ICFP M2 Advanced Quantum Mechanics: Problem set #2: Spatial Correlations

Solution

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1 Reminders on the density matrix and the partial trace

1.1 Partial trace

We first consider one single Hilbert space $\mathscr{E}_A$. Let $(|a_i\rangle)$ be a basis of $\mathscr{E}_A$. We are interested in the vector space $\mathscr{L}(\mathscr{E}_A)$ of linear operators that map $\mathscr{E}_A$ onto itself. The set of operators $(|a_i\rangle\langle a_j|)$ is a basis of $\mathscr{L}(\mathscr{E}_A)$. This basis has a simple interpretation, at least if the dimension of $\mathscr{E}_A$ is finite. Any linear operator M in $\mathscr{L}(\mathscr{E}_A)$ may be expanded as $M = \sum_{i,j} m_{ij} |a_i\rangle\langle a_j|$. Then, the coefficient m_{ij} is the coefficient on the i^{th} line and j^{th} column of the usual matrix representation of M in the basis $(|a_i\rangle)$. The trace of M is defined, as usual, as:

$$\mathrm{Tr}(M) = \sum_i \langle a_i| M |a_i\rangle \ . \tag{1}$$

Next, we consider two Hilbert spaces $\mathscr{E}_A$ and $\mathscr{E}_B$. In the language of quantum information, $\mathscr{E}_A$ and $\mathscr{E}_B$ represent the degrees of freedom accessible to Alice and Bob, respectively. We introduce the joint Hilbert space $\mathscr{E} = \mathscr{E}_A \otimes \mathscr{E}_B$. We are interested in the vector space $\mathscr{L}(\mathscr{E})$ of linear operators that map $\mathscr{E}$ onto itself. Among all the linear operators acting on $\mathscr{E}$, some may be written as $M = M_A \otimes M_B$, where M_A is a linear operator on $\mathscr{E}_A$ and M_B is a linear operator on $\mathscr{E}_B$. For these linear operators, we define the partial trace over $\mathscr{E}_B$ as follows:

$$\begin{array}{cccc} \mathrm{Tr}_B & : & \mathscr{L}(\mathscr{E}) & \to & \mathscr{L}(\mathscr{E}_{\mathscr{A}}) \\ & & M_A \otimes M_B & \mapsto & \mathrm{Tr}_B(M_A \otimes M_B) = \mathrm{Tr}(M_B)\, M_A \ . \end{array} \tag{2}$$

In Eq. (2), the input $M_A \otimes M_B$ is a linear operator acting on $\mathscr{E}$, the quantity $\mathrm{Tr}(M_B)$ is the usual trace of the operator M_B (i.e. a number), and the output $\mathrm{Tr}_B(M_A \otimes M_B)$ is a linear operator acting on $\mathscr{E}_A$. Equation (3) shows, in particular, that the partial trace Tr_B does not depend on any choice of bases for $\mathscr{E}_A$ or for $\mathscr{E}_B$.

Any linear operator acting on $\mathscr{E}$ may be written as a linear combination of operators of the form $M_A \otimes M_B$. Indeed, let $(|a_i\rangle)$ be a basis of $\mathscr{E}_A$ and $(|b_j\rangle)$ a basis of $\mathscr{E}_B$, so that $(|a_i\rangle \otimes |b_j\rangle)$ is a basis of $\mathscr{E}$. Then, the set $(|a_i\rangle\langle a_{i'}| \otimes |b_j\rangle\langle b_{j'}|)$ is a basis of $\mathscr{L}(\mathscr{E})$ whose elements have the required form. Therefore, we may extend the definition of the partial trace Tr_B to all linear operators acting on $\mathscr{E}$ by enforcing its linearity. Then, for any linear operator M acting on $\mathscr{E}$:

$$\mathrm{Tr}(M) = \mathrm{Tr}_A[\mathrm{Tr}_B(M)], \tag{3}$$

i.e. the complete trace (which is a number) may be obtained by first taking the partial trace along $\mathscr{E}_B$, so as to get an operator acting on $\mathscr{E}_A$, and then taking the trace along $\mathscr{E}_A$.

1.2 Reduced density matrix

We assume that Alice and Bob have prepared a joint quantum state determined by the density matrix ρ, which is a linear operator on the joint state $\mathscr{E} = \mathscr{E}_A \otimes \mathscr{E}_B$. Then, Alice and Bob have travelled to different locations that are spatially separated, and they may no longer communicate. Alice has kept her part of the system, described by the Hilbert space $\mathscr{E}_A$, and Bob has kept his, described by the Hilbert space $\mathscr{E}_B$. *Making a distinction between Alice's and Bob's subsystems entails that they are distinguishable.* We shall turn to identical particles starting from Sec. 2.

Alice may acquire information on the state ρ only by performing measurements on her part of the system. These measurements may be described by averages of local operators, i.e. operators which act only on $\mathscr{E}_A$ while leaving the component along $\mathscr{E}_B$ unchanged. In terms of tensor products, these operators read $M_A = M_A \otimes \mathbb{1}_B$. Let us calculate the average value of M_A in the state ρ:

$$\langle M_A \otimes \mathbb{1}_B \rangle = \mathrm{Tr}\left[\rho \left(M_A \otimes \mathbb{1}_B\right)\right] . \tag{4}$$

We wish to show that the average in Eq. (4) depends not on the full density matrix ρ, but rather on a simpler operator, the reduced density matrix ρ_A, which may be deduced from ρ but contains less information than ρ. The operator ρ_A acts on the Hilbert space $\mathscr{E}_A$ (rather than on the larger Hilbert space $\mathscr{E}$), and it gives the average of any local observable $M_A \otimes \mathbb{1}$ through the relation:

$$\langle M_A \otimes \mathbb{1}_B \rangle = \mathrm{Tr}_A(\rho_A \, M_A) . \tag{5}$$

In Eq. (5), ρ_A depends only on ρ and is independent of the considered local operator $M_A \otimes \mathbb{1}_A$.

In order to construct ρ_A, we expand ρ as a sum of tensor products of the following form:

$$\rho = \sum_{i,i',j,j'} \rho_{ii'jj'} \; |a_i\rangle \langle a_{i'}| \otimes |b_j\rangle \langle b_{j'}| \quad = \sum_{jj'} \rho^A_{jj'} \otimes |b_j\rangle \langle b_{j'}| \; . \tag{6}$$

In Eq. (6), the coefficients $\rho_{ii'jj'}$ are numbers, and the first equality follows from $(|a_i\rangle \langle a_{i'}| \otimes |b_j\rangle \langle b_{j'}|)$ being a basis of $\mathscr{L}(\mathscr{E})$. The second equality follows from collecting all terms which contain $|b_j\rangle \langle b_{j'}|$. Hence, the $\rho^A_{jj'}$ are linear operators acting on $\mathscr{E}_A$ defined as:

$$\rho^A_{jj'} = \sum_{ii'} \rho_{ii'jj'} \; |a_i\rangle \langle a_{i'}| \; . \tag{7}$$

We replace Eq. (6) into Eq. (4) to get:

$$\langle M_A \rangle = \sum_{jj'} \mathrm{Tr}\left[\left(\rho^A_{jj'} \otimes |b_j\rangle \langle b'_j|\right) \left(M_A \otimes \mathbb{1}_B\right)\right] = \sum_{jj'} \mathrm{Tr}\left[\left(\rho^A_{jj'} M_A\right) \otimes \left(|b_j\rangle \langle b_{j'}|\right)\right] \; , \tag{8}$$

where the second equality follows from the identity $(S_A \otimes S_B)(T_A \otimes T_B) = (S_A T_A) \otimes (S_B T_B)$.

Next, we take the trace in two steps: first over $\mathscr{E}_{\mathscr{B}}$ and then over $\mathscr{E}_{\mathscr{A}}$, i.e. we use Eq. (3). The quantity $\mathrm{Tr}_B(|b_j\rangle \langle b_{j'}|) = \delta_{jj'}$, with δ_{ij} being the Kronecker symbol, and Eq. (8) reduces to:

$$\langle M_A \rangle = \sum_j \mathrm{Tr}\left(\rho^A_{jj} \, M_A\right) \; . \tag{9}$$

In Eq. (9), both operators inside the trace are linear operators acting on $\mathscr{E}_A$. Finally, we recognise the partial trace $\mathrm{Tr}_B(\rho) = \sum_j \rho^A_{jj}$, as can be seen from the right–hand side of Eq. (6). Thus, the average of the local operator $M_A \otimes \mathbb{1}_A$ satisfies Eq. (5), the operator ρ_A being defined as:

$$\rho_A = \mathrm{Tr}_B(\rho) \; . \tag{10}$$

Equations (5) and (10) are the key results of this section. They show that, by performing measurements on her side of the system (that is to say, by acting on the space $\mathscr{E}_A$ only), Alice cannot access all the information concerning the quantum state ρ. The results of all of her local measurements are piloted by the reduced density matrix ρ_A. Unlike the complete density operator ρ, which is a linear operator acting on the joint Hilbert space $\mathscr{E}$, the reduced density matrix acts on the smaller Hilbert space $\mathscr{E}_A$ encoding the degrees of liberty accessible to Alice. Taking the partial trace over $\mathscr{E}_B$ results in a loss of information on the system. We illustrate this in Sec. 1.3 on an example from quantum information.

1.3 An example from quantum information

We consider the case where the two Hilbert spaces $\mathscr{E}_A$ and $\mathscr{E}_B$ both represent a spin–1/2. We introduce the four Bell states[1], which are (maximally) entangled states of the two particles [1, § 1.3.6]:

$$|\Phi_\pm\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_A |\uparrow\rangle_B \pm |\downarrow\rangle_A |\downarrow\rangle_B\right) , \qquad |\Psi_\pm\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_A |\downarrow\rangle_B \pm |\downarrow\rangle_A |\uparrow\rangle_B\right) \ . \tag{11}$$

We construct the density matrix $\rho = |\Phi_+\rangle\langle\Phi_+|$ corresponding to the pure state $|\Phi_+\rangle$:

$$\rho = |\Phi_+\rangle\langle\Phi_+| = \ \frac{1}{2}\left(|\uparrow\rangle_A |\uparrow\rangle_B + |\downarrow\rangle_A |\downarrow\rangle_B\right)\left(\langle\uparrow|_A \langle\uparrow|_B + \langle\downarrow|_A \langle\downarrow|_B\right) \ . \tag{12}$$

Expanding the product on the right–hand side of Eq. (12), we are left with linear combinations of the four operators $|\uparrow\rangle_A |\uparrow\rangle_B \langle\uparrow|_A \langle\uparrow|_B$, $|\uparrow\rangle_A |\uparrow\rangle_B \langle\downarrow|_A \langle\downarrow|_B$, $|\downarrow\rangle_A |\downarrow\rangle_B \langle\uparrow|_A \langle\uparrow|_B$, $|\downarrow\rangle_A |\downarrow\rangle_B \langle\downarrow|_A \langle\downarrow|_B$. Each of these operators is of the form $M_A \otimes M_B$ (for instance, $|\uparrow\rangle_A |\uparrow\rangle_B \langle\uparrow|_A \langle\uparrow|_B = |\uparrow\rangle_A \langle\uparrow|_A \otimes |\uparrow\rangle_B \langle\uparrow|_B$), hence, we may directly apply Equation (2). We find:

- $\mathrm{Tr}_B(|\uparrow\rangle_A |\uparrow\rangle_B \langle\uparrow|_A \langle\uparrow|_B) = |\uparrow\rangle_A \langle\uparrow|_A$;
- $\mathrm{Tr}_B(|\uparrow\rangle_A |\uparrow\rangle_B \langle\downarrow|_A \langle\downarrow|_B) = \mathrm{Tr}_B(|\downarrow\rangle_A |\downarrow\rangle_B \langle\uparrow|_A \langle\uparrow|_B) = 0$;
- $\mathrm{Tr}_B(|\downarrow\rangle_A |\downarrow\rangle_B \langle\downarrow|_A \langle\downarrow|_B) = |\downarrow\rangle_A \langle\downarrow|_A$.

Thus, the reduced density matrix ρ_A reads:

$$\rho_A = \mathrm{Tr}_B\, \rho = \frac{1}{2}\left(|\uparrow\rangle_A \langle\uparrow|_A + |\downarrow\rangle_A \langle\downarrow|_A\right) \ . \tag{13}$$

Equation (13) shows that, if Alice does not communicate with Bob, the information she may obtain by local measurements on her side of the system does not allow her to distinguish it from a (non coherent) statistical mixture of $|\uparrow\rangle_A$ and $|\downarrow\rangle_A$. Similar calculations show that any of the four Bell states $|\Phi_\pm\rangle$, $|\Psi_\pm\rangle$, would lead to the same reduced density matrix ρ_A given by Eq. (13), which confirms that taking the partial trace along $\mathscr{E}_B$ leads to an important loss of information.

2 Questions 1–4: 1–body density matrix for identical particles

2.1 Invariance of the density operator under particle exchange

We now consider a system of identical particles. The quantum states accessible to one of these particles make up the single–particle Hilbert space $\mathscr{E}$. For now, we use the first quantisation formalism (we shall turn to second quantisation below). Hence, the considered system consists of a fixed number N of particles. The acceptable N–particle wavefunctions $|\Psi\rangle$ are the normalised (anti–)symmetric elements in the N–particle Hilbert space $\mathscr{E}_N = \mathscr{E}^{(1)} \otimes \mathscr{E}^{(2)} \ldots \otimes \mathscr{E}^{(N)}$, where the Hilbert space $\mathscr{E}^{(j)}$ pertains to particle j.

The density matrix describing a pure state $|\Psi\rangle$ is $\rho = |\Psi\rangle\langle\Psi|$. In the basis of spatial positions, this linear operator acting on $\mathscr{E}_N$ is characterised by the matrix elements $\langle \boldsymbol{r}_1, \ldots, \boldsymbol{r}_N|\rho|\boldsymbol{r}'_1, \ldots \boldsymbol{r}'_N\rangle$. Exchanging particles 1, …, N amounts to applying *the same permutation* σ *both on the bra and on the ket of this matrix element*, i.e. to considering $\langle \boldsymbol{r}_{\sigma(1)}, \ldots, \boldsymbol{r}_{\sigma(N)}|\rho|\boldsymbol{r}'_{\sigma(1)}, \ldots \boldsymbol{r}'_{\sigma(N)}\rangle$. Therefore, *both for bosons and for fermions, the density matrix is symmetric* under particle exchange:

$$\text{For any permutation } \sigma,\ \langle \boldsymbol{r}_{\sigma(1)}, \ldots, \boldsymbol{r}_{\sigma(N)}|\rho|\boldsymbol{r}'_{\sigma(1)}, \ldots \boldsymbol{r}'_{\sigma(N)}\rangle = \langle \boldsymbol{r}_1, \ldots, \boldsymbol{r}_N|\rho|\boldsymbol{r}'_1, \ldots \boldsymbol{r}'_N\rangle \ . \tag{14}$$

Equation (14) may be established by writing ρ as a statistical mixture of pure states: $\rho = \sum_i p_i |\Psi_i\rangle\langle\Psi_i|$. For bosons, the states $|\Psi_i\rangle$ are symmetric, and so are the operators $|\Psi_i\rangle\langle\Psi_i|$.

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[1] These are the four states that maximally violate Bell's inequalities, signalling that Quantum Mechanics may not be formulated in terms of local hidden variables.

For fermions, the states $|\Psi_i\rangle$ are antisymmetric, so that exchanging the particles according to the permutation σ replaces $|\Psi_i\rangle$ by $(-)^\sigma |\Psi_i\rangle$ and $\langle\Psi_i|$ by $(-)^\sigma \langle\Psi_i|$, hence, the operator $|\Psi_i\rangle\langle\Psi_i|$ is symmetric. In both cases, ρ is a sum of symmetric operators, so that it is symmetric.

Finally, we cast Eq. (14) into an algebraic relation involving operators only (ie. without any bras or kets). For that purpose, for any permutation σ, we introduce the *permutation operator* P_σ. In order to define P_σ, it is sufficient to specify its action by defining its action on the N–particle product states $|u_1\rangle\otimes|u_2\rangle\otimes\cdots\otimes|u_N\rangle$, with the $|u_i\rangle$'s being single–particle states (all many–particle states may be written as linear combinations of such product states). The convention used at ICFP (J. Dalibard and Y. Castin's lecture notes, F. Chevy's slides, ...) is the following[2]:

$$P_\sigma |u_1\rangle \otimes |u_2\rangle \otimes \cdots \otimes |u_N\rangle \quad = \quad |u_{\sigma(1)}\rangle \otimes |u_{\sigma(2)}\rangle \otimes \cdots \otimes |u_{\sigma(N)}\rangle \ . \tag{15}$$

Thanks to Eq. (15), Eq. (14) reduces to:

$$\text{For any permutation } \sigma, \quad P_\sigma^\dagger \, \rho \, P_\sigma = \rho \ . \tag{16}$$

Permutation operators P_σ are unitary, so that $P_\sigma^\dagger = P_\sigma^{-1}$, and Eq. (16) also means that the density operator ρ commutes with all permutation operators P_σ.

