Quantum Mechanics II

Exercise 4: Second quantization. N-body problems – Solutions

16 October 2019

1. Express two-particle operator $\hat{F} = \frac{1}{2}\sum_{\alpha\neq\beta} \hat{f}^{(2)}(x_\alpha; x_\beta)$ in terms of creation and annihilation operators for the case of bosons as well as fermions.

   Reminder: $\sum_{\alpha=1}^{N} |i\rangle_\alpha \langle j|_\alpha = a_i^\dagger a_j$.

   Solution: Many-particle systems are described by states in the tensor product of one-particle Hilbert spaces. Let $\{|i\rangle\}$ be an orthonormal basis in the one-particle Hilbert space. The matrix form of two-particle operator $\hat{f}^{(2)}$ in the tensor product space of two particles is:

$$\hat{f}^{(2)} = \sum_{ijkl} |i,j\rangle\langle i,j|\hat{f}^{(2)}|k,l\rangle\langle k,l| = \sum_{ijkl} f_{ijkl}|i,j\rangle\langle k,l|$$

   Bosons (fermions) are identical particles therefore for any pair of bosons (fermions) operator $\hat{f}^{(2)}$ will have the same form. Then for the full operator we have

$$\begin{aligned}
\hat{F} &= \frac{1}{2}\sum_{\alpha\neq\beta}\left(\sum_{ijkl} f_{ijkl}|i,j\rangle_{\alpha,\beta}\langle k,l|_{\alpha,\beta}\right) = \frac{1}{2}\sum_{ijkl} f_{ijkl}\sum_{\alpha\neq\beta}|i\rangle_\alpha\langle k_\alpha|\otimes|j\rangle_\beta\langle l|_\beta \\
&= \frac{1}{2}\sum_{ijkl} f_{ijkl}\left(\left(\sum_\alpha |i\rangle_\alpha\langle k_\alpha|\right)\otimes\left(\sum_\beta |j\rangle_\beta\langle l|_\beta\right) - \sum_\beta |i\rangle_\beta \underbrace{\langle k|j\rangle_\beta}_{\delta_{jk}}\langle l|_\beta\right) \\
&= \frac{1}{2}\sum_{ijkl} f_{ijkl}\left(\hat{a}_i^\dagger\hat{a}_k\hat{a}_j^\dagger\hat{a}_l - \hat{a}_i^\dagger\delta_{jk}\hat{a}_l\right),
\end{aligned}$$

   where in the second line we have taken into account the terms corresponding to the interaction of particle with itself as shown in Fig. 1. In the last term, we can replace $\delta_{jk} = [\hat{a}_k, \hat{a}_j^\dagger]$ (for bosons) and $\delta_{jk} = \{\hat{a}_k, \hat{a}_j^\dagger\}$ (for fermions). Thus we obtain:

$$\begin{aligned}
\hat{F} &= \frac{1}{2}\sum_{ijkl} f_{ijkl}\,\hat{a}_i^\dagger\left(\hat{a}_k a_j^\dagger - \hat{a}_k\hat{a}_j^\dagger \pm \hat{a}_j^\dagger\hat{a}_k\right)\hat{a}_l \\
&= \pm\frac{1}{2}\sum_{ijkl} f_{ijkl}\,\hat{a}_i^\dagger\hat{a}_j^\dagger\underbrace{\hat{a}_k\hat{a}_l}_{\pm\hat{a}_l\hat{a}_k} = \frac{1}{2}\sum_{ijkl} f_{ijkl}\,\hat{a}_i^\dagger a_j^\dagger\hat{a}_l\hat{a}_k \blacksquare
\end{aligned}$$

   Note that the order of the sums of operators (first the sum over β and then the sum over α) was chosen arbitrary. It is easy to see that the opposite choice would lead to the exchange of indices of creation and annihilation operators in the final expression as follows $i \leftrightarrow j$ and $k \leftrightarrow l$. However, by commuting two pairs of operators $\hat{a}_j^\dagger\hat{a}_i^\dagger = \pm\hat{a}_i^\dagger\hat{a}_j^\dagger$ and $\hat{a}_k\hat{a}_l = \pm\hat{a}_l\hat{a}_k$ the original result can be we recovered without any change of sign for both, bosons and fermions.

