Karlsruhe Institute of Technology

Institute for Theoretical Condensed Matter physics

Condensed Matter Theory I WS 2022/2023

Prof. Dr. A. Shnirman

Dr. D. Shapiro, Dr. H. Perrin

Sheet 9

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The last task is a bonus exercise. It will be corrected during the tutorial only if we have enough time. In any case, its correction will be uploaded on Ilias with the other exercises.

Category A

1. Correlation functions in ideal Fermi gas $(5 + 10 + 5 + 10 + 5 = 35$ Points)

Consider a 3D system with a finite volume V of N non-interacting fermions in the ground state $|\Psi_0\rangle$. One can express the density operator for particles in the spin state σ using the creation and annihilation operators:

$$\hat{n}(\boldsymbol{r}, \sigma) = \frac{1}{V} \sum_{\boldsymbol{k},\boldsymbol{k}'} e^{-i(\boldsymbol{k}-\boldsymbol{k}')\boldsymbol{r}} a^\dagger_{\boldsymbol{k},\sigma} a_{\boldsymbol{k}',\sigma}.$$

where $\sigma = \downarrow, \uparrow$ is one of the eigenstate of the σ_z operator. The operator $a^\dagger_{\boldsymbol{k},\sigma}$ increases the number of particles in the state $\boldsymbol{k}$ and σ to 1. The operator $a_{\boldsymbol{k},\sigma}$ reduces the number of particles in this state to 0. The creation and annihilation operators satisfy the anti-commutation relations:

$$\{\hat{a}_{\boldsymbol{k},\sigma}, \hat{a}_{\boldsymbol{k}',\sigma'}\} = \{\hat{a}^\dagger_{\boldsymbol{k},\sigma}, \hat{a}^\dagger_{\boldsymbol{k}',\sigma'}\} = 0, \qquad \{\hat{a}^\dagger_{\boldsymbol{k},\sigma}, \hat{a}_{\boldsymbol{k}',\sigma'}\} = \delta_{\sigma,\sigma'}\delta_{\boldsymbol{k},\boldsymbol{k}'}.$$

The ground state of the free Fermi gas can be expressed as follows:

$$|\Psi_0\rangle = \prod_{|\boldsymbol{k}|<k_F,\sigma} \hat{a}^\dagger_{\boldsymbol{k},\sigma}|0\rangle,$$

where all momenta from $|k| = 0$ up to k_F are filled.

(a) Show that, the Fermi momentum in 3D is given by:

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

where

$$n = \frac{N}{V} = \sum_\sigma \langle\Psi_0|\hat{n}(\boldsymbol{r}, \sigma)|\Psi_0\rangle,$$

is the particle density.

We now introduce the fermionic field operators:

$$\hat{\psi}_\sigma(\boldsymbol{r}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{r}} \hat{a}_{\boldsymbol{k},\sigma}, \qquad \hat{\psi}^\dagger_\sigma(\boldsymbol{r}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\boldsymbol{r}} \hat{a}^\dagger_{\boldsymbol{k},\sigma},$$

whose effect are: $\hat{\psi}_\sigma(\boldsymbol{r})$ destroys a particle with spin σ at $\boldsymbol{r}$, while $\hat{\psi}^\dagger_\sigma(\boldsymbol{r})$ creates a particle with spin σ at $\boldsymbol{r}$. Show that these field operators satisfy the canonical anti-commutation relations:

$$\{\hat{\psi}_\sigma(\boldsymbol{r}), \hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}')\} = \delta(\boldsymbol{r}-\boldsymbol{r}')\delta_{\sigma,\sigma'}.$$

Solution:

$$\begin{aligned}
n &= \sum_\sigma \frac{1}{V}\sum_{\boldsymbol{k_1},\boldsymbol{k_2}} e^{-i(\boldsymbol{k_1}-\boldsymbol{k_2})\boldsymbol{r}} \langle 0| \prod_{|\boldsymbol{k}|<k_F,\sigma'} a_{\boldsymbol{k},\sigma'} a^\dagger_{\boldsymbol{k_1},\sigma} \hat{a}_{\boldsymbol{k_2},\sigma} \prod_{|\boldsymbol{k'}|<k_F,\sigma''} a^\dagger_{\boldsymbol{k'},\sigma''} |0\rangle \\
&= \sum_\sigma \frac{1}{V}\sum_{|\boldsymbol{k_1}|,|\boldsymbol{k_2}|<k_F} e^{-i(\boldsymbol{k_1}-\boldsymbol{k_2})\boldsymbol{r}} \langle 0| \prod^{|\boldsymbol{k}|<k_F,\sigma'}_{\sigma'(\boldsymbol{k},\sigma')\neq(\boldsymbol{k_1},\sigma)} a_{\boldsymbol{k},\sigma'} \prod^{|\boldsymbol{k'}|<k_F,\sigma''}_{\sigma'(\boldsymbol{k'},\sigma'')\neq(\boldsymbol{k_2},\sigma)} a^\dagger_{\boldsymbol{k'},\sigma''} |0\rangle \\
&= \sum_\sigma \frac{1}{V}\sum_{|\boldsymbol{k_1}|,|\boldsymbol{k_2}|<k_F} e^{-i(\boldsymbol{k_1}-\boldsymbol{k_2})\boldsymbol{r}} \delta_{\boldsymbol{k_1},\boldsymbol{k_2}} = 2\int_{|\boldsymbol{k}|<k_F} \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3} = \frac{k_F^3}{3\pi^2}
\end{aligned}$$