2.2 Single–particle operators and one–body density matrix

We consider a single–particle operator f acting on the single–particle subspace $\mathscr{E}$. We extend f to the N–particle Hilbert space $\mathscr{E}_N$ by defining the operator F as follows:

$$F = \sum_{i=1}^{N} f^{(i)} \quad = \quad \sum_{i=1}^{N} \mathbb{1}^{(1)} \otimes \ldots \otimes \mathbb{1}^{(i-1)} \otimes f^{(i)} \otimes \mathbb{1}^{(i+1)} \otimes \ldots \otimes \mathbb{1}^{(N)} \ . \tag{17}$$

The operator F defined by Eq. (17) is symmetric with respect to the N particles. In the term of index i in the sum, $f^{(i)}$ acts only on the particle i and all other particles are unaffected.

We wish to calculate the average $\langle F\rangle = \mathrm{Tr}(\rho F)$ of a single–particle F. Just as in the two–subspace case of Sec. 1.2, it is not necessary to know the full density matrix ρ to calculate such an average. We shall show that the averages of all single–particle operators are piloted by a single operator which is much simpler than ρ, and which plays a role similar to that of the reduced density matrix of Sec. 1.2. This operator is the one–body density matrix $\rho^{(1)}$, it acts on the single–particle Hilbert space $\mathscr{E}$, and gives the averages of all one–particle operators throgh the relation (compare with Eq. (5) above):

$$\langle F\rangle = \mathrm{Tr}(\rho^{(1)} f) \ . \tag{18}$$

In Eq. (18), the left–hand side involves the average of an operator acting on the N–particle Hilbert space $\mathscr{E}_N$. However, the right–hand side only involves operators acting on the single–particle Hilbert space $\mathscr{E}$, and the trace $\mathrm{Tr} = \mathrm{Tr}_{\mathscr{E}}$ is taken over that (much smaller) Hilbert space.

In order to construct $\rho^{(1)}$, we start from the general expression for the average of F in terms of ρ, $\langle F\rangle = \mathrm{Tr}(F\rho)$, and use Eq. (17) to obtain:

$$\langle F\rangle = \mathrm{Tr}\left[\rho\left(\sum_{i=1}^{N} f^{(i)}\right)\right] = \sum_{i=1}^{N} \mathrm{Tr}(\rho\, f^{(i)}) \ . \tag{19}$$

Exploiting the symmetry of ρ under particle exchange. We first note that the operator $f^{(i)}$, acting only on particle (i), satisfies $f^{(i)} = P_\sigma^\dagger f^{(1)} P_\sigma$ for any permutation σ such that $\sigma(1) = i$

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[2] Cohen–Tannoudji, Diu, and Laloë [2] use the opposite convention $P_\sigma^{\mathrm{CDL}} = P_\sigma^{-1}$(see their Eq. XIV.B.38).

(simply check that all matrix elements of $f^{(i)}$ and $P_\sigma^\dagger f^{(1)} P_\sigma$ in a basis involving product states $|u_1\rangle \otimes |u_2\rangle \otimes \cdots |u_N\rangle$ coincide). Then:

$$\begin{aligned}
\mathrm{Tr}(\rho\, f^{(i)}) &= \mathrm{Tr}(\rho\, P_\sigma^\dagger f^{(1)} P_\sigma) \\
&= \mathrm{Tr}(P_\sigma \rho P_\sigma^\dagger\, f^{(1)}) \\
&= \mathrm{Tr}(P_{\sigma^{-1}}^\dagger \rho P_{\sigma^{-1}}\, f^{(1)}) \\
&= \mathrm{Tr}(\rho\, f^{(1)}) \ .
\end{aligned} \tag{20}$$

In Eq. (20), the second step follows from $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$, valid for any operators A and B. The third step combines the unitarity of permutation operators, $P_\sigma^\dagger = P_\sigma^{-1}$, with the property[3] $P_\sigma P_{\sigma'} = P_{\sigma' \circ \sigma}$ applied with $\sigma' = \sigma^{-1}$. The final step follows from Eq. (16). Hence, the symmetry of ρ with respect to particle exchange entails that all N terms in the sum of Eq. (19) are equal.

Construction of $\rho^{(1)}$. We now apply Eq. (3) to perform the trace in Eq. (20) in two steps: first over the Hilbert space $\mathscr{E}^{(2)} \otimes \ldots \otimes \mathscr{E}^{(N)}$ (denoted by $\mathrm{Tr}_{2\ldots N}$), and then over the remaining Hilbert space $\mathscr{E}^{(1)}$ (denoted by Tr_1). This yields:

$$\langle F \rangle = \mathrm{Tr}_1 \left[\mathrm{Tr}_{2\ldots N} \left(\rho f^{(1)} \right) \right] = \mathrm{Tr}_1 \left[\left(N\, \mathrm{Tr}_{2\ldots N}\, \rho \right) f^{(1)} \right] \ , \tag{21}$$

where the final step follows from the fact that $f^{(1)}$ acts only on the space $\mathscr{E}^{(1)}$.

Equation (21) confirms that we have constructed the one–body density matrix $\rho^{(1)}$, which reads:

$$\rho^{(1)} = N\ \mathrm{Tr}_{2\ldots N}[\rho] \ . \tag{22}$$

The averages of all one–particle observables F may now be calculated thanks to Eq. (22), i.e. using linear operators which act on the single–particle Hilbert space $\mathscr{E}$ only. The Hilbert space $\mathscr{E}$ is considerably smaller than the N–particle Hilbert space $\mathscr{E}_N$, hence, using the one–body density matrix $\rho^{(1)}$ (rather than the full density matrix ρ) strongly reduces the complexity of the calculations. This simplification helps in numerical problems, where $\rho^{(1)}$ is calculated only once and then yields all one–body averages. It also helps conceptually, because it allows us to think about the N–particle system in terms of one–particle "wavefunctions". A famous example is the case of a Bose–condensed system: in this particular case, $\langle \boldsymbol{r}|\, \rho^{(1)}\, |\boldsymbol{r}'\rangle = \psi_0(\boldsymbol{r})\, \psi_0^*(\boldsymbol{r}')$, where the condensate wavefunction $\psi_0(\boldsymbol{r})$ satisfies the Gross–Pitaevskii equation. Hence, we have replaced the interacting N–particle problem, described by an N–particle wavefunction which obeys the (linear) Schrödinger equation, by a single–particle wavefunction which obeys a (non–linear) equation.

Equation (22) is very similar to Eq. (13) above, with the important difference that there is an extra factor of N on the right–hand side. Hence, the diagonal matrix elements of $\rho^{(1)}$ give the density $n(\boldsymbol{r})$, and $\rho^{(1)}$ is normalised to the total number of particles:

$$\langle \boldsymbol{r}|\, \rho^{(1)}\, |\boldsymbol{r}\rangle = n(\boldsymbol{r}) \quad \text{and} \quad \mathrm{Tr}(\rho^{(1)}) = \int d^3r\ \langle \boldsymbol{r}|\, \rho^{(1)}\, |\boldsymbol{r}\rangle = N \ . \tag{23}$$

2.3 First–order spatial correlations

We now justify that the matrix element $\langle \boldsymbol{r}|\rho^{(1)}\rangle\, |\boldsymbol{r}'\rangle$ gives information about the spatial coherence of the system between the two points $\boldsymbol{r}$ and $\boldsymbol{r}'$. Spatial coherence is a notion that does not rely on the presence of identical particles: it is still meaningful even if the system consists of a single particle. A typical way to probe it is to perform an interference measurement related to Young's double slit setup, i.e. a first–order interference experiment. For this reason, spatial coherence is also called "first–order spatial correlation".

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[3] Note the opposite orderings of σ and σ' on either sign of the equal sign.

In order to make the link between $\langle \boldsymbol{r}|\rho^{(1)}\rangle\,|\boldsymbol{r}'\rangle$ and spatial coherence explicit, we apply Eq. (18) to the specific case where the single–particle operator F corresponds to $f = |\boldsymbol{r'}\rangle\,\langle \boldsymbol{r}|$. We find:

$$\langle F\rangle = \quad \sum_{i=1}^{N} \langle\, |i:\boldsymbol{r'}\rangle\,\langle i:\boldsymbol{r}|\,\rangle \quad = \quad \langle \boldsymbol{r}|\rho^{(1)}|\boldsymbol{r'}\rangle \ , \tag{24}$$

where the last step follows from the property $\mathrm{Tr}(A\,|u\rangle\,\langle v|) = \langle u|A|v\rangle$ which holds for all linear operators A and kets $|u\rangle$, $|v\rangle$.

Let us first consider the case of a single particle in a pure state: $\rho = \rho^{(1)} = |\psi\rangle\,\langle\psi|$. The wavefunction $\psi(\boldsymbol{r})$ may be thought of as a wavepacket with the spatial extent σ. Then, the average $\langle \boldsymbol{r}|\rho^{(1)}|\boldsymbol{r'}\rangle = \psi(\boldsymbol{r})\psi^*(\boldsymbol{r'})$ may be non–zero only if $|\boldsymbol{r}-\boldsymbol{r'}| < \sigma$, which does correspond to the usual definition of spatial coherence for a pure state. If the single particle is prepared in a statistical mixture $\rho = \rho^{(1)}$, then, for $\boldsymbol{r} \neq \boldsymbol{r}'$, the average being non–zero signals that the off–diagonal matrix element of ρ between $\boldsymbol{r}$ and $\boldsymbol{r}'$ is non–zero, which is the standard criterion for coherence in a statistical mixture. Equation (24) generalises this criterion to the case of N identical particles: the state ρ exhibits spatial coherence between the points at $\boldsymbol{r}$ and $\boldsymbol{r}'$ if the process which consists in destroying a particle at $\boldsymbol{r}$ and creating one at $\boldsymbol{r}'$ has a non–zero expectation value.

3 Ideal gases in their ground state (zero temperature)

In this section, we consider ideal quantum gases in the absence of any external electric or magnetic field). The single–particle Hamiltonian reads:

$$h = \frac{\boldsymbol{p^2}}{2m} + U(\boldsymbol{r}) \ . \tag{25}$$

The term $U(\boldsymbol{r})$ is the trapping potential, which acts on each particle in the system individually (this is *not* an interaction term).

3.1 Question 7: Different types of trapping potentials

In the context of cold quantum gases, three types of trapping potentials are routinely considered:

1. *Harmonic traps.* In this case, $U(\boldsymbol{r}) = m(\omega_1^2x^2 + \omega_2^2y^2 + \omega_3^2z^2)/2$. This type of trap may be obtained experimentally through various means: it corresponds to the generic behaviour of a function $U(\boldsymbol{r})$ near a minimum. If the three frequencies $(\omega_i)_{1\leq i\leq 3}$ are equal, the trap is isotropic and the system is rotationally invariant in 3D. If $\omega_3 \gg \omega_{1,2}$, the system is effectively 2D, and may be used to probe e.g. the Berezinskii–Kosterlitz–Thouless crossover. If $\omega_{2,3} \gg \omega_1$, the system is effectively 1D and may be used to probe e.g. the role of integrability.

2. *Box traps.* Here, $U(\boldsymbol{r}) = 0$ inside some large volume V, and $U(\boldsymbol{r}) = +\infty$ outside this volume. Then, the system is uniform inside V and the role of the trapping potential is minimal. This may be achieved experimentally in 3D using a Digital Micromirror Device (DMD), which is very similar to the one used in videoprojectors. In 2D, other techniques are available, such as the projection onto the atomic sample of the image of a suitable mask. This trapping geometry has been used to investigate e.g. the condensation dynamics of an ideal Bose gas, as well as the propagation of sound in a weakly–interacting Bose gas.

3. *Optical lattices.* Here, the potential $U(\boldsymbol{r})$ is spatially periodic. In the most frequent implementation, each lattice site (i.e. spatial period) exhibits a single minimum. This is achieved through the interference of two counterpropagating laser beams in each trapping direction. This type of potential allows for the realisation of *lattice models*, and it has been used to experimentally investigate e.g. the superfluid–to–Mott insulator transition (which will be discussed in Problem 3).

3.2 Question 8: The ideal Bose gas at $T = 0$

Here, we consider the case of non–interacting bosons. We further assume that the ground state of the single–particle Hamiltonian is non–degenerate. Let ϵ_0 be the ground–state energy, and $|\phi_0\rangle$ be the corresponding wavefunction, so that $h\,|\phi_0\rangle = \epsilon_0\,|\phi_0\rangle$.

At $T = 0$, all of the particles of the system are in the ground state[4]. Hence, the system is in a pure state described by the following many–particle wavefunction:

$$|\Psi\rangle = |\phi_0^{(1)}\rangle \otimes \ldots \otimes |\phi_0^{(N)}\rangle \ . \tag{26}$$

Thus, the one–body density matrix reads:

$$\langle \boldsymbol{r}'|\,\rho^{(1)}\,|\boldsymbol{r}\rangle = \langle \boldsymbol{r}'|\ \mathrm{Tr}_{2\ldots N}(|\Psi\rangle\,\langle\Psi|)\,|\boldsymbol{r}\rangle \quad = N\,\phi_0(\boldsymbol{r}')\,\phi_0^*(\boldsymbol{r}) \ . \tag{27}$$

For a uniform system, ϕ_0 does not depend on $\boldsymbol{r}$: we write $\phi_0(\boldsymbol{r}) = \sqrt{n}$, where $n = N/V$ is the spatial density of particles. Then, Eq. (27) yields $\langle \boldsymbol{r}'|\rho^{(1)}|\boldsymbol{r}\rangle = n$. Hence, the off–diagonal elements of the system do not decay with $|\boldsymbol{r} - \boldsymbol{r}'|$. This signals that the coherence length is infinite. This Bose–condensed system is said to exhibit *off–diagonal long range order.*

We now turn to a harmonically trapped system. For simplicity, we assume that the trap is isotropic $\omega_1 = \omega_2 = \omega_3 = \omega_0$. Then, the single–particle ground state wavefunction reads $\phi_0(\boldsymbol{r}) = \exp[-\boldsymbol{r}^2/(2l_0^2)]/\pi^{3/4}$, where the harmonic oscillator length $l_0 = [\hbar/(m\omega_0)]^{1/2}$. Hence, Eq. (27) yields $\langle \boldsymbol{r}'|\rho^{(1)}|\boldsymbol{r}\rangle = N\exp[-(\boldsymbol{r}^2 + \boldsymbol{r}'^2)/(2l_0^2)]/\pi^{3/2}$. Here, the one–body density matrix does not depend only on $(\boldsymbol{r} - \boldsymbol{r}')$, because the system is not translationally invariant. The off–diagonal elements of $\rho^{(1)}$ decay to zero exponentially for $r, r' > l_0$. The coherence length reflects the finite size of the system, which is set by the oscillator length l_0.

3.3 Questions 9–11: The ideal Fermi gas at $T = 0$

3.3.1 Fermionic ground–state wavefunction

We consider a fixed number N of identical fermions of mass m. We assume that they are all in the same internal state ("fully polarised Fermi gas"), so that the spin does not play any role in the thermodynamics of the system.

We focus on the zero–temperature case, $T = 0$, so that the system is in its ground state. In the first–quantisation formalism, the N–particle ground state wavefunction is a determinant involving the N lowest–energy single–particle states $\phi_1(\boldsymbol{r}), \ldots, \phi_N(\boldsymbol{r})$:

$$\psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\boldsymbol{r}_1) & \cdots & \phi_N(\boldsymbol{r}_1) \\ \vdots & & \vdots \\ \phi_1(\boldsymbol{r}_N) & \cdots & \phi_N(\boldsymbol{r}_N) \end{vmatrix} = \sum_{\sigma\in\mathscr{S}_N} \epsilon(\sigma)\phi_{\sigma(1)}(\boldsymbol{r}_1)\cdots\phi_{\sigma(N)}(\boldsymbol{r}_N) \ . \tag{28}$$

In Eq. 28, the right–hand side expresses the determinant in terms of a sum over all permutations σ acting on N elements, i.e. all elements of the symmetric group $\mathscr{S}_N$, weighted by their signatures $\epsilon(\sigma) = \pm 1$.