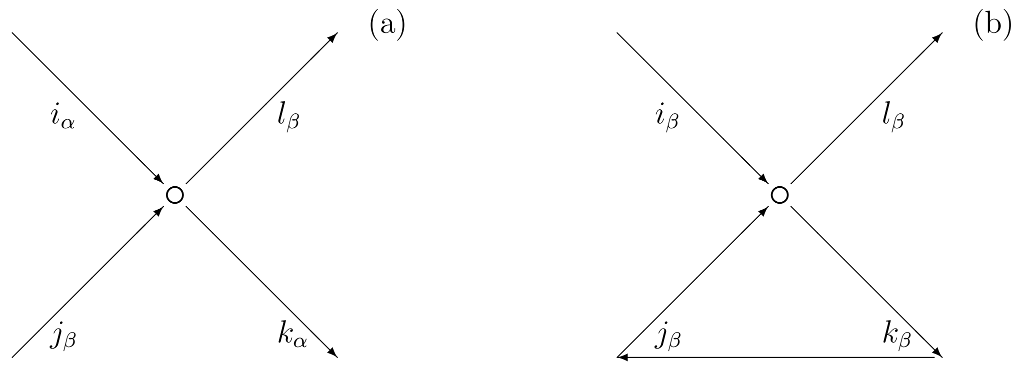

Figure 1: Interaction of two particles (a) and selfinteraction (b).

2. Show that the number operator $\hat{N} = \sum_i \hat{a}_i^\dagger \hat{a}_i$ (for bosons and fermions) commute with the Hamiltonian

$$\hat{H} = \sum_{jk} \hat{a}_j^\dagger \langle i|T|k\rangle \hat{a}_k + \frac{1}{2} \sum_{jklm} \hat{a}_j^\dagger \hat{a}_k^\dagger \langle jk|V|lm\rangle \hat{a}_m \hat{a}_l .$$

<u>Solution:</u> We will check the commutation with each term of the Hamiltonian.

$$\begin{aligned}
\left[\hat{N}, \sum_{jk} \hat{a}_j^\dagger T_{jk} \hat{a}_k\right] &= \sum_{ijk} T_{jk} [\hat{a}_i^\dagger \hat{a}_i, \hat{a}_j^\dagger \hat{a}_k] = \sum_{ijk} T_{jk} (\hat{a}_i^\dagger \underbrace{\hat{a}_i \hat{a}_j^\dagger}_{\delta_{ij} \pm \hat{a}_j^\dagger \hat{a}_i} \hat{a}_k - \hat{a}_j^\dagger \underbrace{\hat{a}_k \hat{a}_i^\dagger}_{\delta_{ik} \pm \hat{a}_i^\dagger \hat{a}_k} \hat{a}_i) \\
&= \sum_{ijk} T_{jk} (\delta_{ij} \hat{a}_i^\dagger \hat{a}_k - \delta_{ik} \hat{a}_j^\dagger \hat{a}_i) \pm \sum_{ijk} T_{jk} (\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_i \hat{a}_k - \hat{a}_j^\dagger \hat{a}_i^\dagger \hat{a}_k \hat{a}_i) \\
&= \sum_{jk} T_{jk} \underbrace{(\hat{a}_j^\dagger \hat{a}_k - \hat{a}_j^\dagger \hat{a}_k)}_{0} \pm \sum_{ijk} T_{jk} (\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_i \hat{a}_k - (\pm \hat{a}_i^\dagger \hat{a}_j^\dagger)(\pm \hat{a}_i \hat{a}_k)) \\
&= \pm \sum_{ijk} T_{jk} \underbrace{(\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_i \hat{a}_k - \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_i \hat{a}_k)}_{0} = 0 .
\end{aligned}$$