The anti-commutation relation of the fermionic field is:

$$\begin{aligned}
\left\{\hat{\psi}_\sigma(\boldsymbol{r}), \hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}')\right\} &= \frac{1}{V}\sum_{\boldsymbol{k},\boldsymbol{k}'} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} \left(\hat{a}_\sigma(\boldsymbol{k})\hat{a}^\dagger_{\sigma'}(\boldsymbol{k}') + \hat{a}^\dagger_{\sigma'}(\boldsymbol{k}')\hat{a}_\sigma(\boldsymbol{k})\right) \\
&= \frac{1}{V}\sum_{\boldsymbol{k},\boldsymbol{k}'} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} \delta_{\sigma\sigma'}\delta_{\boldsymbol{k}\boldsymbol{k}'} \\
&= \delta_{\sigma\sigma'}\frac{1}{V}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} = \delta_{\sigma\sigma'}\int_{\boldsymbol{k}} \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} = \delta_{\sigma\sigma'}\delta(\boldsymbol{r}-\boldsymbol{r}')
\end{aligned}$$

(b) The one-particle correlation function is defined as follows:

$$G_\sigma(\boldsymbol{r}-\boldsymbol{r}') = \langle\Psi_0|\hat{\psi}^\dagger_\sigma(\boldsymbol{r})\hat{\psi}_\sigma(\boldsymbol{r}')|\Psi_0\rangle.$$

This correlation function can be interpreted as the probability amplitude of an electron with spin σ being destroyed at $\boldsymbol{r}'$ and recreated at $\boldsymbol{r}$. Demonstrate that it gives:

$$G_\sigma(\boldsymbol{r}-\boldsymbol{r}') = \frac{3n}{2}\frac{\sin x - x\cos x}{x^3}, \qquad x = k_F|\boldsymbol{r}-\boldsymbol{r}'|.$$

Hint: Use the Fourier transform

Solution:

$$\begin{aligned}
G_\sigma(\boldsymbol{r}-\boldsymbol{r}') &= \frac{1}{V}\sum_{\boldsymbol{k},\boldsymbol{k}'} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} \langle\Psi_0|\hat{a}^\dagger_\sigma(\boldsymbol{k})\hat{a}_\sigma(\boldsymbol{k}')|\Psi_0\rangle = \begin{cases} 1, & \boldsymbol{k}=\boldsymbol{k}', |\boldsymbol{k}|\leqslant k_F \\ 0, & \text{otherwise} \end{cases} \\
&= \frac{1}{V}\sum_{|\boldsymbol{k}|<k_F} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} \\
&= \int_0^{k_F} k^2 dk \int_{-1}^{1} \frac{d\cos\theta}{(2\pi)^2} e^{ik|\boldsymbol{r}-\boldsymbol{r}'|\cos\theta} = \frac{1}{(2\pi)^2|\boldsymbol{r}-\boldsymbol{r}'|^3}\int_0^x z^2 dz \int_{-1}^{1} dy e^{iyz} \\
&= \frac{3n(\sin x - x\cos x)}{2x^3}.
\end{aligned}$$

(c) The two-particle correlation function gives the probability amplitude to find a particle with spin σ' at $\boldsymbol{r}'$ when a particle with spin σ is already at $\boldsymbol{r}$. It is defined as follows:

$$g_{\sigma,\sigma'}(\boldsymbol{r}-\boldsymbol{r}') = \frac{4}{n^2}\langle\Psi_0|\hat{n}(\boldsymbol{r},\sigma)\hat{n}(\boldsymbol{r}',\sigma')|\Psi_0\rangle = \frac{4}{n^2}\langle\Psi_0|\hat{\psi}^\dagger_\sigma(\boldsymbol{r})\hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}')\hat{\psi}_{\sigma'}(\boldsymbol{r}')\hat{\psi}_\sigma(\boldsymbol{r})\Psi_0\rangle.$$