3.3.2 Fermi wavevector for a uniform Fermi gas

The Fermi wavevector k_F is the modulus of the wavevector corresponding to the highest–energy populated mode in the ground state. Its expression directly follows from the Pauli principle: each single–particle state may be populated by at most one atom. In the ground state, the populated single–particle states are the N lowest–energy states, corresponding to the smallest values for $|\boldsymbol{k}|$.

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[4] This is not true for an ideal Fermi gas: see below. Distinguishable particles would also go to the ground state for $T = 0$, but this "thermally frozen" regime occurs for much lower temperatures than for identical bosons.

Uniform 1D Fermi gas. The result obtained in the thermodynamic limit should not depend on the chosen boundary conditions. We choose periodic boundary conditions, so that the single–particle wavefunctions are plane waves $e^{ikx}/\sqrt{L}$ which satisfy $e^{ikL} = 1$, where L is the size of the box. This means that the allowed wavevectors are $k_n = n2\pi/L$, with n spanning all (positive and negative) integers. The corresponding energies are $\hbar^2 k_n^2/(2m)$.

Neglecting the small parity effect, $k_F = 2\pi N/(2L) = \pi\rho$, where the factor 1/2 follows from the fact that the states with wavevectors k and $(-k)$ have the same energy. The Fermi wavevector depends only on the 1D density $\rho = N/L$.

Uniform 3D Fermi gas. We choose periodic boundary conditions applied to a cubic box with volume $V = L^3$. The single–particle states are now plane waves $\exp(i\boldsymbol{k}\cdot\boldsymbol{r})/L^{3/2}$. The allowed wavevectors are $\boldsymbol{k} = 2\pi/L\,(n_1\boldsymbol{e}_x + n_2\boldsymbol{e}_y + n_3\boldsymbol{e}_z)$, with n_1, n_2, and n_3 being (positive or negative) integers. The volume occupied by a single mode is $\delta^3 k = (2\pi/L)^3$.

The Fermi wavevector is now defined by:

$$N = \sum_{|\boldsymbol{k}|\le k_F} 1 = \left(\frac{L}{2\pi}\right)^3 \sum_{|\boldsymbol{k}|\le k_F} \delta^3 k \quad \approx \left(\frac{L}{2\pi}\right)^3 \int_{|\boldsymbol{k}|\le k_F} d^3k \quad = \frac{L^3}{6\pi^2} k_F^3 \ . \tag{29}$$

In Eq. 29, we have replaced the sum over all wavevectors by an integral and used the fact that the volume of a sphere of radius k_F is $4\pi k_F^3/3$. Hence, in the 3D case, the Fermi wavevector reads:

$$k_F = (6\pi^2 n)^{1/3} \ , \tag{30}$$

and, just like in the 1D case, it only depends on the density $n = N/L^3$.

3.3.3 First–order spatial correlation function at $T = 0$

The N–particle density matrix representing the ground state is $\rho_N = |\Psi\rangle\langle\Psi|$. We start from the expression for $g_1(\boldsymbol{r},\boldsymbol{r}')$ in terms of the trace over $N-1$ particles:

$$g_1(\boldsymbol{r},\boldsymbol{r}') = N\,\mathrm{Tr}_{2,\ldots,N}(\rho_N) = N\int d^3r_2\ldots d^3r_N \psi^*(\boldsymbol{r}',\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N)\psi(\boldsymbol{r},\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N) \ . \tag{31}$$

We replace both functions ψ and ψ^* by their expressions in terms of determinants given by Eq. 28. This leads to:

$$\begin{aligned} g_1(\boldsymbol{r},\boldsymbol{r}') = \frac{N}{N!} \sum_{\sigma\in\mathscr{S}_N} \sum_{\tau\in\mathscr{S}_N} & \epsilon(\sigma)\epsilon(\tau)\ \phi^*_{\sigma(1)}(\boldsymbol{r}')\phi_{\tau(1)}(\boldsymbol{r}) \\ & \int d^3r_2\ \phi^*_{\sigma(2)}(\boldsymbol{r}_2)\phi_{\tau(2)}(\boldsymbol{r}_2)\ldots \int d^3r_N\ \phi^*_{\sigma(N)}(\boldsymbol{r}_N)\phi_{\tau(N)}(\boldsymbol{r}_N) \ . \end{aligned} \tag{32}$$

Because of the orthogonality of the single–particle wavefunctions, each of the $(N-1)$ integrals $\int d^3r_k \phi^*_{\sigma(k)}(\boldsymbol{r}_k)\phi_{\tau(k)}(\boldsymbol{r}_k)$ is either one or zero: it reduces to $\delta_{\sigma(k),\tau(k)}$, with δ_{ij} being the Kronecker symbol. If the two permutations σ and τ satisfy $\sigma(k) = \tau(k)$ for $2 \le k \le N$, they also satisfy $\sigma(1) = \tau(1)$, therefore the double sum on σ and τ reduces to a single sum on σ:

$$g_1(\boldsymbol{r},\boldsymbol{r}') = \frac{N}{N!} \sum_{\sigma\in\mathscr{S}_N} \phi^*_{\sigma(1)}(\boldsymbol{r}')\phi_{\sigma(1)}(\boldsymbol{r}) \ . \tag{33}$$

Finally, in order to describe a permutation $\sigma \in \mathscr{S}_N$, we need to give *(i)* the value $\sigma(1)$, which may be any integer from 1 to N, and *(ii)* the image of all other integers $\sigma(k)$ for $k \ge 2$, for which there are $(N-1)!$ possibilities once $\sigma(1)$ has been chosen. This leads to the final expression for $g_1(\boldsymbol{r},\boldsymbol{r}')$:

$$g_1(\boldsymbol{r},\boldsymbol{r}') = \sum_{k=1}^{N} \phi^*_k(\boldsymbol{r}')\phi_k(\boldsymbol{r}) \ . \tag{34}$$

Note that Eq. 34 may be derived in a sraightforward way using the second–quantisation formalism (see Sec. 4.2.2 below).

$g^{(1)}$ **function for a 1D uniform Fermi gas.** We start from Eq. 34 and replace the one–particle wavefunctions $\phi(\boldsymbol{r})$ by plane waves $e^{ikx}/\sqrt{L}$. Using the definition of k_F given in Sec. 3.3.2, we obtain:

$$g^{(1}(x,x') = \sum_{|k|\leq k_F} \frac{e^{ik(x-x')}}{L} \approx \frac{L}{2\pi}\int_{-k_F}^{k_F} dk \frac{e^{ik(x-x')}}{L} \ . \tag{35}$$

Thanks to the parities of the trigonometric functions, this last integral evaluates to:

$$g^{(1)}(x,x') = \frac{1}{\pi}\frac{\sin[k_F(x-x')]}{x-x'} = \rho \, \mathrm{sinc}\left[k_F(x-x')\right] \ . \tag{36}$$

$g^{(1)}$ **function for a 3D uniform Fermi gas.** We start from Eq. 34 with $\phi(\boldsymbol{r}) = \exp(i\boldsymbol{k}\cdot\boldsymbol{r})/L^{3/2}$. Letting $\boldsymbol{R} = \boldsymbol{r} - \boldsymbol{r}'$, we obtain:

$$g^{(1)}(\boldsymbol{R}) = \sum_{|\boldsymbol{k}|\leq k_F} d^3k \frac{\exp(i\boldsymbol{k}\cdot\boldsymbol{r})}{V} = \frac{1}{(2\pi)^3}\int_{|\boldsymbol{k}|\leq k_F} \exp(i\boldsymbol{k}\cdot\boldsymbol{R}) \ . \tag{37}$$

We integrate over d^3k using spherical coordinates of axis $\boldsymbol{R}$:

$$g^{(1)}(\boldsymbol{R}) = \frac{1}{(2\pi)^3}\int_{|\boldsymbol{k}|\leq k_F} dk \int_0^{\pi} k d\theta \int_0^{2\pi} k\sin\theta d\phi \, e^{ikR\cos(\theta)} \ . \tag{38}$$

The integral over $d\phi$ gives a factor 2π, and the integral over θ is elementary:

$$g^{(1)}(\boldsymbol{R}) = \frac{1}{2\pi^2 R^3}\int_0^{k_F R} du \, u \sin u \ . \tag{39}$$

Finally, the remaining integral may be evaluated by parts, leading to:

$$g^{(1)}(\boldsymbol{R}) = n \, \frac{\sin(k_F R) - k_F R\cos(k_F R)}{(k_F R)^3/3} \ . \tag{40}$$

4 Finite temperatures and first steps with interactions

We now turn to the second quantisation formalism, which has three key advantages. First, the total number N of particles need no longer be fixed, so that we may analyse systems using both the canonical ensemble (where N is fixed) and the grand–canonical ensemble (where the average value $\langle N\rangle$ is fixed through the value of the chemical potential μ). Second, second quantisation allows for convenient calculations at non–zero temperatures. Third, the one–body density matrix may be expressed as an average involving the field operator, a definition which holds even in the presence of interactions between the particles.

4.1 Question 12: One–body density matrix in terms of a and $a^\dagger$ operators

In Section 2.3, we have pointed out the link between the one–body density matrix $\rho^{(1)}$ and the single–particle operator $F = \sum_i f^{(i)}$ with $f = |\boldsymbol{r}'\rangle\langle\boldsymbol{r}|$. We have shown that the matrix element $\langle\boldsymbol{r}|\rho^{(1)}|\boldsymbol{r}'\rangle$ of one–body density matrix corresponding to a quantum state defined by the complete density matrix ρ is the average $\langle F\rangle = \mathrm{Tr}(\rho F)$ of the operator F taken in the state ρ (see Eq. (24)):

$$\langle\boldsymbol{r}|\rho^{(1)}|\boldsymbol{r}'\rangle = \langle F\rangle \ . \tag{41}$$

Let us now express the average on the right–hand side of Eq. (41) in terms of second–quantisation operators. We introduce a basis $(|\psi_\alpha\rangle)$ of single–particle states, i.e. of the subspace $\mathscr{E}^{(1)}$. The states $|\psi_\alpha\rangle$ are normalised and orthogonal; at this stage, they satisfy no other constraint. We call

a_α the annihilation operator in the state $|\psi_\alpha\rangle$ and $a_\alpha^\dagger$ the corresponding creation operator. The single–particle operator F may be expressed in terms of these operators as follows:

$$F = \sum_{\alpha,\beta} \langle\psi_\alpha|f|\psi_\beta\rangle \; a_\alpha^\dagger a_\beta \quad = \sum_{\alpha,\beta} \psi_\alpha^*(\boldsymbol{r}')\, \psi_\beta(\boldsymbol{r})\, a_\alpha^\dagger a_\beta \ . \tag{42}$$

In Eq. (42), both indices α and β span all single–particle states $|\psi_\alpha\rangle$. The first equality is a general property of single–particle operators, and it holds both for bosons and for fermions. The second equality follows from the specific choice $f = |\boldsymbol{r}'\rangle\,\langle\boldsymbol{r}|$. Averaging Eq. (42) in the state defined by ρ and using Eq. (41), we find:

$$\langle\boldsymbol{r}|\rho^{(1)}|\boldsymbol{r}'\rangle = \sum_{\alpha,\beta} \psi_\alpha^*(\boldsymbol{r}')\psi_\beta(\boldsymbol{r}) \; \langle a_\alpha^\dagger a_\beta\rangle \ . \tag{43}$$

We shall now apply Eq. (43) to two specific choices of the single–particle basis $(|\psi_\alpha\rangle)$. First, for ideal gases, we shall choose this basis such that the single–particle Hamiltonian is diagonal, which will allow for the explicit calculation of $\rho^{(1)}$ at non–zero temperatures for Boltzmann, Bose, and Fermi statistics. Second, in the general case, we shall choose the *continuous* position basis $|(\boldsymbol{r})\rangle$, yielding an expression of $\rho^{(1)}$ in terms of the field operator $\hat{\Psi}(\boldsymbol{r})$.

4.2 Ideal gases at non–zero temperatures

4.2.1 Ideal gases and second quantisation

The constituents of the ideal gas do not interact which each other, so that the many–particle Hamiltonian H is actually a single–particle operator. Hence, it may be expressed in terms of the single–particle Hamiltonian h acting on the subspace $\mathscr{E}^{(1)}$:

$$H = h^{(1)} + h^{(2)} + \ldots + h^{(N)} \quad = \sum_{\alpha,\beta} \langle\psi_\alpha|h|\psi_\beta\rangle \; a_\alpha^\dagger a_\beta \ . \tag{44}$$

In Eq. (44), $h^{(i)}$ acts only on the particle i, and the states $(|\psi_\alpha\rangle)$ are a basis of the single–particle subspace $\mathscr{E}^{(1)}$ as in Sec. 4.1. The single–particle Hamiltonian h is a hermitian operator, so we may choose a basis of (orthogonal and normalised) states $(|\phi_\alpha\rangle)$ in which it is diagonal: $h\,|\phi_\alpha\rangle = \epsilon_\alpha\,|\phi_\alpha\rangle$, where ϵ_α is the energy corresponding to the single–particle state $|\phi_\alpha\rangle$. Choosing the basis $(|\phi_\alpha\rangle)$ in Eq. (44) and using the property $\langle\psi_\alpha|h|\psi_\beta\rangle = \delta_{\alpha\beta}\,\epsilon_\alpha$, we obtain an expression for H involving *a sum over a single index* α:

$$H = \sum_\alpha \epsilon_\alpha\, a_\alpha^\dagger a_\alpha \quad = \sum_\alpha \epsilon_\alpha\, \hat{n}_\alpha \ , \tag{45}$$

the operator $\hat{n}_\alpha = a_\alpha^\dagger a_\alpha$ being the particle number operator in the mode α. Equation (45) reflects the intuition behind the many–particle Hamiltonian of an ideal gas: the contribution to the total energy of the single–particle state α is its energy ϵ_α multiplied by its occupation number n_α.

Equation (45) shows that H conserves the occupation number in each mode, in the sense that the commutator $[H, \hat{n}_\alpha] = 0$ for any single–particle state α. This conservation property is expressed in terms of *a true commutator both for bosons and for fermions.* It reflects the fact that H and the particle–number operators $\hat{n}_\alpha$ may be simultaneously diagonalised in the same many–particle basis. This basis is the set of Fock states $(|(n_\alpha)\rangle)$, which have both well-defined energies and well–defined particle numbers in each mode. A given Fock states is defined by giving the sequence (n_α) of *integers* specifying the occupation number in each mode. Hence, they satisfy:

$$\hat{n}_\gamma\,|(n_\alpha)\rangle = n_\gamma\,|(n_\alpha)\rangle \quad \text{and} \quad H\,|(n_\alpha)\rangle = \left(\sum_\alpha \epsilon_\alpha n_\alpha\right) |(n_\alpha)\rangle \ . \tag{46}$$

We now show that, at thermal equilibrium, the many–body density matrix ρ is diagonal in the Fock–state basis $(|(n_\alpha)\rangle)$, both in the canonical ensemble and in the grand–canonical ensemble.

Canonical ensemble. In this ensemble, the total number of particles N is fixed. Therefore, the acceptable Fock states $|(n_\alpha)\rangle$ satisfy $\sum_\alpha n_\alpha = N$. The N–particle Hilbert space is spanned by all acceptable Fock states. The Hamiltonian H is diagonal in the Fock–state basis, because Fock states have a well–defined energy. Therefore, for any value of the inverse temperature $\beta = 1/(k_\mathrm{B}T)$, the operator $\exp(-\beta H)$ is also diagonal in this basis:

$$\exp(-\beta H)\ |(n_\alpha)\rangle = \exp\left(-\beta \sum_\alpha n_\alpha \epsilon_\alpha\right)\ |(n_\alpha)\rangle\ . \tag{47}$$

We introduce the canonical partition function Z_C, which is a number defined by:

$$Z_C = \mathrm{Tr}[\exp(-\beta H)] = \sum_{(n_\alpha)} \exp\left(-\beta \sum_\alpha n_\alpha \epsilon_\alpha\right)\ , \tag{48}$$

where the sum is taken over all Fock states with the total particle number N, i.e. over all integer sequences (n_α) such that $\sum_\alpha n_\alpha = N$. The many–particle density matrix in the canonical ensemble is $\rho_C = \exp(-\beta H)/Z_C$. It is the product of a number $(1/Z_C)$ by an operator which is diagonal in the Fock–state basis $(\exp(-\beta H))$, so that it is itself diagonal in the Fock–state basis.