$$\begin{aligned}
\left[\hat{N}, \sum_{jklm} \hat{a}_j^\dagger \hat{a}_k^\dagger \langle jk|V|lm\rangle \hat{a}_m \hat{a}_l\right] &= \sum_{ijkm} V_{jklm} [\hat{a}_i^\dagger \hat{a}_i, \hat{a}_j^\dagger \hat{a}_k^\dagger \hat{a}_m \hat{a}_l] \\
&= \sum_{ijklm} V_{jklm} (\hat{a}_i^\dagger \underbrace{\hat{a}_i \hat{a}_j^\dagger}_{\delta_{ij} \pm \hat{a}_j^\dagger \hat{a}_i} \hat{a}_k^\dagger \hat{a}_m \hat{a}_l - \hat{a}_j^\dagger \hat{a}_k^\dagger \hat{a}_m \underbrace{\hat{a}_l \hat{a}_i^\dagger}_{\delta_{il} \pm \hat{a}_i^\dagger \hat{a}_l} \hat{a}_i) \\
&= \sum_{ijklm} V_{jklm} (\delta_{ij} \hat{a}_i^\dagger \hat{a}_k^\dagger \hat{a}_m \hat{a}_l - \delta_{il} \hat{a}_j^\dagger \hat{a}_k^\dagger \hat{a}_m \hat{a}_i) \\
&\pm \sum_{ijklm} V_{jklm} (\hat{a}_i^\dagger \hat{a}_j^\dagger \underbrace{\hat{a}_i \hat{a}_k^\dagger}_{\delta_{ik} \pm a_k^\dagger \hat{a}_i} \hat{a}_m \hat{a}_l - \hat{a}_j^\dagger \hat{a}_k^\dagger \underbrace{\hat{a}_m \hat{a}_i^\dagger}_{\delta_{im} \pm a_i^\dagger \hat{a}_m} \hat{a}_l \hat{a}_i) \\
&= \sum_{jklm} V_{jklm} \underbrace{(a_j^\dagger \hat{a}_k^\dagger \hat{a}_m \hat{a}_l - \hat{a}_j^\dagger \hat{a}_k^\dagger \hat{a}_m \hat{a}_l)}_{0}
\end{aligned}$$

$$
\begin{aligned}
&\pm \sum_{ijklm} V_{jklm}(\delta_{ik}\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_m \hat{a}_l - \delta_{im}\hat{a}_j^\dagger \hat{a}_k^\dagger \hat{a}_l \hat{a}_i) \\
&+ \sum_{ijklm} V_{jklm}(\hat{a}_i^\dagger \hat{a}_j^\dagger a_k^\dagger \hat{a}_i \hat{a}_m \hat{a}_l - \hat{a}_j^\dagger \underbrace{\hat{a}_k^\dagger \hat{a}_i^\dagger}_{\pm \hat{a}_i^\dagger \hat{a}_k^\dagger} \hat{a}_m \underbrace{\hat{a}_l \hat{a}_i}_{\pm \hat{a}_i \hat{a}_l}) \\
&= \pm \sum_{jklm} V_{jklm}(\hat{a}_k^\dagger \hat{a}_j^\dagger \hat{a}_m \hat{a}_l - \underbrace{\hat{a}_j^\dagger \hat{a}_k^\dagger}_{\pm a_k^\dagger \hat{a}_j^\dagger} \underbrace{\hat{a}_l \hat{a}_m}_{\pm \hat{a}_m \hat{a}_l}) \\
&+ \sum_{ijklm} V_{jklm}(\hat{a}_i^\dagger \hat{a}_j^\dagger a_k^\dagger \hat{a}_i \hat{a}_m \hat{a}_l - \underbrace{\hat{a}_j^\dagger \hat{a}_i^\dagger}_{\pm \hat{a}_i^\dagger \hat{a}_j^\dagger} \hat{a}_k^\dagger \underbrace{\hat{a}_m \hat{a}_i}_{\pm \hat{a}_i \hat{a}_m} \hat{a}_l) \\
&= \pm \sum_{jklm} V_{jklm}(\underbrace{\hat{a}_k^\dagger \hat{a}_j^\dagger \hat{a}_m \hat{a}_l - a_k^\dagger \hat{a}_j^\dagger \hat{a}_m \hat{a}_l}_{0}) \\
&+ \sum_{ijklm} V_{jklm}(\underbrace{\hat{a}_i^\dagger \hat{a}_j^\dagger a_k^\dagger \hat{a}_i \hat{a}_m \hat{a}_l - \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k^\dagger \hat{a}_i \hat{a}_m \hat{a}_l}_{0}) = 0 \blacksquare
\end{aligned}
$$