Show that in the case where $\sigma \neq \sigma'$ (for any $\boldsymbol{r}$ and $\boldsymbol{r}'$)

$$g_{\sigma,\sigma'}(\boldsymbol{r}-\boldsymbol{r}') = 1.$$

Solution:

$$\begin{aligned}
g_{\sigma_1\sigma_2}(\boldsymbol{r}_1-\boldsymbol{r}_2) &= \frac{4}{n^2V^2}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_1'} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_1')\cdot\boldsymbol{r}_1}\sum_{\boldsymbol{k}_2,\boldsymbol{k}_2'} e^{i(\boldsymbol{k}_2-\boldsymbol{k}_2')\cdot\boldsymbol{r}_2}\langle\Psi_0|\hat{a}^\dagger_{\sigma_1}(\boldsymbol{k}_1)\hat{a}^\dagger_{\sigma_2}(\boldsymbol{k}_2)\hat{a}_{\sigma_2}(\boldsymbol{k}_2')\hat{a}_{\sigma_1}(\boldsymbol{k}_1')|\Psi_0\rangle \\
&= \frac{4}{n^2V^2}\sum_{|\boldsymbol{k}_1|,|\boldsymbol{k}_1'|<k_F} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_1')\cdot\boldsymbol{r}_1}\sum_{|\boldsymbol{k}_2|,|\boldsymbol{k}_2'|<k_F} e^{i(\boldsymbol{k}_2-\boldsymbol{k}_2')\cdot\boldsymbol{r}_2}\delta_{\boldsymbol{k}_1\boldsymbol{k}_1'}\delta_{\boldsymbol{k}_2\boldsymbol{k}_2'} \\
&= \frac{4}{n^2}\left[\int_{|\boldsymbol{k}|<k_F}\frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3}\right]^2 = 1
\end{aligned}$$

(d) Show that only when we are in the case $\sigma = \sigma'$ the two -particle correlation function can be expressed using the one-particle correlation function such that:

$$g_{\sigma,\sigma}(\boldsymbol{r}-\boldsymbol{r}') = 1 - \frac{4}{n^2}\left[G_\sigma(\boldsymbol{r}-\boldsymbol{r}')\right]^2.$$

Compare this result with the one of question (d) and and think about what all this has to do with the Pauli principle.

Solution:

$$\begin{aligned}
g_{\sigma\sigma}(\boldsymbol{r}_1-\boldsymbol{r}_2) &= \frac{4}{n^2V^2}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_1'} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_1')\cdot\boldsymbol{r}_1}\sum_{\boldsymbol{k}_2,\boldsymbol{k}_2'} e^{i(\boldsymbol{k}_2-\boldsymbol{k}_2')\cdot\boldsymbol{r}_2}\langle\Psi_0|\hat{a}^\dagger_{\sigma}(\boldsymbol{k}_1)\hat{a}^\dagger_{\sigma}(\boldsymbol{k}_2)\hat{a}_{\sigma}(\boldsymbol{k}_2')\hat{a}_{\sigma}(\boldsymbol{k}_1')|\psi_0\rangle \\
&= \frac{4}{n^2V^2}\sum_{|\boldsymbol{k}_1|,|\boldsymbol{k}_1'|<k_F} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_1')\cdot\boldsymbol{r}_1}\sum_{|\boldsymbol{k}_2|,|\boldsymbol{k}_2'|<k_F} e^{i(\boldsymbol{k}_2-\boldsymbol{k}_2')\cdot\boldsymbol{r}_2}\left[\delta_{\boldsymbol{k}_1\boldsymbol{k}_1'}\delta_{\boldsymbol{k}_2\boldsymbol{k}_2'} - \delta_{\boldsymbol{k}_2\boldsymbol{k}_1'}\delta_{\boldsymbol{k}_1\boldsymbol{k}_2'}\right] \\
&= \frac{4}{n^2V^2}\sum_{|\boldsymbol{k}_1|,|\boldsymbol{k}_2|<k_F} 1 - e^{i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)} \\
&= 1 - \frac{4}{n^2}G^2_\sigma(\boldsymbol{r}_1-\boldsymbol{r}_2).
\end{aligned}$$

We notice that when particle are in the same spin state, we have a decrease of the probability amplitude to observe both particles next to each others due to Pauli repulsion.

(e) To understand the Pauli principle, calculate the following integral:

$$\frac{n}{2}\int d^3r\left[g_{\sigma,\sigma}(\boldsymbol{r}-\boldsymbol{r}') - 1\right].$$

How do you interpret the result ?

Solution:

$$\frac{n}{2}\int d^3r\,[g_{\sigma\sigma}(r)-1] = -\frac{9n}{2}\int d^3r\frac{(\sin k_F r - k_F r\cos k_F r)^2}{k_F^6 r^6}$$

$$= -\frac{18\pi n}{k_F^3}\int_0^\infty dx\frac{(\sin x - x\cos x)^2}{x^4} = -1.$$

This result stands for the negative correlation between fermions. One electron repulses another one due to the Pauli principle. In other words, having created the fermion with a spin σ at the position $\mathbf{r}$ we have less probability to observe another electron with the same spin in a vicinity of $\mathbf{r}$.