Grand–canonical ensemble. In this ensemble, the total particle number N is not rigorously fixed, but its average value $\langle \hat{N}\rangle$ is, through the choice of the chemical potential μ. We consider the operator $H - \mu\hat{N}$, which reads:

$$H - \mu\hat{N} = \left(\sum_\alpha \epsilon_\alpha \hat{n}_\alpha\right) - \mu\left(\sum_\alpha \hat{n}_\alpha\right) \quad = \sum_\alpha (\epsilon_\alpha - \mu)\ \hat{n}_\alpha\ , \tag{49}$$

where we have used both Eq. (45) and the relation $\hat{N} = \sum_\alpha \hat{n}_\alpha$. Equation (49) shows that $H - \mu\hat{N}$ is diagonal in the Fock–state basis. Therefore, so is the operator $\exp[-\beta(H - \mu\hat{N})]$ for any inverse temperature β:

$$\exp[-\beta(H - \mu\hat{N})]\ |(n_\alpha)\rangle = \exp\left[-\beta\left(\sum_\alpha (\epsilon_\alpha - \mu) n_\alpha\right)\right]\ |(n_\alpha)\rangle\ . \tag{50}$$

We introduce the grand–canonical partition function Z_{GC}, which is a number defined by:

$$Z_{GC} = \mathrm{Tr}\left[\exp[-\beta(H - \mu\hat{N})]\right] \quad = \sum_{(n_\alpha)} \exp\left[-\beta \sum_\alpha (\epsilon_\alpha - \mu) n_\alpha\right]\ . \tag{51}$$

Unlike for the canonical ensemble, there is no constraint on the occupation numbers (n_α) of the specific states (other than the Pauli exclusion for fermions). Therefore, Z_{GC} factorises into a product of grand–canonical partition functions $Z_{GC}^{(\alpha)}$ for each mode:

$$Z_{GC} = \prod_\alpha Z_{GC}^{(\alpha)} \quad \text{with} \quad Z_{GC}^{(\alpha)} = \exp\left[-\beta \sum_{n_\alpha} (\epsilon_\alpha - \mu) n_\alpha\right]\ . \tag{52}$$

The factorisation of Eq. (52) is the key feature which makes the grand–canonical ensemble particularly suited to the description of ideal quantum gases. We turn to the grand–canonical density matrix, defined by $\rho_{GC} = \exp(-\beta(H - \mu\hat{N}))/Z_{GC}$. It is a number $(1/Z_{GC})$ multiplied by an operator which is diagonal in the Fock–state basis $(\exp[-\beta(H - \mu\hat{N})])$, therefore it is itself diagonal in the Fock–state basis.

4.2.2 Question 15: One–body density matrix for ideal gases

We now show that, for ideal gases, if the one–body density matrix $\rho^{(1)}$ is expanded in terms of the creation and annihilation operators for the single–particle states $|\phi_\alpha\rangle$ which are eigenstates of the single–particle Hamiltonian h, then Eq. (43) *only involves a sum over a single index* α spanning all single–particle states.

We start from the general expression, in terms of the many–body density matrix ρ, for the average $\langle a^\dagger_\alpha a_\beta\rangle$ which appears in Eq. (43): $\langle a^\dagger_\alpha a_\beta\rangle = \mathrm{Tr}[\rho\, a^\dagger_\alpha a_\beta]$. This trace may be evaluated in any many–particle basis. We choose to work in the Fock–state basis $|(n_\gamma)\rangle$:

$$\langle a^\dagger_\alpha a_\beta\rangle = \sum_{(n_\gamma)} \langle (n_\gamma)|\rho a^\dagger_\alpha a_\beta|(n_\gamma)\rangle \quad = \sum_{(n_\gamma)} \langle (n_\gamma)|\rho|(n_\gamma)\rangle \; \langle (n_\gamma)|a^\dagger_\alpha a_\beta|(n_\gamma)\rangle \ , \tag{53}$$

where the second step follows from ρ being diagonal in the Fock–state basis (see Sec. 4.2.1). The matrix element on the right is the scalar product between the states $a_\alpha\,|(n_\gamma)\rangle$ and $a_\beta\,|(n_\gamma)\rangle$. Both of these states have well–defined occupation numbers in each single–particle mode, meaning that they are both proportional to Fock states. Their overlap may be non–zero only if they are proportional to the same Fock state, which requires $\alpha = \beta$. Hence:

$$\langle a^\dagger_\alpha a_\beta\rangle = \delta_{\alpha\beta}\,\langle a^\dagger_\alpha a_\alpha\rangle = \delta_{\alpha\beta}\,\langle \hat{n}_\alpha\rangle \ . \tag{54}$$

Therefore, in the case of ideal gases described in the single–particle basis which diagonalises the single–particle Hamiltonian h, Eq. (43) reduces to:

$$\langle \boldsymbol{r}|\rho^{(1)}|\boldsymbol{r}'\rangle = \sum_\alpha \pi_\alpha\,\phi^*_\alpha(\boldsymbol{r}')\phi_\alpha(\boldsymbol{r}) \quad \text{with} \quad \pi_\alpha = \langle \hat{n}_\alpha\rangle \ . \tag{55}$$

Equation (55) encompasses our previous results concerning the one–body density matrix of ideal gases. For bosons at zero temperature, the ground state of the system corresponds to N particles in the state ϕ_0 (and no particles in the excited states), so that $\pi_0 = N$ and Eq. (55) reduces to Eq. (27). For spin–polarised fermions at zero temperature, the ground state is a Fermi sea, so that $\pi_\alpha = 1$ for all states such that $\epsilon_\alpha < E_F$ and $\pi_\alpha = 0$ otherwise, thus Eq. (55) reduces to Eq. (34).

In Eq. (55), the populations $\phi_\alpha = \langle \hat{n}_\alpha\rangle$ are the average values of the particle number operator in the considered many–body state ρ. They are all positive and satisfy $\sum_\alpha \pi_\alpha = N = \langle \hat{N}\rangle$. If $\rho = |(n_\alpha)\rangle\,\langle (n_\alpha)|$ represents a pure Fock state, then $\pi_\alpha = n_\alpha$ is an integer for any α. However, the (π_α) need not be integers. For example, if ρ is a thermal state for an ideal quantum gas described in the grand–canonical ensemble, then the populations reflect the quantum statistics:

$$\text{For bosons,} \quad \pi_\alpha = \frac{1}{e^{\beta(\epsilon_\alpha-\mu)}-1} \ ; \qquad \text{For fermions,} \quad \pi_\alpha = \frac{1}{e^{\beta(\epsilon_\alpha-\mu)}+1} \ . \tag{56}$$

We shall now use Eqs. (55) and (56) to calculate the one–body density matrix at non–zero temperature for uniform ideal gases obeying Boltzmann statistics, Bose statistics, and Fermi statistics.

4.2.3 Question 16: $g^{(1)}$ function for a uniform classical gas

The single–particle Hamiltonian is $h = \boldsymbol{p}^2/(2m)$, its eigenstates are plane waves $\exp(i\boldsymbol{k}\cdot\boldsymbol{r})/\sqrt{V}$, and the corresponding energies are $p^2/(2m)$ with $\boldsymbol{p} = \hbar\boldsymbol{k}$. The occupation numbers satisfy the Maxwell–Boltzmann distribution, i.e. the population of a single–particle state with the wavevector $\boldsymbol{k}$ is proportional to $\exp(-\beta E)$, with $E = p^2/2m$ and $\beta = 1/(k_B T)$:

$$\pi(\boldsymbol{p}) = \alpha\,\exp(-\beta p^2/2m) \ . \tag{57}$$

The prefactor α is determined by the total number of particles:

$$N = \iint \frac{d^3x\,d^3p}{h}\pi(\boldsymbol{p}) = \alpha \iint \frac{d^3x\,d^3p}{h}\exp(-\beta p^2/2m) \ , \tag{58}$$

where the integral is taken over all phase space. The integral over d^3x gives the total volume V. The integral over d^3p may be performed using polar coordinates, letting $u = \beta p^2/(2m)$, and finally remembering that $\Gamma(3/2) = \sqrt{\pi}/2$. Introducing the thermal de Broglie wavelength $\Lambda_T = h/\sqrt{2\pi m k_B T}$, we obtain:

$$\pi(\boldsymbol{p}) = N\frac{\Lambda_T^3}{V}\ \exp(-\beta p^2/2m)\ . \tag{59}$$

We now use Eq. (55):

$$g^{(1)}(\boldsymbol{r},\boldsymbol{r}') = \sum_\alpha \pi_\alpha\ \phi^*_\alpha(\boldsymbol{r}')\phi_\alpha(\boldsymbol{r}) = \frac{N\Lambda_T^3}{V}\int \frac{d^3k}{(2\pi)^3}\ \exp(i\boldsymbol{k}\cdot\boldsymbol{R})\ \exp[-\beta\hbar^2k^2/(2m)]\ , \tag{60}$$

with $\boldsymbol{R} = \boldsymbol{r}' - \boldsymbol{r}$. Equation 60 shows that $g^{(1)}(\boldsymbol{r},\boldsymbol{r}')$ is the Fourier transform of a Gaussian of width $mk_BT/\hbar^2$, i.e. $g^{(1)}(\boldsymbol{r},\boldsymbol{r}')$ is a Gaussian of width $\hbar^2/(mk_BT)$. We finally find:

$$\rho^{(1)}(\boldsymbol{R}) = \rho\ \exp(-\pi R^2/\Lambda_T^2)\ . \tag{61}$$

4.2.4 Question 17: $g^{(1)}$ function for a uniform 3D Bose gas

Thermodynamics. We consider a uniform system with periodic boundary conditions. Hence, the single–particle states are the plane waves $\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \exp(i\boldsymbol{k}\cdot\boldsymbol{r})/\sqrt{V}$, where V. These states are labelled by the wavevector $\boldsymbol{k}$ and correspond to the single–particle energies $\epsilon_{\boldsymbol{k}} = \hbar^2\boldsymbol{k}^2/(2m)$. The thermodynamics of the uniform 3D Bose gas are conveniently described by expressing the chemical potential in terms of the density. For a sufficiently large system, the predictions of all thermodynamic ensembles coincide. We describe the gas in the grand–canonical ensemble[5], where the analysis is the simplest thanks to the uncoupling between the single–particle modes. The total number N of particles satisfies:

$$N = \sum_{\boldsymbol{k}} \pi_{\boldsymbol{k}}\ , \quad \text{where} \quad \pi_{\boldsymbol{k}} = \frac{1}{e^{\beta(\epsilon_k-\mu)}-1} = \frac{1}{z^{-1}e^{\beta\epsilon_k}-1}\ . \tag{62}$$

In Eq. (62), the population $\pi_{\boldsymbol{k}}$ of the single–particle state $|\phi_{\boldsymbol{k}}\rangle$ satisfies the Bose–Einstein distribution with the inverse temperature $\beta = 1/(k_\mathrm{B}T)$ and the chemical potential μ. We have also introduced the fugacity $z = e^{\beta\mu}$. In order for all populations $\pi_{\boldsymbol{k}}$ to be positive, the chemical potential μ must be smaller than all ϵ_k's, i.e. μ must be negative, which means $0 < z < 1$.

In the thermodynamic limit, the difference between consecutive values of $\boldsymbol{k}$ is very small: $2\pi/L$ in each direction, which corresponds to the small k–space volume $(2\pi)^3/V$. We wish to replace the discrete sum in Eq. (62) by an integral, using the following substitution where we have made apparent the small k–space volume we have just derived:

$$\sum_{\boldsymbol{k}} F(\boldsymbol{k}) \approx \int \frac{d^3k}{(2\pi)^3/V}\ F(\boldsymbol{k})\ . \tag{63}$$

For that purpose, the contribution π_0 of the ground state (wavefunction $\phi_0(\boldsymbol{r}) = 1/\sqrt{V}$) must be carefully accounted for. Indeed, for z close to 1 (i.e. for $\mu \to 0^-$), $\pi_0 = 1/(z^{-1}-1)$ becomes very large. This contribution is completely neglected in the integral approximation: Indeed, exploiting the fact that $\pi_{\boldsymbol{k}} = \pi_k$ depends on the modulus $k = |\boldsymbol{k}|$ only, we may write $\int d^3k\pi_k = \int dk\, 4\pi k^2\pi_k$, so that the weight affected to π_0 vanishes like k^2. Hence, whenever the population of π_0 is macroscopic (that is, when it is comparable to N, which occurs for all temperatures below the critical condensation temperature T_B), $\pi_0 = 1/(z^{-1}-1)$ must be explicitly retained in the sum over all modes:

$$N = \pi_0\ +\int \frac{d^3k}{(2\pi)^3/V}\ \frac{1}{z^{-1}\,e^{\beta\epsilon_k}-1}\ . \tag{64}$$

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[5] The grand–canonical ensemble is fully applicable for the calculation of quantities related to $\rho^{(1)}$. However, it is treacherous when used to calculate quantities related to $\rho^{(2)}$ in the presence of a condensate [3] [4, § 3.3].

We now expand the integrand in increasing powers of z:

$$\frac{1}{z^{-1}\,e^{\beta\epsilon_k}-1}=\frac{z\,e^{-\beta\epsilon_k}}{1-z\,e^{-\beta\epsilon_k}}\quad=\sum_{l=1}^{\infty}z^l\,e^{-l\beta\epsilon_k}\ , \tag{65}$$

the convergence of the series on the right–hand side being ensured by the condition $z<1$. Replacing Eq. (65) into Eq. (62) and integrating the series term by term, we find:

$$N=\pi_0+\frac{V}{\Lambda_T^3}\,g_{3/2}(z)\ ,\quad \text{where}\quad g_{3/2}(z)=\sum_{l=1}^{\infty}\frac{z^l}{l^{3/2}}\ . \tag{66}$$

In Eq. (66), the function $g_{3/2}(z)$ is called 'polylogarithm' or 'Bose function' of order 3/2. It is a monotonously increasing function of z which behaves like $g_{3/2}(z)\approx z$ for small z; it reaches the finite value $\zeta(3/2)=2.61$ for $z\to 1$.

Two cases are now possible depending on the value of the temperature T. First, for large T (more specifically, for T greater than the critical condensation temperature T_B), π_0 is negligible compared to N, and Eq. (66) reduces to:

$$\text{For } T>T_B,\quad n\Lambda_T^3=g_{3/2}(z)\ . \tag{67}$$

The parameter $n\Lambda_T^3$ appearing in Eq. (67) is called the 'phase–space density' and plays a key role in the description of cold quantum gases, bosonic or fermionic. We may write $n\Lambda_T^3=(\Lambda_T/n^{-1/3})^3$, so that the phase–space density is directly related to the ratio of the coherence length Λ_T of a single particle to the mean interparticle spacing $n^{-1/3}$. Quantum effects are expected if the coherence length exceeds the interparticle spacing, i.e. for phase–space densities $n\Lambda_T^3\gtrsim 1$. More specifically, if T decreases, then Λ_T increases, and therefore so does z. For bosons, Eq. (67) remains valid as long as $z<1$. The Bose transition occurs for $z=1$, at which point $g_{3/2}(z)$ reaches its maximum value $\zeta(3/2)$, corresponding to the temperature T_B such that:

$$n\Lambda_{T_B}^3=\zeta(3/2)\ ,\quad \text{which means:}\quad k_\mathrm{B}T_B=\frac{\hbar^2}{mn^{-2/3}}\,\frac{2\pi}{[\zeta(3/2)]^{2/3}}\ . \tag{68}$$

Apart from the numerical prefactor $2\pi/[\zeta(3/2)]^{2/3}\approx 3.31$, the critical temperature $k_\mathrm{B}T_B$ is the kinetic energy $\hbar^2/(mn^{-2/3})$ corresponding to the mean interparticle spacing $n^{-1/3}$.