3. Bose-Einstein Condensate (BEC) in a harmonic trap.

   Consider N bosons of spin zero in an isotropic harmonic trap of angular frequency ω. The interactions between particles are neglected and the mean number of particles at the energy level E is given by the Bose-Einstein law

$$n_E = \frac{1}{e^{(E-\mu)/k_b T} - 1},$$

   where μ is chemical potential and T is temperature.

   Show that:

   (a) The chemical potential satisfies $\mu < \frac{3}{2}\hbar\omega$.

   Solution: The number of particles is a non negative number, therefore, from the definition of n_E we have

$$n_E \geq 0 \Leftrightarrow e^{(E-\mu)/k_b T} - 1 > 0 \Leftrightarrow (E-\mu)/k_b T > 0 \Leftrightarrow E > \mu.$$

   The energy levels, which for bosons in the three dimensional trap are

$$E_n = \left(n + \frac{3}{2}\right)\hbar\omega.$$

   The last inequality should hold for all levels therefore,

$$E_n \geq E_0 = \frac{3}{2}\hbar\omega > \mu \blacksquare$$

   (b) The number of particles N outside the fundamental level of the trap satisfies

$$N \leq F(\xi) = \sum_{n=1}^{\infty} \frac{(n+1)(n+2)}{2(e^{n\xi} - 1)}, \qquad \xi = \frac{\hbar\omega}{k_b T}.$$

   Reminder: The degeneracy of the energy level $E_n = (n + \frac{3}{2})\hbar\omega$ is

$g_n = \frac{1}{2}(n+1)(n+2)$.

Solution: The number of particles N outside the fundamental level in the trap is given by the sum over all other energy levels

$$N' = \sum_{n=1}^{\infty} g_n n_{E_n} = \frac{1}{2}\sum_{n=1}^{\infty}(n+1)(n+2)(e^{(E_n-\mu)}-1)^{-1}$$

where g_n and n_{E_n} are degeneracy and the mean number of particles at level n. Starting from the inequality on μ proven in 4 a) we obtain

$$\begin{aligned}
-\mu \geq -\frac{3}{2}\hbar \;\; &\Leftrightarrow \;\; E_n - \mu \geq E_n - \frac{3}{2}\hbar\omega = n\hbar\omega \\
&\Leftrightarrow \;\; e^{(E_n-\mu)/k_\mathrm{B}T} \geq e^{n\hbar\omega/k_\mathrm{B}T} \\
&\Leftrightarrow \;\; \left(e^{(E_n-\mu)/k_\mathrm{B}T}-1\right)^{-1} \leq \left(e^{n\xi}-1\right)^{-1}, \quad \xi = \frac{\hbar\omega}{k_\mathrm{B}T}.
\end{aligned}$$

Using the last inequality in the expression for N' we have:

$$N' = \frac{1}{2}\sum_{n=1}^{\infty}(n+1)(n+2)(e^{(E_n-\mu)}-1)^{-1} \leq \sum_{n=1}^{\infty}\frac{(n+1)(n+2)}{2(e^{n\xi}-1)} = F(\xi) \blacksquare$$

(c) In the limit $k_\mathrm{B}T \gg \hbar\omega$ the discrete sum in the definition of $F(\xi)$ can be replaced by an integral. Show that the number of particles outside the fundamental level is majorized by

$$N'_{\max} = \zeta(3)\left(\frac{k_bT}{\hbar\omega}\right)^3,$$

where the Rieman $\zeta(n)$ fonction.