2. Thermodynamic perturbation theory (5 + 10 = 15 Points)

We consider a gas of spinless bosons of mass m in a volume $V = L^3$, with periodic boundary conditions for the wave functions. The particles interact via a potential $U(\vec{r}_1 - \vec{r}_2) = U_0\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)$ with $U_0 > 0$. The interaction part of the Hamiltonian ($\widehat{H} = \widehat{H}_0 + \widehat{U}$) has the following form in secondary quantization representation:

$$\widehat{U} = \frac{U_0}{2V}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4}\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3-\boldsymbol{k}_4}\,\hat{a}^\dagger_{\boldsymbol{k}_3}\hat{a}^\dagger_{\boldsymbol{k}_4}\hat{a}_{\boldsymbol{k}_2}\hat{a}_{\boldsymbol{k}_1}$$

The chemical potential μ and the temperature T are given.

(a) Consider $\widehat{U}$ as a small perturbation and show that the first-order correction in U_0 to the grand canonical potential is given by

$$\delta\Omega = \langle\widehat{U}\rangle_{H_0} = \frac{\mathrm{tr}\left\{\widehat{U}e^{-\beta\left(\widehat{H}_0-\mu\widehat{N}\right)}\right\}}{\mathrm{tr}\left\{e^{-\beta\left(\widehat{H}_0-\mu\widehat{N}\right)}\right\}}\ .$$

(b) Calculate $\delta\Omega$. The relevant matrix element can be generated either by different states $\vec{k}_1 \neq \vec{k}_2$ or by the same state $\vec{k}_1 = \vec{k}_2$. Consider these two cases separately.

Solution: (a) The grand thermodynamic potential is (we assume hereafter $k_\mathrm{B} = 1$)

$$\Omega = -\beta\ln Z$$

where $\beta = T^{-1}$ is the inverse temperature and Z is the partition function. It reads

$$Z = \mathrm{tr}\Big[e^{-\beta(H_0-\mu N+U)}\Big].$$

Now we expand Z up to the first order in U. Using the cyclic permutations of operators under the trace sign, we have for the matrix exponent:

$$\mathrm{tr}\Big[e^{-\beta(H_0-\mu N+U)}\Big] = \sum_{n=0}^\infty\frac{(-\beta)^n}{n!}\Big[\mathrm{tr}\big((H_0-\mu N)^n\big) + n\,\mathrm{tr}\big(U(H_0-\mu N)^{n-1}\big) + ...\Big].$$

The first order correction by U yields after the resummation:

$$Z \approx Z_0 - \beta \mathrm{tr}\Big[Ue^{-\beta(H_0-\mu N)}\Big]$$

where the unperturbed partition function is $Z_0 = \mathrm{tr}\Big[e^{-\beta(H_0-\mu N)}\Big]$. Now we expand the potential Ω in the first order by U:

$$\Omega = -\beta \ln\Big(Z_0 - \beta \mathrm{tr}\Big[Ue^{-\beta(H_0-\mu N)}\Big]\Big) = -\beta \ln\Big(Z_0\Big(1 - Z_0^{-1}\beta \mathrm{tr}\Big[Ue^{-\beta(H_0-\mu N)}\Big]\Big)\Big) \approx$$

$$\approx -\beta \ln Z_0 + Z_0^{-1}\mathrm{tr}\Big[Ue^{-\beta(H_0-\mu N)}\Big] = \Omega_0 + \langle U\rangle_{H_0}.$$

Finally, we have for the first order correction $\delta\Omega \equiv \Omega - \Omega_0 = \langle U\rangle_{H_0}$.

(b) Let us calculate $\langle U\rangle_{H_0}$ explicitly at $\boldsymbol{k}_1 \neq \boldsymbol{k}_2$:

$$\langle U\rangle_{H_0,\boldsymbol{k}_1\neq\boldsymbol{k}_2} = \frac{U_0}{2V}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4}^{\boldsymbol{k}_1\neq\boldsymbol{k}_2} \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3,\boldsymbol{k}_4}\langle \hat{a}^\dagger_{\boldsymbol{k}_3}\hat{a}^\dagger_{\boldsymbol{k}_4}\hat{a}_{\boldsymbol{k}_2}\hat{a}_{\boldsymbol{k}_1}\rangle =$$

$$= \frac{U_0}{2V}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4}^{\boldsymbol{k}_1\neq\boldsymbol{k}_2} \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3-\boldsymbol{k}_4}\left(\delta_{\boldsymbol{k}_1,\boldsymbol{k}_4}\delta_{\boldsymbol{k}_2,\boldsymbol{k}_3} + \delta_{\boldsymbol{k}_1,\boldsymbol{k}_3}\delta_{\boldsymbol{k}_2,\boldsymbol{k}_4}\right) N_{\boldsymbol{k}_1}N_{\boldsymbol{k}_2} =$$

$$= \frac{U_0}{V}\sum_{\boldsymbol{k}_1\neq\boldsymbol{k}_2} N_{\boldsymbol{k}_1}N_{\boldsymbol{k}_2}.$$

Here, $N_{\boldsymbol{k}} \equiv \langle \hat{a}^\dagger_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}}\rangle$ is the distribution function of bosons.