Second, for small T (more specifically, for $T<T_B$), z is always equal to 1. Hence, the populations $\pi_{\boldsymbol{k}}$ of all states but $|\phi_{\boldsymbol{0}}\rangle$ are maximal: the thermal component of the Bose gas is said to be 'saturated'. The maximum thermal population $N_T=N-\pi_0$ satisfies:

$$\frac{N_T}{N}=\frac{V}{N\Lambda_T^3}\,g_{3/2}(1)\quad=\frac{\zeta(3/2)}{n\lambda_{T_B}^3}\,\frac{\Lambda_{T_B}^3}{\Lambda_T^3}\quad=(T/T_B)^{3/2}\ . \tag{69}$$

In Eq. (69), the first step follows from Eq. (66) with $z=1$, and the last one uses Eq. (68). All particles in excess of this maximum value go to the ground state, leading to a value of π_0 which is of the order of N. Writing $\pi_0=N-N_T$, we finally obtain the condensate fraction π_0/N:

$$\text{For } T<T_B,\quad \pi_0/N=1-\left(\frac{T}{T_B}\right)^{3/2}\ . \tag{70}$$

Reduced density matrix. We start from the general expression for $g^{(1)}(\boldsymbol{r},\boldsymbol{r}')$:

$$g^{(1)}(\boldsymbol{r},\boldsymbol{r}')=\sum_{\boldsymbol{k}}\pi_{\boldsymbol{k}}\,\phi_{\boldsymbol{k}}^*(\boldsymbol{r}')\phi_{\boldsymbol{k}}(\boldsymbol{r})\quad=\sum_{\boldsymbol{k}}\pi_{\boldsymbol{k}}\,\frac{\exp[i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')]}{V}\ , \tag{71}$$

where the $\pi_{\boldsymbol{k}}$'s are given by Eq. (62). As expected from the translational symmetry of the problem, $g^{(1)}(\boldsymbol{R})$ depends only on $\boldsymbol{R}=\boldsymbol{r}-\boldsymbol{r}'$. Following Eq. (64), we explicitly retain the contribution of π_0 and replace the sum over all other modes by an integral:

$$g^{(1)}(\boldsymbol{R})=\frac{\pi_0}{V}+\int\frac{d^3k}{(2\pi)^3}\,\frac{1}{z^{-1}e^{\beta\epsilon_k}-1}\,\exp[i\boldsymbol{k}\cdot\boldsymbol{R}]\ . \tag{72}$$

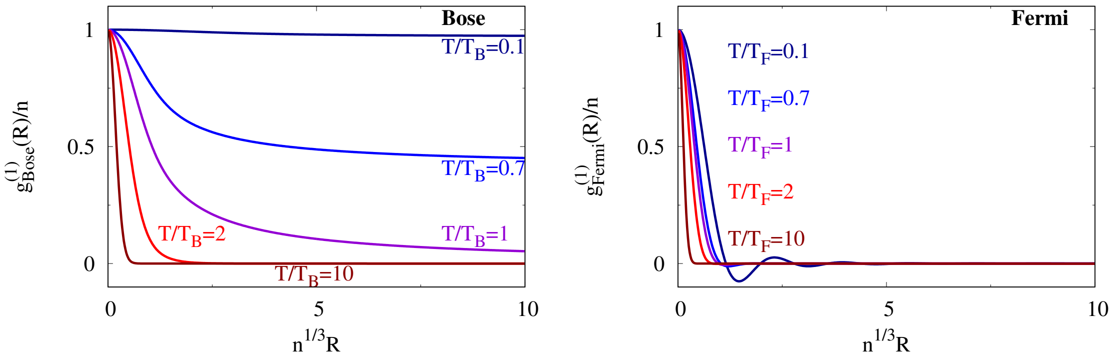

Figure 1 First–order spatial correlation functions $g^{(1)}(R)$ of uniform an ideal quantum gases. The bosonic case is shown on the left and the fermionic one on the right. In both cases, distances $R = |\boldsymbol{r} - \boldsymbol{r}'|$ are expressed in units of the mean interparticle distance $n^{-1/3}$, and $g^{(1)}(R)$ in units of the uniform density n.

We expand the Bose factor using Eq. (65), and integrate the series term by term to finally obtain:

$$\frac{g^{(1)}_{\text{Bose}}(R)}{n} = \frac{\pi_0}{N} + \frac{1}{n\Lambda_T^3} \sum_{l=1}^{\infty} \frac{z^l}{l^{3/2}} \exp\left(-\frac{\pi}{l}\frac{R^2}{\Lambda_T^2}\right) \ , \tag{73}$$

where n is the uniform density of the gas. The final result depends on $R = |\boldsymbol{R}|$, as expected from the rotational symmetry. The bosonic first–order spatial correlation function $g^{(1)}_{\text{Bose}}$ is shown on the left panel of Fig. 1. Let us now discuss Eq. (73) for various temperature regimes. For very high T, the fugacity z is small, and we may retain only the leading term in the sum of Eq. (73), which coincides with the classical result of Eq. (61). For temperatures which are not so high, but still greater than T_B, the condensate fraction π_0/N vanishes. Multiple terms in the sum over l may survive, but they all decay exponentially with a characteristic length set by Λ_T: hence, the coherence length is $\sim \Lambda_T$. We now turn to the case of temperatures $T < T_B$. Then, a condensate is present, so that $\pi_0/N > 0$. The first–order correlation function no longer vanishes for $R \to \infty$: instead, it reaches the asymptotic value π_0/N. Thus, the coherence length is infinite, which signals that the system remains coherent over a *long spatial range*. In other words, a Bose–condensed system exhibits an *order* identified by the fact that *off–diagonal* elements of the reduced density matrix remain non–zero for $R \to \infty$. Therefore, Bose–Einstein condensation is also referred to as *off-diagonal long–range order.*

4.2.5 $g^{(1)}$ function for a uniform Fermi gas

Thermodynamics. The single–particle wavefunctions $|\phi_{\boldsymbol{k}}\rangle$ and energies $\epsilon_{\boldsymbol{k}}$ are the same as in Sec. 4.2.4. However, the populations $\pi_{\boldsymbol{k}}$ now reflect Fermi statistics:

$$N = \sum_{\boldsymbol{k}} \pi_{\boldsymbol{k}} \ , \quad \text{where} \quad \pi_{\boldsymbol{k}} = \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1} = \frac{1}{z^{-1}e^{\beta\epsilon_k} + 1} \ . \tag{74}$$

For high temperatures, the fugacity $z > 0$ is very small just like for Bose gases: this means that μ is negative and large compared to $k_{\text{B}}T$ or, equivalently, that the system is well described by Boltzmann statistics. However, the low–temperature behaviour of the chemical potential is very different from its bosonic counterpart. The chemical potential μ is defined as the energy required to add a particle to the system. For fermions at very low temperature, the many–particle system is a ‘Fermi sea’ where all single–particle states are occupied up to the maximum energy E_F (see Sec. 3.3). Therefore, adding a particle to the system costs an energy very close to E_F, meaning that $\mu = E_F$. Hence, the fugacity $z \approx \exp(\beta E_F)$ goes to $+\infty$ in the limit of very low temperatures.

Thus, unlike for bosons (for which $z_{\rm Bose} < 1$), for fermions, z spans all positive values from $z = 0$ (reached for very large T) to $z = +\infty$ (reached for $T = 0$).

All populations $\pi_{\boldsymbol{k}} \leq 1$, reflecting Pauli's exclusion principle, so that no single–particle state may become macroscopically occupied. Therefore, we may apply Eq. (63) to replace the discrete sum over an integral spanning all modes:

$$N = \int \frac{d^3k}{(2\pi)^3/V} \, \frac{1}{z^{-1}\, e^{\beta\epsilon_k} + 1} \; . \tag{75}$$

In Eq. (75), the integrand depends only on k, and the change of variables $x = \beta\epsilon_k = \beta\hbar^2 k^2/(2m)$ in the integral shows that the phase–space density $n\Lambda_T^3 = N\Lambda_T^3/V$ depends only on z:

$$n\Lambda_T^3 = f_{3/2}(z) \quad = \frac{1}{\Gamma(3/2)} \int_0^{+\infty} dx \, \frac{x^{1/2}}{z^{-1} e^x + 1} \; . \tag{76}$$

It is tempting to expand the Fermi factor in increasing powers of z as for bosons (see Eq. (65)):

$$f_{3/2}(z) = -g_{3/2}(-z) \quad = -\sum_{l=1}^{\infty} \frac{(-z)^l}{l^{3/2}} \; . \tag{77}$$

However, the series of Eq. (77) only converges for $z \leq 1$, whereas the low–temperature regime where the quantum effects are strongest is reached for $z > 1$. There, the Fermi factor may not be expanded in powers of z, and $f_{3/2}(z)$ must be defined[6] through the integral of Eq. (76).

For fermions, no phase transition occurs for low temperatures. However, an order of magnitude for the temperature below which quantum effects are important is given by the Fermi temperature T_F, defined in terms of the Fermi energy E_F by $k_{\rm B}T_F = E_F$. Thanks to Eq. (30), we find:

$$E_F = k_{\rm B}T_F = \frac{\hbar^2}{mn^{-2/3}} \, \frac{(6\pi^2)^{2/3}}{2} \; . \tag{78}$$

The Fermi temperature T_F has a very similar structure to that of the Bose temperature T_B defined by Eq. (68). It involves the same typical kinetic energy $\hbar^2/(mn^{-2/3})$, but the numerical prefactor is different: $(6\pi^2)^{2/3}/2 \approx 7.60$. It satisfies $n\Lambda_{T_F}^3 = 4/(3\sqrt{\pi}) = 0.752$, confirming that quantum effects become important for phase–space densities $n\Lambda_T^3 \gtrsim 1$ as for bosons.

Reduced density matrix. We start from the general expression of Eq. (71), where the populations $\pi_{\boldsymbol{k}}$ now obey Fermi statistics and are given by Eq. (74). We replace the discrete sum over all modes $\boldsymbol{k}$ by an integral following the procedure of Eq. (63). This leads to:

$$g^{(1)}(\boldsymbol{R}) = \int \frac{d^3k}{(2\pi)^3} \, \frac{1}{z^{-1}\exp(\beta\epsilon_k) + 1} \, \exp(i\boldsymbol{k}\cdot\boldsymbol{R}) \; , \tag{79}$$

where we have set $\boldsymbol{R} = \boldsymbol{r} - \boldsymbol{r}'$ in accordance with the translational symmetry. Just like in the zero–temperature case of Sec. 3.3.3, we integrate over d^3k using spherical coordinates of axis $\boldsymbol{R}$. Changing the integration variable to $u = kR$, we obtain:

$$\frac{g^{(1)}_{\rm Fermi}(R)}{n} = \frac{1}{2\pi^2}\,\frac{1}{n\Lambda_T^3}\left(\frac{\Lambda_T}{R}\right)^3 \int_0^{\infty} du \, \frac{u\,\sin u}{z^{-1}\exp\left(\frac{1}{4\pi}\frac{\Lambda_T^2}{R^2}u^2\right) + 1} \; , \tag{80}$$

showing that $g^{(1)}_{\rm Fermi}(R)$ depends only on $R = |\boldsymbol{R}|$, as expected from the rotational symmetry. For $z < 1$, the integrand may be expanded into a power series in z which we then integrate term by term. This leads to an expression which is very similar to the bosonic prediction of Eq. (73):

$$\text{For } z < 1, \qquad \frac{g^{(1)}_{\rm Fermi}(R)}{n} = \frac{1}{n\Lambda_T^3}\,(-)\sum_{l=1}^{\infty}\frac{(-z)^l}{l^{3/2}}\,\exp\left(-\frac{\pi}{l}\,\frac{R^2}{\Lambda_T^2}\right) \; . \tag{81}$$

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[6] In the quantum regime of large z, an asymptotic expansion of $f_{3/2}(z)$ may be obtained through a Sommerfeld expansion [5, § 11.1].

In the high–temperature limit, corresponding to $z \ll 1$, only the leading term survives in the sum of Eq. (81), and $g^{(1)}_{\mathrm{Fermi}}(R)$ coincides with the classical prediction of Eq. (61), just like $g^{(1)}_{\mathrm{Bose}}(R)$. In the quantum regime, where $z > 1$, the series of Eq. (81) does not converge, and $g^{(1)}_{\mathrm{Fermi}}(R)$ must be evaluated numerically starting from the integral of Eq. (80). The one–body density matrix for a uniform and ideal gas of fermions is represented on the right panel of Fig. 1. For large temperatures $T \gg T_F$, the coherence length is Λ_T. For $T \ll T_F$, it is given by the inverse Fermi wavevector $1/k_F$, and remains finite for $T = 0$. Hence, unlike their bosonic counterparts, low–temperature Fermi gases do not exhibit any spectacular first–order coherence effects.

4.3 One–body density matrix in terms of the field operator

4.3.1 Definition and usage of the field operator

The field operator $|\hat{\Psi}(\boldsymbol{r})\rangle$ is defined as the annihilation operator corresponding to the single–particle state $|\boldsymbol{r}\rangle$, and its transpose conjugate operator is the corresponding creation operator:

$$\hat{\Psi}(\boldsymbol{r}) = a_{|\boldsymbol{r}\rangle} \quad \text{and} \quad \hat{\Psi}^\dagger(\boldsymbol{r}) = a^\dagger_{|\boldsymbol{r}\rangle} \ . \tag{82}$$

The new notation as a function rather than as an index reflects the fact that the basis $(|\boldsymbol{r}\rangle)$ is a *continuous basis* (rather than an enumerable one, such as that of the harmonic oscillator eigenstates). The (minor) difference in between enumerable and continuous bases is that, in the latter case, the (anti–)commutation relations between $\hat{\Psi}(\boldsymbol{r})$ and $\hat{\Psi}^\dagger(\boldsymbol{r})$ involve Dirac Delta peaks rather than discrete Kronecker Delta symbols:

$$[\hat{\Psi}(\boldsymbol{r}), \hat{\Psi}(\boldsymbol{r}')]_\pm = 0, \quad [\hat{\Psi}^\dagger(\boldsymbol{r}), \hat{\Psi}^\dagger(\boldsymbol{r}')]_\pm = 0, \quad [\hat{\Psi}(\boldsymbol{r}), \hat{\Psi}^\dagger(\boldsymbol{r}')]_\pm = \delta(\boldsymbol{r} - \boldsymbol{r}'). \tag{83}$$

The single–particle basis $(|\boldsymbol{p}\rangle)$ is also a continuous basis, for which we may likewise define the field operator $\hat{\Psi}(\boldsymbol{p})$:

$$\hat{\Psi}(\boldsymbol{p}) = a_{|\boldsymbol{p}\rangle} \quad \text{and} \quad \hat{\Psi}^\dagger(\boldsymbol{p}) = a^\dagger_{|\boldsymbol{p}\rangle} \ . \tag{84}$$

It satisfies the corresponding commutation relations:

$$[\hat{\Psi}(\boldsymbol{p}), \hat{\Psi}(\boldsymbol{p}')]_\pm = 0, \quad [\hat{\Psi}^\dagger(\boldsymbol{p}), \hat{\Psi}^\dagger(\boldsymbol{p}')]_\pm = 0, \quad [\hat{\Psi}(\boldsymbol{p}), \hat{\Psi}^\dagger(\boldsymbol{p}')]_\pm = \delta(\boldsymbol{p} - \boldsymbol{p}'). \tag{85}$$

Just like any other creation operator, $\hat{\Psi}^\dagger(\boldsymbol{r})$ transforms like a ket. Therefore, in order to expand $\hat{\Psi}^\dagger(\boldsymbol{r})$ onto the creation operators for any other (enumerable or continuous) single–particle basis $(|\psi_\alpha\rangle)$, we first derive the transformation law for single–particle kets using the closure relation:

$$|\boldsymbol{r}\rangle = \sum_\alpha |\psi_\alpha\rangle \langle\psi_\alpha|\boldsymbol{r}\rangle \quad = \sum_\alpha \psi^*_\alpha(\boldsymbol{r}) \ |\psi_\alpha\rangle \ . \tag{86}$$

Replacing $|\boldsymbol{r}\rangle$ by $\hat{\Psi}^\dagger(\boldsymbol{r})$ and $|\psi_\alpha\rangle$ by $a^\dagger_\alpha$ in Eq. (86), we obtain the transformation law for $\hat{\Psi}^\dagger(\boldsymbol{r})$:

$$\hat{\Psi}^\dagger(\boldsymbol{r}) = \sum_\alpha \ \psi^*_\alpha(\boldsymbol{r})\, a^\dagger_\alpha \ . \tag{87}$$

Then, taking the transpose conjugate of Eq. (87) yields the transformation law for $\hat{\Psi}(\boldsymbol{r})$:

$$\hat{\Psi}(\boldsymbol{r}) = \sum_\alpha \ \psi_\alpha(\boldsymbol{r})\, a_\alpha \ . \tag{88}$$

The relevance of the field operator $\hat{\Psi}(\boldsymbol{r})$ stems from the fact that it may be used to express the many–particle Hamiltonian in second–quantised form. The complete many–body Hamiltonian $H = K + U + V$ is usually the sum of three operators: the trapping potential $U = \sum_i u^{(i)}$ and the kinetic energy $K = \sum_i k^{(i)}$ (which are both single–particle operators), and the two–body interaction term V (which is a two–body operator). We examine these three terms in turn.