Reminder:

$$\int_0^{\infty}\frac{x^{\alpha-1}}{e^x-1}\mathrm{d}x = \Gamma(\alpha)\zeta(\alpha), \qquad \Gamma(3) = 2!, \qquad \zeta(3) \approx 1.202.$$

Solution: In the limit $k_\mathrm{B}T \gg \hbar\omega$, variable $x = \frac{\hbar\omega}{k_\mathrm{B}T}n = \xi n$ changes almost continuously with n and therefore the sum in the definition of $F(\xi)$ can be replaced by the integral

$$F(\xi) = \int_0^{\infty}\frac{\left(\frac{x}{\xi}+1\right)\left(\frac{x}{\xi}+2\right)}{2(e^x-1)}\frac{dx}{\xi} = \frac{1}{2\xi}\int_0^{\infty}\frac{\left(\frac{x^2}{\xi^2}+3\frac{x}{\xi}+2\right)}{e^x-1}dx.$$

Note that in the limit $k_\mathrm{B}T \gg \hbar\omega$ we have $\xi \ll 1$ and therefore

$$\frac{1}{\xi^2} \gg \frac{1}{\xi} \gg 1.$$

Keeping only the highest order term we obtain

$$F(\xi) \approx \frac{1}{2\xi^3}\int_0^{\infty}\frac{x^2}{e^x-1}dx = \frac{1}{2\xi^3}\Gamma(3)\zeta(3)$$

Then using $\Gamma(3) = 2! = 2$ we come to

$$F(\xi) \approx \zeta(3)\left(\frac{k_{\mathrm{B}}T}{\hbar\omega}\right)^3,$$

which gives us

$$N'_{\max} = \zeta(3)\left(\frac{k_{\mathrm{B}}T}{\hbar\omega}\right)^3$$

(d) What happens if we place in the trap more than $N'_{\max}$ particles? At which temperature this phenomenon can be observed in a trap of frequency $\frac{\omega}{2\pi} = 100$ Hz containing 10^6 atoms?

Solution: If more than N' atoms are in the trap the excess number of bosons will be at the fundamental level. This phenomenon is called Bose-Einstein condensation. By inverting the result of 4 c) we obtain the temperature of such transition:

$$T = \left(\frac{N'}{\zeta(3)}\right)^{1/3}\frac{\hbar\omega}{k_{\mathrm{B}}} \simeq 4,52\cdot 10^{-7}K,$$

taking into account the following numbers

$$\begin{cases} N'_{\max} = 10^6 \\ \zeta(3) \approx 1.202 \\ \hbar\omega = h\nu = 6,63\cdot 10^{-34}\cdot 100[\mathrm{J}\cdot\mathrm{s}\cdot\mathrm{Hz}] \\ k_{\mathrm{B}} = 1.38\cdot 10^{-23}[\mathrm{J}\cdot\mathrm{K}^{-1}]. \end{cases}$$

The relation shows us that by decreasing the temperature we decrease the number of bosons which can be outside the fundamental level. Even if initially we had $N < N'$ by decreasing temperature we can decrease N' such that $N > N'$, and therefore, $N - N'$ bosons will necessarily occupy the fundamental level (go to the BE condensate).

4. Fermi gas : non-interacting fermions at low (zero) temperature.

- "non-interacting" particles - the energy of the particles is only kinetic.
- "low temperature" - the particles occupy the lowest possible energy levels.

Consider N non-interacting fermions of spin s at low temperature confined in a three-dimensional (cubic) box with the edge length L:

(a) Find the relation between the density of the Fermi gas ρ and the *Fermi momentum* p_F asuming that the number of fermions N is large. Use the momentum quantization of a free particle in a box with the momentum eigenvalues $\vec{p} = \frac{2\pi\hbar}{L}\vec{n}$, where $\vec{n} = (n_1, n_2, n_3)$ and all $n_i \neq 0$ integer. Take into account the maximal number of fermions of spin s which can occupy the same energy level.

