in Eq. (9), that is, with a *single sum* over the index $\alpha$.
    HINT: First, justify that $\rho^{(1)}$ is a hermitian linear operator.

20. The ideal gas model of questions 8 and 16 describes weakly–interacting Bose gases. Which other quantum system also exhibits off–diagonal long–range order? What is its key difference with respect to the model studied in this section?

## Further reading

INTRODUCTORY

- The density matrix is defined and reviewed in Ref. [2, Appendix D].
- An accessible introduction to identical particles in Quantum Mechanics may be found in Ref. [3, chap. 4].
- The properties of quantum gases are reviewed in Ref. [4], chapters 8, 11 (fermions), and 12 (bosons).
- The correlation functions $g^{(1)}$ and $g^{(2)}$ are defined in an elementary way in Ref. [5, §23.2].
- Section 20.4 of Ref. [6] provides an introduction to the Poisson distribution applied to classical gases.

MORE ADVANCED

- The one–body and two–body density matrices are defined in Ref. [1, chap. 2]. This chapter also contains an introduction to off–diagonal long–range order in the context of Bose–Einstein condensation.
- The correlation functions $g^{(1)}$ and $g^{(2)}$ for Fermi gases are analysed in Ref. [7, §1.2 & §1.3].

## References

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