Consider now the case $\boldsymbol{k}_1 = \boldsymbol{k}_2$:

$$\langle U\rangle_{H_0,\boldsymbol{k}_1=\boldsymbol{k}_2} = \frac{U_0}{2V}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_3,\boldsymbol{k}_4} \delta_{2\boldsymbol{k}_1-\boldsymbol{k}_3,\boldsymbol{k}_4}\langle \hat{a}^\dagger_{\boldsymbol{k}_3}\hat{a}^\dagger_{\boldsymbol{k}_4}\hat{a}_{\boldsymbol{k}_1}\hat{a}_{\boldsymbol{k}_1}\rangle = \frac{U_0}{2V}\sum_{\boldsymbol{k}}\langle \hat{a}^\dagger_{\boldsymbol{k}}\hat{a}^\dagger_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}}\rangle.$$

For two indistinguishable particles, we have $\langle \hat{a}^\dagger_{\boldsymbol{k}}\hat{a}^\dagger_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}}\rangle = 2\langle \hat{a}^\dagger_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}}\rangle^2$ (this result also reflects the well-known Wick theorem). We obtain

$$\langle U\rangle_{H_0,\boldsymbol{k}_1=\boldsymbol{k}_2} = 2\frac{U_0}{2V}\sum_{\boldsymbol{k}} N^2_{\boldsymbol{k}}$$

Summing up the both results, we have:

$$\delta\Omega = \langle U\rangle_{H_0} = \langle U\rangle_{H_0,\boldsymbol{k}_1\neq\boldsymbol{k}_2} + \langle U\rangle_{H_0,\boldsymbol{k}_1=\boldsymbol{k}_2} = \frac{U_0N^2}{V}.$$

3. Operators in the secondary quantized representation (bonus exercise) (25 Points)

In the lecture, the second quantization for bosonic operators $\hat{F}^{(1)} = \sum_a \hat{f}^{(1)}_{x_a}$ has been derived: $\hat{F}^{(1)} = \sum_{ij}\langle i|\hat{f}^{(1)}|j\rangle\, \hat{b}^\dagger_i\hat{b}_j$. Here, $|i\rangle$ are the single particle states and the operator

$\hat{f}^{(1)}_{x_a}$ acts on coordinates x_a. The diagonal elements ($i = j$) of the bosonic operators are given by

$$\langle N_1, N_2, \ldots |\hat{F}^{(1)}|N_1, N_2, \ldots\rangle = \sum_i N_i \langle i|\hat{f}^{(1)}|i\rangle, \tag{1}$$

where $|N_1, N_2, ...\rangle = \left(\frac{N_1!N_2!\ldots}{N!}\right)^{1/2} \sum_P \phi_{P_1}(x_1)\phi_{P_2}(x_2)\ldots\phi_{P_N}(x_N)$ is the symmetrized bosonic wavefunction. $\phi_i(x_i)$ are the single particle wave functions (i is a quantum number). The non-diagonal elements ($i \neq j$) are

$$\langle \ldots, N_i, \ldots, N_j - 1, \ldots |\hat{F}^{(1)}| \ldots, N_i - 1, \ldots, N_j, \ldots\rangle = \sqrt{N_i N_j}\, \langle i|\hat{f}^{(1)}|j\rangle \tag{2}$$

where $N = \sum_i N_i$. Analogously to the single-particle operators, the two-particle bosonic operators $\hat{F}^{(2)}$ are introduced

$$\hat{F}^{(2)} = \frac{1}{2} \sum_{iklm} \langle ik|\hat{f}^{(2)}|lm\rangle\, \hat{a}^\dagger_i \hat{a}^\dagger_k \hat{a}_m \hat{a}_l \tag{3}$$

with the matrix elements $\langle ik|\hat{f}^{(2)}|lm\rangle = \iint dx_1\, dx_2\, \phi^\star_i(x_1)\, \phi^\star_k(x_2)\, \hat{f}^{(2)}\, \phi_l\,(x_1)\, \phi_m(x_2)$.

Derive the expression for $\hat{F}^{(2)} = \sum_{a<b} f^{(2)}_{ab}$ of the form (3) where the operator acts on coordinates x_a and x_b. To do that, find the expressions for two-particle operators that are analogous to (1) and (2). Distinguish whether $f^{(2)}$ acts twice on the same single-particle state or on two different ones.

Solution:

Single-particle operators

In the lecture, the single-particle operators in second quantization picture have been derived. For single-particle operators, there are two possible matrix elements, diagonal and non-diagonal. For two-particle operators there are, however, multiple diagonal and off-diagonal matrix elements.