Trapping potential. The general rule for expressing single–particle operators (first equality of Eq. (42)) combined with the transformation law of Eq. (88) leads to the following expression for the trapping potential term:

$$\hat{U} = \int d^3r \, u(\boldsymbol{r}) \, \hat{\Psi}^\dagger(\boldsymbol{r}) \, \hat{\Psi}(\boldsymbol{r}) \; . \tag{89}$$

Kinetic energy. We focus here on the single–particle kinetic energy operator, $k = \boldsymbol{p}^2/(2m)$, and the corresponding many–body operator, $K = \sum_i k^{(i)}$. Our main goal is to cast k in the form:

$$k = \int d^3r \; |\boldsymbol{r}\rangle \left(-\frac{\hbar^2}{2m} \, \boldsymbol{\nabla}^2_{\boldsymbol{r}} \right) \langle \boldsymbol{r}| \; . \tag{90}$$

The corresponding many–body operator is then obtained from Eq. (90) through the usual rules:

$$K = \int d^3r \, \hat{\Psi}^\dagger(\boldsymbol{r}) \left(-\frac{\hbar^2}{2m} \, \boldsymbol{\nabla}^2_{\boldsymbol{r}} \right) \hat{\Psi}(\boldsymbol{r}) \; . \tag{91}$$

Using the hermitian character[7] of $\boldsymbol{p} = -i\hbar\nabla_{\boldsymbol{r}}$, Eq. (91) may be rewritten in the following form:

$$K = +\frac{\hbar^2}{2m} \int d^3r \, (\boldsymbol{\nabla}_{\boldsymbol{r}} \hat{\Psi}^\dagger(\boldsymbol{r})) \cdot (\boldsymbol{\nabla}_{\boldsymbol{r}} \hat{\Psi}(\boldsymbol{r})) \; . \tag{92}$$

In order to obtain Eq. (90), we first expand the single–particle operator k in the position basis:

$$k \quad = \quad \int d^3r_1 d^3r_2 \; |\boldsymbol{r}_1\rangle \, \langle \boldsymbol{r}_1|k|\boldsymbol{r}_2\rangle \, \langle \boldsymbol{r}_2| \quad = \quad \int d^3r_1 d^3r_2 \; \langle \boldsymbol{r}_1|k|\boldsymbol{r}_2\rangle \, |\boldsymbol{r}_1\rangle \, \langle \boldsymbol{r}_2| \; . \tag{93}$$

Equation (93) involves a double sum on $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$, whereas the sought Eq. (90) is diagonal in $\boldsymbol{r}$. The next step is the calculation of the matrix element $\langle \boldsymbol{r}_1|k|\boldsymbol{r}_2\rangle$. It is not straightforward to express the operator $k = \boldsymbol{p}^2/(2m)$ in the position basis ($|\boldsymbol{r}\rangle$); however, k is diagonal in the momentum basis ($|\boldsymbol{p}\rangle$). The relation between these two bases may be summarised by two closure relations and an overlap[8]:

$$\int d^3r \; |\boldsymbol{r}\rangle \, \langle \boldsymbol{r}| = 1, \quad \int d^3p \; |\boldsymbol{p}\rangle \, \langle \boldsymbol{p}| = 1, \quad \langle \boldsymbol{r}|\boldsymbol{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} \, \exp(i\boldsymbol{p}\cdot\boldsymbol{r}/\hbar) \; . \tag{94}$$

We introduce the closure relation on the momentum basis within the matrix element $\langle \boldsymbol{r}_1|k|\boldsymbol{r}_2\rangle$:

$$\langle \boldsymbol{r}_1|k|\boldsymbol{r}_2\rangle \quad = \langle \boldsymbol{r}_1|\frac{\boldsymbol{p}^2}{2m}|\boldsymbol{r}_2\rangle \quad = \langle \boldsymbol{r}_1| \, \frac{\boldsymbol{p}^2}{2m} \left(\int d^3p \, |\boldsymbol{p}\rangle \, \langle \boldsymbol{p}| \right) |\boldsymbol{r}_2\rangle \quad = \int d^3p \; \langle \boldsymbol{r}_1|\frac{\boldsymbol{p}^2}{2m}|\boldsymbol{p}\rangle \, \langle \boldsymbol{p}|\boldsymbol{r}_2\rangle \; . \tag{95}$$

We now exploit the fact that $|\boldsymbol{p}\rangle$ is the eigenstate of the operator $\boldsymbol{p}$ with the eigenvalue $\boldsymbol{p}$:

$$\langle \boldsymbol{r}_1|k|\boldsymbol{r}_2\rangle \quad = \quad \int d^3p \, \frac{\boldsymbol{p}^2}{2m} \; \langle \boldsymbol{r}_1|\boldsymbol{p}\rangle \, \langle \boldsymbol{p}|\boldsymbol{r}_2\rangle \quad = \quad \int d^3p \, \frac{\boldsymbol{p}^2}{2m} \, \frac{\exp(i\boldsymbol{p}\cdot\boldsymbol{R}/\hbar)}{(2\pi\hbar)^3} \; . \tag{96}$$

In establishing the last equality of Eq. (96), we have used the last of Eqs. (94) and introduced $\boldsymbol{R} = \boldsymbol{r}_1 - \boldsymbol{r}_2$. The Fourier transform appearing on the right–hand side of Eq. (96) is readily calculated by recognising a second–order derivative with respect to $\boldsymbol{R}$:

$$\begin{aligned} \langle \boldsymbol{r}_1|k|\boldsymbol{r}_2\rangle &= \int d^3p \, \left(-\frac{\hbar^2}{2m} \right) \boldsymbol{\nabla}^2_{\boldsymbol{R}} \left[\frac{\exp(i\boldsymbol{p}\cdot\boldsymbol{R}/\hbar)}{(2\pi\hbar)^3} \right] \\ &= -\frac{\hbar^2}{2m} \, \boldsymbol{\nabla}^2_{\boldsymbol{R}} \left[\int d^3p \, \frac{\exp(i\boldsymbol{p}\cdot\boldsymbol{R}/\hbar)}{(2\pi\hbar)^3} \right] \; . \end{aligned} \tag{97}$$

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[7] The hermitian character of $\boldsymbol{p}$ is not always straightforward to establish. In the most usual scenario, it follows from the assumption that wavefunctions vanish sufficiently quickly for large distances.

[8] Many different conventions are used in the literature for Eqs. (94), and it is important to be consistent in the choice of the normalisation factors. We follow the convention of Ref. [6, §II.E.1, Eqs. E-5 and E-9].

We now recall two well–known properties of the Dirac peak δ:

$$\delta(x) = \int \frac{dk}{2\pi}\, e^{ikx} \qquad \text{and} \qquad \delta(\alpha x) = \frac{1}{\alpha}\delta(x) \text{ for any constant } \alpha > 0. \tag{98}$$

These allow for the calculation of the integral within the brackets on the second line of Eq. (97):

$$\langle \boldsymbol{r}_1 | k | \boldsymbol{r}_2 \rangle = -\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2_{\boldsymbol{R}} \left[\delta(\boldsymbol{R})\right] \ . \tag{99}$$

Recalling that $\boldsymbol{R} = \boldsymbol{r}_1 - \boldsymbol{r}_2$, and using the chain rule for the gradient twice, the gradient in Eq. (99) may be taken with respect to either $\boldsymbol{r}_1$ or $\boldsymbol{r}_2$, with no change in the sign:

$$\langle \boldsymbol{r}_1 | k | \boldsymbol{r}_2 \rangle \quad = \quad -\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2_{\boldsymbol{r}_1} \left[\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)\right] \quad = \quad -\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2_{\boldsymbol{r}_2} \left[\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)\right] \ . \tag{100}$$

We choose to use $\boldsymbol{\nabla}_{\boldsymbol{r}_2}$, and inject Eq. (100) into Eq. (93) to obtain:

$$k = \int d^3r_1 d^3r_2 \ |\boldsymbol{r}_1\rangle \langle \boldsymbol{r}_2| \left(-\frac{\hbar^2}{2m}\right) \boldsymbol{\nabla}^2_{\boldsymbol{r}_2} \left[\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)\right] \ . \tag{101}$$

We now perform two consecutive integrations by parts to transfer the gradients acting on the Dirac peak onto the operator $|\boldsymbol{r}_1\rangle \langle \boldsymbol{r}_2|$. Each integration by parts adds a minus sign; therefore, the two consecutive integrations by parts have no net effect on the sign:

$$k = \int d^3r_1 d^3r_2 \ |\boldsymbol{r}_1\rangle \left(-\frac{\hbar^2}{2m}\right) \boldsymbol{\nabla}^2_{\boldsymbol{r}_2} \left[\, \langle \boldsymbol{r}_2| \,\right] \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2) \ . \tag{102}$$

Finally, the Dirac peak $\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)$ eliminates the integral on $\boldsymbol{r}_1$, and we conclude:

$$k = \int d^3r_2 \ |\boldsymbol{r}_2\rangle \left(-\frac{\hbar^2}{2m}\right) \boldsymbol{\nabla}^2_{\boldsymbol{r}_2} \langle \boldsymbol{r}_2| \ , \tag{103}$$

which coincides with Eq. (90).

Pairwise interaction. We now turn to the interaction term $\hat{V}$, which describes the pairwise interaction between the particles. This is a two–body operator which reads, in first–quantised notation:

$$\hat{V} = \sum_{i \neq j} v^{(i,j)} \ , \tag{104}$$

where the operator $v^{(i,j)}$ acts on the particles i and j only. In terms of the creation and annihilation operators related to the single–particle basis $|\psi_\alpha\rangle$, the two–particle operator V reads:

$$\hat{V} = \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle \, a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \ . \tag{105}$$

The ordering of the creation and annihilation operators appearing on the right–hand side of Eq. (105) is important in the fermionic case. The mnemonic rule of the ‘stack of plates’, which is equivalent to the pop/push terminology of a stack in computer science, helpfully links it to the ordering of the single–particle states in the matrix element $\langle \alpha\beta | v | \gamma\delta \rangle$. Any (fermionic) ket $|\alpha_1, \alpha_2, \ldots, \alpha_j, \ldots\rangle$ may be understood as a stack where the single–particle states $|\alpha_j\rangle$ play the role of the plates: the plate at the top of the stack appears on the left and the one at the bottom of the stack appears on the right. Annihilation operations behave like “pop” operations on the stack: the top plate should be broken first and the bottom plate last, like in a Greek restaurant. Recall that in the composition of two linear operators U and V acting on a vector $|\Psi\rangle$, $VU|\Psi\rangle = V \circ U |\Psi\rangle$, U first acts on $|\Psi\rangle$ and then V acts on $U|\Psi\rangle$. Hence, the annihilation of the two–state ket $|\gamma\delta\rangle$ corresponds to $a_\delta a_\gamma$. Conversely, creation operators behave like “push” operations on the stack: if a plate is added to the stack, it is added at the top and pushes all other plates towards the bottom. Hence, if a single–particle state is added to the stack, it appears on the left and pushes all the other states towards the right. Thus, the creation of the two-state ket $|\alpha\beta\rangle$ corresponds to $a_\alpha^\dagger a_\beta^\dagger$. The matrix element $\langle\alpha\beta|v|\gamma\delta\rangle$ should be read from right to left: it describes the annihilation of the two–state ket $|\gamma\delta\rangle$ followed by the creation of the two–state ket $|\alpha\beta\rangle$. Therefore, it corresponds to the sequence of operators $a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma$, in accordance with Eq. (105).

We finally specialise Eq. (105) to case where $(|\psi_\alpha\rangle)$ is the position basis $(|\boldsymbol{r}\rangle)$, and obtain the expression of V in terms of the field operator $\hat{\Psi}(\boldsymbol{r})$:

$$\hat{V} = \int d^3r_1 d^3r_2 \, v(\boldsymbol{r}_1 - \boldsymbol{r}_2) \, \hat{\Psi}^\dagger(\boldsymbol{r}_1)\hat{\Psi}^\dagger(\boldsymbol{r}_2)\hat{\Psi}(\boldsymbol{r}_2)\hat{\Psi}(\boldsymbol{r}_1) \ . \tag{106}$$

4.3.2 Question 13: One–body density matrix in terms of the field operator

We now show that the one–body density matrix elements may be expressed as an average of a product of two field operators in the considered quantum state:

$$\langle\boldsymbol{r}|\rho^{(1)}|\boldsymbol{r}'\rangle = \langle\hat{\Psi}^\dagger(\boldsymbol{r}')\Psi(\boldsymbol{r})\rangle \ , \tag{107}$$

an expression which is frequently taken as the definition for the one–body density matrix or first–order correlation functions in advanced textbooks. We give two different proofs for Eq. (107).

First proof. We start from Eq. (43), valid for any single–particle basis $|(\psi_\alpha)\rangle$, in braket notation:

$$\langle\boldsymbol{r}|\rho^{(1)}|\boldsymbol{r}'\rangle = \sum_{\alpha,\beta} \langle\psi_\alpha|\boldsymbol{r}'\rangle \, \langle\boldsymbol{r}|\psi_\beta\rangle \, \langle a_\alpha^\dagger a_\beta\rangle \ . \tag{108}$$

We now specialise to the single–particle basis $(|\psi_\alpha\rangle) = (|\boldsymbol{r}\rangle)$. We replace the running indices α and β by $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$, respectively, and use the definition of the field operator (Eq. (82)) to obtain:

$$\langle\boldsymbol{r}|\rho^{(1)}|\boldsymbol{r}'\rangle = \int d^3r_1 d^3r_2 \, \langle\boldsymbol{r}_1|\boldsymbol{r}'\rangle \, \langle\boldsymbol{r}|\boldsymbol{r}_2\rangle \, \langle\hat{\Psi}^\dagger(\boldsymbol{r}_1)\hat{\Psi}(\boldsymbol{r}_2)\rangle \ . \tag{109}$$

The matrix elements $\langle\boldsymbol{r}'|\boldsymbol{r}_1\rangle = \delta(\boldsymbol{r}_1 - \boldsymbol{r}')$ and $\langle\boldsymbol{r}_2|\boldsymbol{r}\rangle = \delta(\boldsymbol{r}_2 - \boldsymbol{r})$ select the specific positions of $\boldsymbol{r}_1 = \boldsymbol{r}'$ and $\boldsymbol{r}_2 = \boldsymbol{r}$ in the integral, so that Eq. (109) reduces to the sought Eq. (107).

Second proof. The quantities $\phi_\alpha^*(\boldsymbol{r}')$ and $\psi_\beta(\boldsymbol{r})$ are numbers, so that we may write Eq. (43) in the following form:

$$\langle\boldsymbol{r}|\rho^{(1)}|\boldsymbol{r}'\rangle = \left\langle \left(\sum_\alpha \psi_\alpha^*(\boldsymbol{r}') \, a_\alpha^\dagger\right) \left(\sum_\beta \psi_\beta(\boldsymbol{r}) \, a_\beta\right) \right\rangle \ . \tag{110}$$

We recognise the expression for $\hat{\Psi}^\dagger(\boldsymbol{r}')$ (given by Eq. (87)) inside the first set of parentheses and that for $\hat{\Psi}(\boldsymbol{r})$ (given by Eq. (88)) inside the second set, so that Eq. (107) follows immediately.

5 Interacting systems

5.1 Question 18: Various types of interaction

5.1.1 Between two neutral atoms

Two neutral atoms interact via an isotropic and short–ranged interaction. For two alkali atoms in their ground state, the long–range interaction is an *attractive* van der Waals interaction [2, Complement $\mathrm{C_{XI}}$], i.e the interaction potential $V(r) = -C_6/r^6$, with r being the interatomic distance and $C_6 > 0$. This long–range attractive part is due to the fluctuations of the dipoles

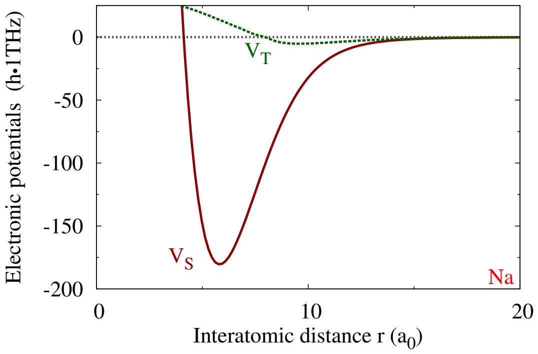

Figure 2 The two potentials $V_S(r)$ and $V_T(r)$ characterising the interaction between two ground–state ^{23}Na atoms. The interatomic distance r is expressed in terms of the Bohr radius $a_0 = 52.9\,\mathrm{fm}$; the energies $V_{S,T}(r)$ are expressed in units of $h \cdot 1\,\mathrm{THz}$.

of each atom inducing a non–vanishing dipole moment on the other atom: this is a second–order effect, which explains the dependence with $1/r^6$ (rather than $1/r^3$ for two permanent dipoles). For small interatomic distances, the interaction is repulsive owing to the Pauli exclusion principle affecting the overlapping electron clouds. Hence, a rough approximation to the interaction between two ground–state alkali atoms may be obtained through a Lennard–Jones potential $V_{\mathrm{LJ}}(r)$:

$$V_{\mathrm{LJ}}(r) = E_{\mathrm{min}} \left[\left(\frac{r_m}{r} \right)^{12} - 2 \left(\frac{r_m}{r} \right)^{6} \right] . \tag{111}$$

The potential of Eq. (111) reaches the minimum $-E_{\mathrm{min}}$ for the interatomic distance $r = r_m$.