Reminder: Fermi momentum is the maximal absolute value of the momentum of a fermionic particle in the Femi gas.

Solution: The total hamiltonian of N independent fermions is a sum of N individual hamiltonians of single fermion in a box (in our case), because there is no interaction. The eigenstates of each individual hamiltonian are plane waves

$\phi_{\mathbf{p}}(\mathbf{r}) = e^{i\mathbf{pr}}/L^3$, to which is associated one of $2s+1$ spin states corresponding to a particular projection $m_s\hbar$ ($m_s = -s, -s+1, \dots, s$) of spin on a chosen axis. The three-dimensional momentum is given by $\mathbf{p} = (2\pi\hbar/L)\mathbf{n}$, where $\mathbf{n} = (n_1, n_2, n_3)$ is a three-dimensional vector of integers (positive or negative). The fundamental level of the total system is achieved when the particles fill in all possible states with lowest energies and therefore momenta. Then the absolute values of all momenta are bounded by *Fermi momentum* $|\mathbf{p}| < p_F$. The sum of the filled states is equal to N.

$$N = \sum_{\mathbf{p}(|\mathbf{p}|<p_F)} (2s+1).$$

For large N the sum may be replaced by integral over the sphere of radius p_F:

$$N \simeq (2s+1)\frac{L^3}{(2\pi\hbar)^3}\int_{|\mathbf{p}|<p_F} \mathrm{d}^3\mathbf{p} = (2s+1)\frac{L^3}{(2\pi\hbar)^3}\frac{4}{3}\pi p_F^3 = \frac{2s+1}{6\pi^2}\left(\frac{Lp_F}{\hbar}\right)^3.$$

The the gas density $\rho = N/L^3$ is related to p_F as

$$\rho = \frac{2s+1}{6\pi^2}\left(\frac{p_F}{\hbar}\right)^3.$$

(b) Express the average energy of the fermions in terms of the *Fermi energy* ε_F corresponding to Fermi momentum p_F.

Solution: The Fermi energy for a particle of mass m is given in terms of the Fermi momentum as $\epsilon_F = p_F^2/2m$. Since the energy of non-interacting particles is only kinetic, and for a large number of particles ($N \gg (2s+1)$), if a particle is added to a Fermi gas of $N-1$ particles, the total energy of the gas increases by an ammount equal to the Fermi energy

$$\epsilon_F(N) = \frac{1}{2m_e}\left(\frac{6\pi^2\hbar^3 N}{L^3(2s+1)}\right)^{2/3}.$$

Hence, the average energy of the gas is approximately given by

$$\langle E\rangle = \frac{1}{N}\int_0^N \epsilon_F(N')dN' = \frac{3}{5}\epsilon_F(N).$$

(c) Express the Fermi energy as a function of the density of fermions and deduce an expression of the Fermi energy for electrons.

NB: The Fermi energy of electrons can attain large values ($\varepsilon_F = 3eV$ in sodium metal) which is much higher than the kinetic energy of the thermal motion at room temperature ($k_{\mathrm{B}}T \approx 0,025$ eV). That is why the "zero temperature" approximation is applicable for the conduction electrons in metals even at room temperature.

Solution: Using the relation between the density of particles and the Fermi momentum we have for electrons ($s = 1/2$):

$$\rho_e = \frac{1}{3\pi^2}\left(\frac{p_F}{\hbar}\right)^3 = \frac{1}{3\pi^2\hbar^3}(2m\epsilon_F)^{3/2},$$

and finally

$$\epsilon_F = \frac{\hbar^2\left(3\rho_e\pi^2\right)^{3/2}}{2m_e}.$$

Note. Applications of the Fermi gas model:

- conduction electrons in a metal
- semi-conductors
- electronic degenerate gas in white dwarfs
- electronic degenerate gas in neutron stars