First we repeat how the one-particle operators work. The single-particle states are $\phi_i(x)$, where i is a quantum number (e.g. momentum) and x is the coordinate (e.g. location). The symmetric product state is then given as

$$\Psi_s(N_1, N_2, \ldots) = \sqrt{\frac{N_1!N_2!\ldots}{N!}} \sum_{P \in S^\star_N} \Big[\phi_{P(1)}(1)\phi_{P(2)}(2)\, \ldots\, \phi_{P(N)}(N)\Big]$$

In this notation, large numbers denote the coordinates, e.g., $3 \equiv x_3$. The number $P(3)$ denotes a permuted quantum number at the position 3.

The scalar product is defined as usual in quantum mechanics:

$$\int dX \phi^\star_{P(i)}(X)\phi_{\tilde{P}(j)}(X) \equiv \langle P(i)|\tilde{P}(j)\rangle\ .$$

For demonstration purposes we check the norm of the symmetrized bosonic many-body state:

$$\begin{aligned}
\langle\Psi_s|\Psi_s|\Psi_s|\Psi_s\rangle &= \frac{N_1!N_2!\ldots}{N!}\sum_{P,\tilde{P}}\underbrace{\langle P(1)|\tilde{P}(1)\rangle\langle P(2)|\tilde{P}(2)\rangle\ldots}_{\delta_{P,\tilde{P}}} \\
&= \frac{N_1!N_2!\ldots}{N!}\sum_{P} \\
&= \frac{N_1!N_2!\ldots}{N!}\;\frac{N!}{N_1!N_2!\ldots} = 1
\end{aligned}$$

The sum $\sum_P 1 = \frac{N!}{N_1!N_2!\ldots}$ takes into account all allowed permutations. The not allowed one is a permutation of two particles that occupy the same coordinate. (Such a situation can not happen for fermions because of the Pauli principle.) Since the set of allowed permutations is not S_N (all permutations), we introduced $P \in S_N^\star$ in the definition of Ψ_s.

In the following we write simply $|\Psi_s(N_1, N_2, \ldots)\rangle \equiv |N_1, N_2, \ldots\rangle$.

Now we finally start with single-particle operators. First, consider the diagonal elements for bosons:

$$\langle F^{(1)}\rangle = \sum_{a=1}^{N}\langle f^{(1)}_{x_a}\rangle$$

where

$$\begin{aligned}
\langle N_1, N_2, \ldots|\, f^{(1)}_{x_a}\, |N_1, N_2, \ldots\rangle &= \frac{N_1!N_2!\ldots}{N!}\sum_{P,\tilde{P}}\langle P(1)|\tilde{P}(1)\rangle\ldots\langle P(a)|f^{(1)}_{x_a}|\tilde{P}(a)\rangle\ldots \\
&= \frac{N_1!N_2!\ldots}{N!}\sum_{P}\langle P(a)|f^{(1)}_{x_a}|\tilde{P}(a)\rangle
\end{aligned}$$

In the last step the following has happened: the operator at the position a does not act on any other positions. Because of the orthonormality of the single-particle states, the following applies $P(1) = \tilde{P}(1)$, $P(2) = \tilde{P}(2)$ etc. Only for $P(a)$ and $\tilde{P}(a)$ this does not applies because $f^{(1)}$ is not necessarily diagonal in $\phi_i(X)$. However, if $P = \tilde{P}$ for all but one of the numbers from $1\ldots N$ holds, then this last number is also fixed: $P(a) = \tilde{P}(a)$, so $P = \tilde{P}$ still applies to all $1\ldots N$.

We build a permutation P by choosing the quantum numbers $1, \ldots, N$ for $i = P(a)$ that contribute to a sum $\sum_{i=1}^{N}$. Now the sum runs over all permutations except the remaining $N-1$ numbers, that results in $(N-1)!$ identical contributions. But again we have to extract wrong permutations. Here you have to note that from the original N_i particles in the i-th state only $N_i - 1$ are available. Finally we obtain

$$\begin{aligned}
\langle N_1, N_2, \ldots | \, f^{(1)}_{x_a} \, | N_1, N_2, \ldots \rangle &= \frac{N_1! N_2! \ldots}{N!} \sum_{i=1}^{N} \langle i | f^{(1)} | i \rangle \frac{(N-1)!}{N_1! \ldots (N_i - 1)! \ldots} \\
&= \sum_{i=1}^{N} \frac{N_i}{N} \langle i | f^{(1)} | i \rangle
\end{aligned}$$

We get the final result by taking the sum over a: enters:

$$\langle N_1, N_2, \ldots | \, F^{(1)} \, | N_1, N_2, \ldots \rangle = \sum_{a=1}^{N} \sum_{i=1}^{N} \frac{N_i}{N} \langle i | f^{(1)} | i \rangle = \sum_{i} N_i \langle i | f^{(1)} | i \rangle$$