A more accurate analysis of the interaction between two alkali atoms should include the role of the electronic spins, which lead to the presence of an *exchange interaction* [7, chap. 32]. Each atom carries a single outer electron. The two outer electrons may combine to form either a singlet state (S) with the total two–electron spin $S = 0$, or a triplet state (T) with $S = 1$. Hence, there are actually two different interatomic potentials $V_S(r)$ and $V_T(r)$, which share the same long–range behaviour $-C_6/r^6$ but differ for intermediate distances. These are illustrated on Fig. 2 in the case of two ground–state ^{23}Na atoms. Both the singlet and the triplet potential wells support bound states. The highest–energy bound states play a key role in the low–energy scattering properties of the two atoms. For large r, the total electronic spin $\boldsymbol{S}$ is not a good quantum number, because the atomic electronic spins $\boldsymbol{s}_{1,2}$ couple to the corresponding nuclear spins $\boldsymbol{i}_{1,2}$, giving rise to the atomic hyperfine structure. The hyperfine coupling term $(\boldsymbol{s}_1 \cdot \boldsymbol{i}_1 + \boldsymbol{s}_2 \cdot \boldsymbol{i}_2)$ does not commute with the total electronic spin $\boldsymbol{S}$. This yields a coupling between the singlet and triplet two–atom wavefunctions, which gives rise to low–energy scattering resonances called Feshbach resonances.

We call R the range of the interaction potentials $V_{S,T}$. For atoms of mass m interacting via the van der Waals interaction $-C_6/r^6$, this range may be estimated by comparing C_6/R^6 to the typical kinetic energy $\hbar^2/(mR^2)$:

$$\frac{C_6}{R^6} = \frac{\hbar^2}{mR^2}, \quad \text{which leads to} \quad R = \left(\frac{mC_6}{\hbar^2} \right)^{1/4} . \tag{112}$$

If the mean interatomic distance $n^{-1/3}$ is much larger than R, i.e. if $nR^3 \ll 1$, the system is said to be dilute. Then, the short–range details of the interaction potential do not matter, and the interaction may be modelled in terms of an effective contact potential:

$$V_{\mathrm{eff}}(r) = \frac{4\pi\hbar^2}{m}\, a\, \delta(r) , \tag{113}$$

where the scattering length a is chosen to reproduce the low–energy scattering properties of the real potential $V(r)$. For two atoms in their ground states, the real interaction is always attractive at large distances (see Fig. 2), but *the effective interaction may be either attractive or repulsive.* The case $a > 0$ corresponds to a repulsive effective interaction, whereas $a < 0$ signals that the effective interaction is attractive. The sign of a, and hence the attractive or repulsive nature of the effective interaction, depend on the position of the highest–energy bound state in the real potential well $V(r)$. In all cases, the scattering cross–section σ is proportional to a^2.

A Feshbach resonance may be exploited to tune the value of a to arbitrarily large or small, positive or negative values of a. If $|a|$ is much larger than the mean interatomic spacing, i.e. if $n|a|^3 \gg 1$, the system is said to be strongly interacting. Note that the system may be simultaneously dilute ($nR^3 \ll 1$) and strongly interacting ($n|a|^3 \gg 1$). This requires the following double condition on the mean interparticle spacing $n^{-1/3}$:

$$R \ll n^{-1/3} \ll |a| \; . \tag{114}$$

This regime, called the 'unitary' limit, is particularly relevant for recent experiments on cold atomic gases, be they Bose or Fermi. For example, the unitary Fermi *gas* [8, § 26.5.4] is readily brought into the superfluid regime, where it exhibits properties which are closely related to those of the superfluid phase of *liquid* ^{4}He (which is the bosonic isotope of helium, whereas ^{3}He is a fermion) [9, 10]. The unitary Bose gas presents challenging instabilities due to increased three–body and four–body loss processes (which are less problematic in the fermionic case thanks to Pauli exclusion), and it is currently the object of intense theoretical and experimental investigation.

5.1.2 Between two dipoles

Some more recent applications of atomic Physics require interatomic interactions which are longer–ranged than the van der Waals interaction of Eq. (111) or its idealised contact version (Eq. (113)). An important example is the construction of two–qubit quantum gates [1, chap. 1.3.2], which are fundamental components required for quantum information processing and some modern formulations of quantum simulation. A way to achieve such longer–ranged interactions is to resort to cold gases exhibiting dipole–dipole interactions [4, chap. 25]. We consider two dipolar particles which carry the (electric or magnetic) dipole moments $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$, respectively. If the two particles are separated by the vector $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$, then the Dipole–Dipole Interaction (DDI) reads:

$$V_{\mathrm{DDI}}(\boldsymbol{r}) = \frac{\boldsymbol{d}_1 \cdot \boldsymbol{d}_2 - 3(\boldsymbol{d}_1 \cdot \hat{\boldsymbol{r}})(\boldsymbol{d}_2 \cdot \hat{\boldsymbol{r}})}{r^3} \; , \tag{115}$$

with $\hat{\boldsymbol{r}} = \boldsymbol{r}/r$ being the unit vector giving the direction of $\boldsymbol{r}$. Equation (115) reveals two important differences of the DDI with respect to the van der Waals interaction. First, the DDI interaction is *longer–ranged*, because it decays for large distances like $1/r^3$ rather than like $1/r^6$. Second, it is *anisotropic*. In order to make the anisotropy more apparent, let us specialise Eq. (115) to the case where both dipoles are polarised in the same direction, $\boldsymbol{d}_1 = \boldsymbol{d}_2 = d\boldsymbol{e}_z$. The polarisation $\boldsymbol{e}_z$ is set by an external electric field for particles carrying an electric dipole moment, and magnetic for particles carrying a magnetic dipole moment. We call θ the angle between the polarisation direction $\boldsymbol{e}_z$ and the interatomic vector $\boldsymbol{r}$. Then, Eq. (115) reduces to:

$$V_{\mathrm{DDI}}(\boldsymbol{r}) = \frac{d^2}{r^3}(1 - 3\cos^2\theta) \; , \tag{116}$$

where the anisotropy is reflected by the explicit dependence on θ. The interaction potential of Eq. (116) is partly repulsive and partly attractive. Indeed, let us call $\theta_c^{\mathrm{DDI}} = \arccos(1/\sqrt{3})$. Then, if $\theta > \theta_c$, then V_{DDI} behaves like $+1/r^3$, which is repulsive, leading to stable dipolar systems. By contrast, if $\theta < \theta_c$, then V_{DDI} behaves like $-1/r^3$, which is attractive, leading to unstable dipolar systems where all particles tend to collapse towards the same point. In order to avoid such instabilities, dipolar systems are usually confined to 2D or 1D geometries thanks to strongly confining potentials in one spatial direction (2D 'pancake'–like geometry) or in two spatial directions (1D 'cigar'–like geometry).

In the absence of an external electric field, the electronic distribution of an atom in its ground state is spherically symmetric. The presence of a permanent electric dipole moment would select a specific direction, thus violating the spherical symmetry. Hence, *atoms in their ground state* *do not carry a permanent electric dipole moment.* However, they may carry a non–negligible permanent magnetic dipole moment. This hold for e.g. bosonic ^{52}Cr and fermionic ^{161}Dy (neither of those atoms belongs to the alkali group). Quantum–degenerate dipolar gases have recently been brought to quantum degeneracy (that is, below T_B for bosons and below T_F for fermions), and their properties are undergoing intense theoretical and experimental scrutiny.

Another way to access the DDI is to replace atoms by heteronuclear diatomic molecules [11]. The ground state of these composite objects is not constrained by spherical symmetry, so that they may be polar. The first experimental realisation of a quantum degenerate gas of such polar molecules has very recently been reported with fermionic $\mathrm{K}-\mathrm{Rb}$ molecules.

A third way to exploit dipolar interactions is to turn to Rydberg atomic states [12]. These states are characterised by one electron being in a highly–excited state. For alkali atoms such as ^{87}Rb, the excited electron is the one on the outer shell. Such a Rydberg state has a well–defined value of the electronic angular momentum l and, hence, a definite spatial parity, which forbids the presence of a diagonal electric dipole moment. However, off–diagonal dipole moments are not forbidden: quite on the contrary, they are huge for large values of $l \gtrsim 50$. For large interatomic distances, these off–diagonal dipole moments yield strong van der Waals interactions, whose van der Waals length R defined by Eq. (112) may exceed the interparticle spacing. For smaller interatomic distances, Rydberg atoms interact through the anisotropic DDI of Eq. (115) (see e.g. Ref. [13, §II.B]).

5.1.3 Between two charged particles

Two charged particles interact via the Coulomb interaction:

$$V_{\text{Coulomb}}(r) = \frac{1}{4\pi\epsilon_0}\,\frac{q_1 q_2}{r}\ , \tag{117}$$

where q_1 and q_2 are the charges of the two interacting particles. The Coulomb interaction is isotropic and long–ranged. It is attractive if $q_1 q_2 < 0$ and repulsive if $q_1 q_2 > 0$. In both cases, the scattering states and bound states of the two–particle system are well known — the bound states exist only in the attractive case and correspond to the discrete energy levels of the hydrogen atom [14, §11.3].

Ions may be trapped and manipulated in a similar way as for neutral atoms. Their long–range interaction is an added complication for experiments, but it may be put to good use in the field of quantum simulation and quantum information processing, where two–qubit gates with excellent fidelity and efficiency have been realised.

Electrons, which carry the charge $-|e|$, are ubiquitous in condensed–matter systems. In many cases, rough but relevant descriptions of condensed–matter phenomena may be obtained by neglecting the interaction between them. This is the ‘independent electron approximation’, whose relevance stems from the fact that interactions in many–electron systems tend to be screened. The electrons themselves interact via the Coulomb interaction, but the system may be described in terms of fictitious ‘quasi–particles’, or ‘dressed electrons’, which interact only very weakly.

5.2 Question 4: Symmetries of $\rho^{(1)}$ for uniform gases

In this section, the trapping potential vanishes ($U(\boldsymbol{r}) = 0$), and no external magnetic field is present (so that the single–particle kinetic energy is $\boldsymbol{p}^2/(2m)$). However, we do allow arbitrary two–particle interactions which only depend on the relative distance between the two particles (and not on their spin states), $V_I(|\boldsymbol{r}-\boldsymbol{r}'|)$, and whose strength and range are arbitrary. We further assume that the system is fully polarised, i.e. all particles are in the same spin state, so that it drops out of the analysis. Our goal is to show that, under these assumptions, the first–order correlation function $g_1(\boldsymbol{r},\boldsymbol{r}')$ depends only on $|\boldsymbol{r}-\boldsymbol{r}'|$. This means in particular that, for such a uniform system, $g_1(\boldsymbol{r},\boldsymbol{r}')$ is real for all $\boldsymbol{r}$ and $\boldsymbol{r}'$.

5.2.1 Invariance under translations

Our first step is to exploit the translational symmetry. The N–particle Hamiltonian H does not commute with the single–particle linear momenta $\boldsymbol{p}_1$, …, $\boldsymbol{p}_N$, because the interactions between the particles mix these momenta. However, because of the translational invariance, H does commute with the *total linear momentum* $\boldsymbol{P} = \boldsymbol{p}_1 + \ldots + \boldsymbol{p}_N$. Therefore, so does the N–body density matrix ρ, both in the canonical ensemble ($\rho_{\mathrm{C}} = \exp(-\beta H)/Z$) and in the grand–canonical ensemble ($\rho_{\mathrm{GC}} = \exp[-\beta(H - \mu N)]/Z$). Hence, the matrix elements of ρ in the momentum basis, $\langle \boldsymbol{p}_1, \ldots, \boldsymbol{p}_N | \rho | \boldsymbol{p}'_1, \ldots, \boldsymbol{p}'_N \rangle$, are non–zero only if the total momenta corresponding to the ket and the bra are equal: $\boldsymbol{p}_1 + \ldots + \boldsymbol{p}_N = \boldsymbol{p}'_1 + \ldots + \boldsymbol{p}'_N$. We are particularly interested in the matrix elements appearing in the partial trace $\mathrm{Tr}_{2\ldots N}(\rho)$ evaluated in the momentum–state basis:

$$\langle \boldsymbol{p}_1 | \rho^{(1)} | \boldsymbol{p}'_1 \rangle = N \, \langle \boldsymbol{p}_1 | \, \mathrm{Tr}_{2\ldots N}(\rho) | \boldsymbol{p}'_1 \rangle = \int d\boldsymbol{p}_2 \ldots d\boldsymbol{p}_N \; \langle \boldsymbol{p}_1, \boldsymbol{p}_2, \ldots, \boldsymbol{p}_N | \; \rho \; | \boldsymbol{p}'_1, \boldsymbol{p}_2, \ldots, \boldsymbol{p}_N \rangle \ . \tag{118}$$

The matrix elements appearing in Eq. (118) are those for which $\boldsymbol{p}_2 = \boldsymbol{p}'_2, \ldots, \boldsymbol{p}_N = \boldsymbol{p}'_N$. Therefore, in order for $\langle \boldsymbol{p}_1 | \rho^{(1)} | \boldsymbol{p}'_1 \rangle$ to be non–zero, the conservation of total momentum requires that $\boldsymbol{p}_1 = \boldsymbol{p}'_1$. Thus, $\rho^{(1)}$ is diagonal in the single–particle momentum basis ($\boldsymbol{p}$). In other words, $\rho^{(1)}$ commutes with the operator $\boldsymbol{p}$, namely $[\rho^{(1)}, \boldsymbol{p}] = 0$. The commutator appearing here is a true commutator, regardless of the bosonic or fermionic nature of the particles.

We now introduce the translation operator $T_{\boldsymbol{r}_0} = \exp(-i\boldsymbol{r}_0 \cdot \boldsymbol{p}/\hbar)$. The action of $T_{\boldsymbol{r}_0}$ on a spatial ket $|\boldsymbol{r}\rangle$ is to shift it by $\boldsymbol{r}_0$: $T_{\boldsymbol{r}_0} \, |\boldsymbol{r}\rangle = |\boldsymbol{r} + \boldsymbol{r}_0\rangle$. The operator $T_{\boldsymbol{r}_0}$ is unitary, so that $T^{\dagger}_{\boldsymbol{r}_0} = T_{-\boldsymbol{r}_0}$. The reduced density matrix $\rho^{(1)}$ commutes with the operator $\boldsymbol{p}$, hence, it commutes with $T_{\boldsymbol{r}_0}$ for any vector $\boldsymbol{r}_0$, and we may write:

$$\langle \boldsymbol{r}' | \rho^{(1)} | \boldsymbol{r} \rangle = \langle \boldsymbol{r}' | T^{\dagger}_{\boldsymbol{r}_0} \; \rho^{(1)} \; T_{\boldsymbol{r}_0} | \boldsymbol{r} \rangle = \langle \boldsymbol{r}' + \boldsymbol{r}_0 | \rho^{(1)} | \boldsymbol{r} + \boldsymbol{r}_0 \rangle \ . \tag{119}$$

We choose $\boldsymbol{r}_0 = -\boldsymbol{r}'$ in Eq. (119) to obtain:

$$\langle \boldsymbol{r}' | \rho^{(1)} | \boldsymbol{r} \rangle = \langle \boldsymbol{0} | \rho^{(1)} | \boldsymbol{r} - \boldsymbol{r}' \rangle \ , \quad \text{which means} \quad g^{(1)}(\boldsymbol{r}, \boldsymbol{r}') = g^{(1)}(\boldsymbol{r} - \boldsymbol{r}') \ . \tag{120}$$

5.2.2 Invariance under rotations

We now turn to the rotational invariance. The N–particle Hamiltonian H commutes with the *projection of the total angular momentum* along the quantisation axis $\boldsymbol{e}_z$, $L_z = l_{z1} + \ldots + l_{zN}$. We repeat the reasoning above, replacing the momentum basis with the following one: $(|r_1, l_1, l_{z1}; \ldots; r_N, l_N, l_{zN}\rangle)$. Here, the quantum number l_j defines the modulus of the single–particle angular momentum $\boldsymbol{l}_j$ through the relation $\boldsymbol{l}_j^2 = l_j(l_j + 1)$. We consider a matrix element of $\rho^{(1)}$ in the corresponding single–particle basis, $(|r_1, l_1, l_{1z}\rangle)$:

$$\begin{aligned} \langle r_1 l_1 l_{1z} | \rho^{(1)} | r'_1 l'_1 l'_{1z} \rangle = N \, \langle r_1 l_1 l_{1z} | \, \mathrm{Tr}_{2\ldots N}(\rho) | r'_1 l'_1 l'_{1z} \rangle = \sum_{l_2, \ldots, l_N} \sum_{l_{z2}, \ldots, l_{zN}} \int dr_2 \ldots dr_N \\ \langle r_1 l_1 l_{1z}; r_2 l_2 l_{2z}; \ldots r_N l_N l_{Nz} | \; \rho \; | r'_1 l'_1 l'_{1z}; r_2 l_2 l_{2z}; \ldots r_N l_N l_{Nz} \rangle \ . \end{aligned} \tag{121}$$

In order for $\langle r_1 l_1 l_{1z} | \rho^{(1)} | r'_1 l'_1 l'_{1z} \rangle$ to be non–zero, the conservation of the total angular momentum projection requires $l_{1z} + l_{2z} + \ldots + l_{Nz} = l'_{1z} + l_{2z} + \ldots + l_{Nz}$, that is, $l_{1z} = l'_{1z}$. Hence, $\rho^{(1)}$ commutes with the single–particle operator l_z. The direction $\boldsymbol{e}_z$ plays no role in this argument, so that $\rho^{(1)}$ also commutes with the operators l_x and l_y.