Now to the off-diagonal matrix elements:

$$\begin{aligned}
&\langle \ldots, N_i, \ldots, N_j - 1, \ldots | \, f^{(1)}_{x_a} \, | \ldots, N_i - 1, \ldots, N_j, \ldots \rangle \\
= \; & \frac{N_1! \ldots N_{i-1}! N_{i+1}! \ldots N_{j-1}! N_{j+1}! \ldots}{N!} \sqrt{N_i! (N_i - 1)! N_j! (N_j - 1)!} \times \\
& \sum_{P, \tilde{P}} \langle P(1) | \tilde{P}(1) \rangle \; \langle P(2) | \tilde{P}(2) \rangle \; \ldots \; \langle P(a) | f^{(1)}_{x_a} | \tilde{P}(a) \rangle \ldots
\end{aligned}$$

In this case, we choose $P(a) = i$ and $\tilde{P}(a) = j$. All further permutations P and $\tilde{P}$ must be equal (with the same argumentation as with the diagonal elements):

$$= \frac{N_1! \ldots N_{i-1}! N_{i+1}! \ldots N_{j-1}! N_{j+1}! \ldots}{N!} \sqrt{N_i! (N_i - 1)! N_j! (N_j - 1)!} \sum_{P} \langle i | f^{(1)} | j \rangle$$

Again, only $N - 1$ particles are allowed to be permuted. We have to divide by the numbers of wrong permutations of $N_i - 1$ and $N_j - 1$ particles:

$$\begin{aligned}
= \; & \frac{N_1! \ldots N_{i-1}! N_{i+1}! \ldots N_{j-1}! N_{j+1}! \ldots}{N!} \sqrt{N_i! (N_i - 1)! N_j! (N_j - 1)!} \langle i | f^{(1)} | j \rangle \times \\
& \frac{(N-1)!}{N_1! \ldots (N_i - 1)! (N_j - 1)! \ldots} \\
= \; & \frac{\sqrt{N_i N_j}}{N} \langle i | f^{(1)} | j \rangle
\end{aligned}$$

The summation over a again eliminates the N in the denominator and we find for the off-diagonal matrix element: $\langle F^{(1)} \rangle = \sqrt{N_i N_j} \, \langle i | \, f^{(1)} \, | j \rangle$.

The operator can be written as

$$F^{(1)} = \sum_{ij} \langle i | \, f^{(1)} \, | j \rangle \, a_i^\dagger a_j$$

because

$$\begin{aligned}
& \sum_{ij} \langle N_1, N_2, \ldots | \, \langle i | \, f^{(1)} \, | j \rangle \, a_i^\dagger a_j \, | N_1, N_2, \ldots \rangle \\
& \qquad = \sum_{ij} \langle i | \, f^{(1)} \, | j \rangle \, \sqrt{N_i N_j} \delta_{ij} = \sum_{i} \langle i | \, f^{(1)} \, | i \rangle \, N_i
\end{aligned}$$

and

$$\sum_{ij} \langle \ldots, N_i, \ldots, N_j - 1, \ldots | \, \langle i | \, f^{(1)} \, | j \rangle \, a_i^\dagger a_j \, | \ldots, N_i - 1, \ldots, N_j, \ldots \rangle$$

$$= \langle i | \, f^{(1)} \, | j \rangle \, \sqrt{N_i N_j}$$

for the non-diagonal elements. The sums are omitted here, since there is only one contribution, and exactly when $a_i^\dagger$ acts on the state i and a_j on the state j. One gets 0 in the opposite case due to the orthogonality of the states.

Two-particle operators:

In this part we arrive at two-particle operators, $F^{(2)} = \sum\limits_{a<b} f^{(2)}$. Note the sum $\sum\limits_{a<b}$ will yield a factor $N(N-1)/2$.

<u>Diagonal elements for bosons:</u>

$$\langle N_1, N_2, \ldots | \, f^{(2)}_{x_a x_b} \, | N_1, N_2, \ldots \rangle = \frac{N_1! N_2! \ldots}{N!} \sum_{P, \tilde{P}} \ldots \langle P(a) P(b) | f^{(2)}_{x_a x_b} | \tilde{P}(a) \tilde{P}(b) \rangle$$

$$= \frac{N_1! N_2! \ldots}{N!} \sum_{P} \langle P(a) P(b) | f^{(2)}_{x_a x_b} | \tilde{P}(b) \tilde{P}(a) \rangle$$

Here we have to distinguish between the two cases: either $f^{(2)}$ acts on two single-particle states with the same quantum number i or on two single-particle states with the different quantum numbers i and j:

$$\langle N_1, N_2, \ldots | \, f^{(2)}_{x_a x_b} \, | N_1, N_2, \ldots \rangle =$$

$$= \begin{cases} \dfrac{N_1! N_2! \ldots}{N!} \sum\limits_i \langle ii | f^{(2)} | ii \rangle \dfrac{(N-2)!}{N_1! \ldots (N_i - 2)! \ldots} = \sum\limits_i \dfrac{N_i (N_i - 1)}{N(N-1)} \langle ii | f^{(2)} | ii \rangle \\ = \ldots = \sum\limits_{ij} \dfrac{N_i N_j}{N(N-1)} \Big(\langle ij | f^{(2)} | ji \rangle + \langle ij | f^{(2)} | ij \rangle \Big) \end{cases}$$

We also obtain

$$\langle F^{(2)} \rangle = \sum_{a<b} \sum_i \frac{N_i (N_i - 1)}{N(N-1)} \langle ii | f^{(2)} | ii \rangle = \frac{1}{2} \sum_i \langle ii | f^{(2)} | ii \rangle N_i (N_i - 1) \tag{4}$$

and

$$\langle F^{(2)} \rangle = \frac{1}{2} \sum_{i \neq j} \Big(\langle ij | f^{(2)} | ji \rangle + \langle ij | f^{(2)} | ij \rangle \Big) N_i N_j \; . \tag{5}$$

One more comment concerning the permutations. We calculated $\sum\limits_P$ as follows: We choose $i = P(a)$ and $j = P(b)$ (and vice versa) from the set $1 \ldots N$. The remaining $(N-2)$ numbers are permuted, which results in the factor $(N-2)!$. The matrix element

(4) is zero due to the Pauli principle. Calculating (5) we should be careful with the fermion permutation sign. As a result, we obtain:

$$\langle N_1, N_2, \ldots |\, f^{(2)}_{x_a x_b}\, | N_1, N_2, \ldots \rangle = \frac{1}{N!} \sum_{P,\tilde{P}} (-1)^{\chi_P} (-1)^{\chi_{\tilde{P}}} \ldots \langle P(a)P(b)| f^{(2)}_{x_a x_b} |\tilde{P}(a)\tilde{P}(b)\rangle$$

$$= \frac{1}{N!} \sum_{i=1}^{N} \sum_{\substack{j=1\\ j\neq i}}^{N} \Big(\langle ij|f^{(2)}|ij\rangle - \langle ij|f^{(2)}|ji\rangle \Big)(N-2)!$$

$$\boxed{\langle F^{(2)}\rangle \;=\; \sum_{i,j} \frac{1}{2}\Big(\langle ij|f^{(2)}|ij\rangle - \langle ij|f^{(2)}|ji\rangle \Big)}$$

Non-diagonal elements for bosons:

$$\langle N_i, \ldots, N_j, \ldots, N_l - 1 |\, f^{(2)}_{x_a x_b}\, | N_i - 1, \ldots, N_j, \ldots, N_l \rangle =$$

$$\frac{N_1! \ldots, N_j! \ldots}{N!} \sqrt{N_i!(N_i-1)!N_l!(N_l-1)!} \sum_{P,\tilde{P}} \ldots \langle P(a)P(b)| f^{(2)}_{x_a x_b} |\tilde{P}(a)\tilde{P}(b)\rangle$$

$$= \frac{\cdots}{\cdots} \sqrt{\cdots} \sum_j \Big(\langle ij|f^{(2)}|lj\rangle + \langle ij|f^{(2)}|jl\rangle \Big) \frac{(N-2)!}{N_1! \ldots (N_i-1)!(N_j-1)!(N_l-1)! \ldots}$$

$$= \sum_j \frac{N_j\sqrt{N_i N_l}}{N(N-1)} \Big(\langle ij|f^{(2)}|lj\rangle + \langle ij|f^{(2)}|jl\rangle \Big)$$

$$\boxed{\langle F^{(2)}\rangle = \sum_j \frac{1}{2} N_j \sqrt{N_i N_l} \Big(\langle ij|f^{(2)}|lj\rangle + \langle ij|f^{(2)}|jl\rangle \Big)}$$

Analogously, the following non-diagonal matrix elements can be found for bosons:

$$\langle \ldots N_i \ldots N_j - 1 \ldots N_l \ldots N_m - 1 \ldots |\, F^{(2)}\, | \ldots N_i - 1 \ldots N_j \ldots N_l - 1 \ldots N_m \ldots \rangle$$
$$= \frac{1}{2}\sqrt{N_i N_j N_l N_m} \Big(\langle il|f^{(2)}|jm\rangle + \langle il|f^{(2)}|mj\rangle \Big) \quad (6)$$

and

$$\langle \ldots N_i \ldots N_l - 2 \ldots |\, F^{(2)}\, | \ldots N_i - 2 \ldots N_l \ldots \rangle$$
$$= \frac{1}{2}\sqrt{N_i(N_i-1)N_l(N_l-1)}\; \langle ii|f^{(2)}|ll\rangle \quad (7)$$