We now introduce the rotation operator $R_{\theta\hat{\boldsymbol{n}}} = \exp(-i\theta \, \hat{\boldsymbol{n}} \cdot \boldsymbol{l}/\hbar)$. The action of $R_{\theta\hat{\boldsymbol{n}}}$ on a spatial ket $|\boldsymbol{r}\rangle$ is to rotate it about the direction defined by $\hat{\boldsymbol{n}}$ by the angle θ: $R_{\theta\hat{\boldsymbol{n}}} \, |\boldsymbol{r}\rangle = |\mathscr{R}_{\theta\hat{\boldsymbol{n}}} \, \boldsymbol{r}\rangle$ (here, $R_{\theta\hat{\boldsymbol{n}}}$ acts on the single–particle Hilbert space, whereas $\mathscr{R}_{\theta\hat{\boldsymbol{n}}}$ is the geometrical rotation in real 3D space). The operator $R_{\theta\hat{\boldsymbol{n}}}$ is unitary, so that $R^{\dagger}_{\theta\hat{\boldsymbol{n}}} = R_{-\theta\hat{\boldsymbol{n}}}$. The reduced density matrix $\rho^{(1)}$ commutes with the operators l_x, l_y, and l_z, hence, it commutes with $R_{\theta\hat{\boldsymbol{n}}}$ for any direction $\hat{\boldsymbol{n}}$ and angle θ. Starting from Eq. (120) with $\boldsymbol{R} = \boldsymbol{r} - \boldsymbol{r}'$, we may write:

$$\langle \boldsymbol{r}' | \rho^{(1)} | \boldsymbol{r} \rangle = \langle \boldsymbol{0} | R^{\dagger}_{\theta\hat{\boldsymbol{n}}} \, \rho^{(1)} \; R_{\theta\hat{\boldsymbol{n}}} | \boldsymbol{R} \rangle = \langle \boldsymbol{0} | \; \rho^{(1)} \; | \mathscr{R}_{\theta\hat{\boldsymbol{n}}} \boldsymbol{R} \rangle \ . \tag{122}$$

For a given $\boldsymbol{R} = \boldsymbol{r} - \boldsymbol{r}'$, we choose $\boldsymbol{n}$ and θ in Eq. (122) such that $\mathscr{R}_{\theta\hat{\boldsymbol{n}}}\boldsymbol{R} = |\boldsymbol{R}|\boldsymbol{e}_z$. Hence,

$$\langle \boldsymbol{r}'|\rho^{(1)}|\boldsymbol{r}\rangle = \langle \boldsymbol{0}|\, \rho^{(1)}\, |\mathscr{R}_{\theta\hat{\boldsymbol{n}}}|\boldsymbol{R}|\boldsymbol{e}_z\rangle \ , \quad \text{which means} \quad g^{(1)}(\boldsymbol{r},\boldsymbol{r}') = g^{(1)}(|\boldsymbol{r}-\boldsymbol{r}'|) \ . \tag{123}$$

Finally, the fact that $g^{(1)}(\boldsymbol{r},\boldsymbol{r}')$ is real for all $\boldsymbol{r}$ and $\boldsymbol{r}'$ follows from:

$$g^{(1)}(\boldsymbol{r},\boldsymbol{r}') = g^{(1)}(|\boldsymbol{r}-\boldsymbol{r}'|) = g^{(1)}(\boldsymbol{r}',\boldsymbol{r}) = [g^{(1)}(\boldsymbol{r},\boldsymbol{r}')]^* \ . \tag{124}$$

5.3 Diagonalisation of the one–body density operator

5.3.1 Hermiticity of the one–body density operator

We first prove that the one–body density operator $\rho^{(1)}$ is hermitian: $\rho^{(1)\dagger} = \rho^{(1)}$. We provide two *independent* proofs of this result: one in terms of first quantisation and another one in the language of second quantisation.

Proof in terms of first quantisation. We prove the equality of the matrix elements $\langle \boldsymbol{r}|\rho^{(1)\dagger}\boldsymbol{r}'\rangle$ and $\langle \boldsymbol{r}|\rho^{(1)}\boldsymbol{r}'\rangle$ in the single–particle position basis $|\boldsymbol{r}\rangle$. For that purpose, we write:

$$\begin{aligned}
\langle \boldsymbol{r}|\rho^{(1)\dagger}|\boldsymbol{r}'\rangle &= \Big[\langle \boldsymbol{r}'|\rho^{(1)}|\boldsymbol{r}\rangle\Big]^* \\
&= \left[N\int d^3r_2\dots d^3r_N\ \langle \boldsymbol{r}',\boldsymbol{r}_2,\dots,\boldsymbol{r}_N|\,\rho\,|\boldsymbol{r},\boldsymbol{r}_2,\dots,\boldsymbol{r}_N\rangle\right]^* \\
&= N\int d^3r_2\dots d^3r_N\ [\langle \boldsymbol{r}',\boldsymbol{r}_2,\dots,\boldsymbol{r}_N|\,\rho\,|\boldsymbol{r},\boldsymbol{r}_2,\dots,\boldsymbol{r}_N\rangle]^* \\
&= N\int d^3r_2\dots d^3r_N\ \langle \boldsymbol{r},\boldsymbol{r}_2,\dots,\boldsymbol{r}_N|\,\rho^\dagger\,|\boldsymbol{r}',\boldsymbol{r}_2,\dots,\boldsymbol{r}_N\rangle \\
&= N\int d^3r_2\dots d^3r_N\ \langle \boldsymbol{r},\boldsymbol{r}_2,\dots,\boldsymbol{r}_N|\,\rho\,|\boldsymbol{r}',\boldsymbol{r}_2,\dots,\boldsymbol{r}_N\rangle \\
&= \langle \boldsymbol{r}|\rho^{(1)}|\boldsymbol{r}'\rangle \ .
\end{aligned} \tag{125}$$

The first step is the definition of the transpose conjugate operator $\rho^{(1)\dagger}$ in terms of its matrix elements. The second step follows from the definition of $\rho^{(1)}$, the partial trace $\mathrm{Tr}_{2\dots N}$ being performed in the N–particle position basis. The third step simply uses the linearity of the conjugation of a complex number. The fourth step is the definition of the transpose conjugate operator $\rho^\dagger$. The fifth step expresses that the full density matrix ρ is hermitian. The sixth and final step follows from the definition of the matrix element $\langle \boldsymbol{r}|\rho^{(1)}|\boldsymbol{r}'\rangle$ of the reduced density operator $\rho^{(1)}$.

Proof in terms of second quantisation. This proof is independent of the preceding one. It requires a preliminary mathematical step. We are used to calculating expectation values $\langle M\rangle$ for Hermitian operators M, in which case $\langle M\rangle$ is real. By contrast, the expectation value of a non–hermitian operator may be non–real, and it satisfies $\langle M^\dagger\rangle = \langle M\rangle^*$. Indeed:

$$\begin{aligned}
\langle M^\dagger\rangle &= \mathrm{Tr}[\rho\, M^\dagger] \\
&= \mathrm{Tr}[(M\,\rho^\dagger)^\dagger] \\
&= \mathrm{Tr}[(M\,\rho)^\dagger] \\
&= \mathrm{Tr}[M\,\rho]^\star \\
&= \mathrm{Tr}[\rho\, M]^\star \\
&= \langle M\rangle^\star
\end{aligned} \tag{126}$$

In Eq. (126), the first step is the definition of the expectation value in terms of the (full) density operator ρ. The second step exploits the general property $(AB)^\dagger = B^\dagger A^\dagger$ of the Hermitian conjugate of a product of two operators A and B. The third step follows from the fact that the density operator ρ is always Hermitian. The fourth step follows from the definition $A^\dagger = {}^tA^*$ of the Hermitian conjugate $A^\dagger$ of A in terms of transposition (t) and complex conjugation ($*$). The fifth step reflects $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$, which holds for any two operators A and B. The sixth and final step is analogous to the first one.

Next, we consider the non–Hermitian operator $\hat{\Psi}^\dagger(\boldsymbol{r})\hat{\Psi}(\boldsymbol{r}')$ and obtain:

$$\begin{aligned}\langle \boldsymbol{r}|\rho^{(1)}|\boldsymbol{r}'\rangle &= \langle \hat{\Psi}^\dagger(\boldsymbol{r}')\hat{\Psi}(\boldsymbol{r})\rangle \\ &= \langle \Big(\hat{\Psi}^\dagger(\boldsymbol{r})\hat{\Psi}(\boldsymbol{r}')\Big)^\dagger\rangle \\ &= \langle \Big(\hat{\Psi}^\dagger(\boldsymbol{r})\hat{\Psi}(\boldsymbol{r}')\Big)\rangle^* \\ &= \langle \boldsymbol{r}'|\rho^{(1)}|\boldsymbol{r}\rangle^* \\ &= \langle \boldsymbol{r}|\rho^{(1)\dagger}|\boldsymbol{r}'\rangle \ ,\end{aligned} \tag{127}$$

where the first and fourth step follow from Eq. (107), whereas the third step follows from Eq. (126).

5.3.2 Question 19: Diagonalisation of the one–body density operator

The operator $\rho^{(1)}$ is hermitian, hence, it may be diagonalised in an orthonormal basis. Thus, there is a basis $(|\phi_\alpha\rangle)$ of the single–particle Hilbert space $\mathscr{E}^{(1)}$ which consists of (orthogonal and normalised) eigenstates of $\rho^{(1)}$:

$$\rho^{(1)}\,|\phi_\alpha\rangle = \pi_\alpha\,|\phi_\alpha\rangle\,, \quad \text{meaning that} \quad \rho^{(1)} = \sum_\alpha \pi_\alpha\,|\phi_\alpha\rangle\,\langle\phi_\alpha| \ , \tag{128}$$

where the real number π_α is the eigenvalue corresponding to the eigenstate $|\phi_\alpha\rangle$. Therefore, the matrix elements $\langle \boldsymbol{r}|\rho^{(1)}|\boldsymbol{r}'\rangle$ satisfy the same expression as for an ideal gas (see Eq. (55) above):

$$\langle \boldsymbol{r}|\rho^{(1)}|\boldsymbol{r}'\rangle = \sum_\alpha \pi_\alpha\,\phi^*_\alpha(\boldsymbol{r}')\phi_\alpha(\boldsymbol{r}) \ , \tag{129}$$

that is, the expansion of $\rho^{(1)}$ in terms of the wavefunctions $\phi_\alpha(\boldsymbol{r})$ involves only a single sum on the index α.

5.3.3 Positivity of the one–body density operator and Penrose criterion for condensation

We know from Eq. (23) that $\mathrm{Tr}[\rho^{(1)}] = N$. Hence, the π_α appearing in Eq. (128) satisfy:

$$\sum_\alpha \pi_\alpha = N \ . \tag{130}$$

We now show that the real numbers π_α are all positive, i.e. that the hermitian operator $\rho^{(1)}$ is positive. We follow the standard procedure, i.e. we consider an arbitrary ket $|\psi\rangle$ in the space $\mathscr{E}^{(1)}$ and calculate $\langle\psi|\rho^{(1)}|\psi\rangle$. For that purpose, we start from Eq. (22) and expand the partial trace $\mathrm{Tr}_{2\ldots N}$ in the position basis (but any N–particle basis would do just as well):

$$\langle\psi|\rho^{(1)}|\psi\rangle = N\int d^3r_2\ldots dr_N\,\langle\psi,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N|\rho|\psi,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N\rangle \ . \tag{131}$$

The many–body density matrix is a positive operator, hence, all of its diagonal matrix elements appearing in Eq. (131) are positive. Therefore, $\langle\psi|\rho^{(1)}|\psi\rangle \geq 0$. Then, choosing $|\psi\rangle$ to be one of the eigenstates $|\phi_\alpha\rangle$, we find $0 \leq \langle\phi_\alpha|\rho^{(1)}|\phi_\alpha\rangle = \pi_\alpha$, so that all eigenvalues π_α are positive. Hence, we may call the eigenstates $|\phi_\alpha\rangle$ ‘single–particle wavefunctions’ and interpret the corresponding eigenvalues π_α as their populations.

This interpretation of Eq. (129) yields a criterion, due to Penrose, for whether or not a Bose–Einstein condensate is present in the system. The system is said to be Bose–condensed if one at least of the populations π_α is macroscopic, i.e. of the order of N. This definition is applicable at zero and non–zero temperatures, both in the absence and in the presence of interactions. In the uniform case, where the wavefunctions $\phi_\alpha(\boldsymbol{r})$ are not constrained to vanish for large r because no trapping potential is imposed onto the system, this criterion coincides with the definition for off–diagonal long–range order given in Sec. 4.2.4.

For an ideal Bose gas at $T = 0$, $\pi_0 = N$ and the system is Bose–condensed. For temperatures $0 < T < T_B$, the condensate fraction $\pi_0/N < 1$, but it still remains sizeable ($\pi_0/N = 1-(T/T_B)^{3/2}$ for the uniform Bose gas of Sec. 4.2.4: see Eq. Eq. (70)). However, for $T > T_B$, the ground state is no longer macroscopically populated, and all $\pi_\alpha \ll N$ in the thermodynamic limit.

5.3.4 Question 20: Quantum depletion

We now briefly discuss the role of repulsive interactions on the condensate fraction π_0/N. These interactions cause the population π_0 to decrease with respect to N, a phenomenon known as 'quantum depletion'. Atomic gases in the presence of weak repulsive interactions are characterised by a small value of the adimensional parameter na^3 (with $a > 0$). In the uniform case at $T = 0$, the condensate fraction at $T = 0$ is $\pi_0/N = 1 - \gamma(na^3)^{1/3}$ with $\gamma = 8/(3\sqrt{\pi}) \approx 1.5$, a result which may be obtained using well–understood analytical techniques based on the Bogoliubov approach [4, Section 4.3]. There, the quantum depletion is very small. It has recently been measured unambiguously for the first time in an experiment specially designed to bring the depleted fraction up to a few percent. The situation is very different for liquid ^{4}He. There, the system is not dilute, in the sense that nR^3, where R is the range of the interaction, is not small compared to 1 — this is why the system behaves as a liquid rather than as a gas. Therefore, the previous estimate for π_0/N no longer holds. In liquid helium, π_0/N is not accurately given by known analytical techniques, it should be either measured or calculated numerically. In both cases, we find $\pi_0/N \sim 0.1$, i.e. the role of interactions is so strong that the condensate is almost fully depleted [4, Section 8.4]. Nevertheless, liquid Helium does behave as a superfluid. This means that the condensate fraction and the superfluid fraction do not coincide, an intriguing point which has spawned many interesting recent developments, in particular towards lower–dimensional systems (where the transition to a condensed phase is replaced by a crossover to the superfluid regime) and stronger–interacting quantum gases (where the Bogoliubov approach is not applicable).

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