Homework 1

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1. Give the wave-function in first quantization which corresponds to the Fock-vector

$$|2,0,2,0,0,\dots\rangle$$

of four particles and the fermionic wave-function corresponding to

$$|1,0,1,1,1,0,0,\dots\rangle$$

Solution. The state $|2,0,2,0,0,\dots\rangle$ is a bosonic state since more than 1 particle is in the same state.

$$|2,0,2,0,0,\dots\rangle = \frac{1}{\sqrt{2!}}(\hat{a}_1^\dagger)^2\frac{1}{\sqrt{2!}}(\hat{a}_3^\dagger)^2\,|0\rangle$$

$$\begin{aligned}\phi(x_1,x_2,\dots) &= \frac{1}{\sqrt{4!}}\,\langle 0|\hat{\Psi}(x_1)\hat{\Psi}(x_2)\hat{\Psi}(x_3)\hat{\Psi}(x_4)|2,0,2,0,0,\dots\rangle\\ &= \frac{1}{\sqrt{4!}}\frac{1}{\sqrt{2!}}\frac{1}{\sqrt{2!}}\,\langle 0|\hat{\Psi}(x_1)\hat{\Psi}(x_2)\hat{\Psi}(x_3)\hat{\Psi}(x_4)(\hat{a}_1^\dagger)^2(\hat{a}_3^\dagger)^2|0\rangle\end{aligned}$$

$$\hat{\Psi}(x_i) = \sum_j \varphi_j(x_i)\hat{a}_j$$

$$\begin{aligned}\phi(x_1,x_2,\dots) &= \frac{1}{96}\sum_j\sum_k\sum_l\sum_m \langle 0|\varphi_j(x_1)\hat{a}_j\varphi_k(x_2)\hat{a}_k\varphi_l(x_3)\hat{a}_l\varphi_m(x_4)\hat{a}_m(\hat{a}_1^\dagger)^2(\hat{a}_3^\dagger)^2|0\rangle\\ &= \frac{1}{96}\sum_{j,k,l,m}\varphi_j(x_1)\varphi_k(x_2)\varphi_l(x_3)\varphi_m(x_4)\,\langle 0|\hat{a}_j\hat{a}_k\hat{a}_l\hat{a}_m(\hat{a}_1^\dagger)^2(\hat{a}_3^\dagger)^2|0\rangle\end{aligned}$$

$$\left[\hat{a}_k,\hat{a}_l^\dagger\right] = \delta_{kl},\ \ \hat{a}_k\,|0\rangle = 0$$

$$\begin{aligned}\langle 0|\hat{a}_j\hat{a}_k\hat{a}_l\hat{a}_m(\hat{a}_1^\dagger)^2(\hat{a}_3^\dagger)^2|0\rangle &= \langle 0|\hat{a}_j\hat{a}_k\hat{a}_l\hat{a}_m\hat{a}_1^\dagger\hat{a}_1^\dagger\hat{a}_3^\dagger\hat{a}_3^\dagger|0\rangle\\ &= \langle 0|\hat{a}_j\hat{a}_k\hat{a}_l(\delta_{m1}+\hat{a}_1^\dagger\hat{a}_m)\hat{a}_1^\dagger\hat{a}_3^\dagger\hat{a}_3^\dagger|0\rangle\\ &= \delta_{m1}\,\langle 0|\hat{a}_j\hat{a}_k\hat{a}_l\hat{a}_1^\dagger\hat{a}_3^\dagger\hat{a}_3^\dagger|0\rangle\\ &+ \langle 0|\hat{a}_j\hat{a}_k\hat{a}_l\hat{a}_1^\dagger\hat{a}_m\hat{a}_1^\dagger\hat{a}_3^\dagger\hat{a}_3^\dagger|0\rangle\\ &= \delta_{m1}\,\langle 0|\hat{a}_j\hat{a}_k(\delta_{l1}+\hat{a}_1^\dagger\hat{a}_l)\hat{a}_3^\dagger\hat{a}_3^\dagger|0\rangle\\ &+ \langle 0|\hat{a}_j\hat{a}_k\hat{a}_l\hat{a}_1^\dagger(\delta_{m1}+\hat{a}_1^\dagger\hat{a}_m)\hat{a}_3^\dagger\hat{a}_3^\dagger|0\rangle\\ &= \delta_{m1}\delta_{l1}\,\langle 0|\hat{a}_j\hat{a}_k\hat{a}_3^\dagger\hat{a}_3^\dagger|0\rangle\\ &+ \delta_{m1}\,\langle 0|\hat{a}_j\hat{a}_k\hat{a}_1^\dagger\hat{a}_l\hat{a}_3^\dagger\hat{a}_3^\dagger|0\rangle\\ &+ \delta_{m1}\,\langle 0|\hat{a}_j\hat{a}_k\hat{a}_l\hat{a}_1^\dagger\hat{a}_3^\dagger\hat{a}_3^\dagger|0\rangle\\ &+ \langle 0|\hat{a}_j\hat{a}_k\hat{a}_l\hat{a}_1^\dagger\hat{a}_1^\dagger\hat{a}_m\hat{a}_3^\dagger\hat{a}_3^\dagger|0\rangle\\ &= \delta_{m1}\delta_{l1}\,\langle 0|\hat{a}_j(\delta_{k3}+\hat{a}_3^\dagger\hat{a}_k)\hat{a}_3^\dagger|0\rangle\\ &+ \delta_{m1}\,\langle 0|\hat{a}_j\hat{a}_k\hat{a}_1^\dagger(\delta_{l3}+\hat{a}_3^\dagger\hat{a}_l)\hat{a}_3^\dagger|0\rangle\\ &+ \delta_{m1}\,\langle 0|\hat{a}_j\hat{a}_k(\delta_{l1}+\hat{a}_1^\dagger\hat{a}_l)\hat{a}_3^\dagger\hat{a}_3^\dagger|0\rangle\\ &+ \langle 0|\hat{a}_j\hat{a}_k\hat{a}_l\hat{a}_1^\dagger\hat{a}_1^\dagger(\delta_{m3}+\hat{a}_3^\dagger\hat{a}_m)\hat{a}_3^\dagger|0\rangle\\ &= \delta_{m1}\delta_{l1}\delta_{k3}\,\langle 0|\hat{a}_j\hat{a}_k\hat{a}_3^\dagger|0\rangle + \delta_{m1}\delta_{l1}\,\langle 0|\hat{a}_j\hat{a}_3^\dagger\hat{a}_k\hat{a}_3^\dagger|0\rangle\\ &+ \delta_{m1}\delta_{l3}\,\langle 0|\hat{a}_j\hat{a}_k\hat{a}_1^\dagger\hat{a}_3^\dagger|0\rangle + \delta_{m1}\,\langle 0|\hat{a}_j\hat{a}_k\hat{a}_1^\dagger\hat{a}_3^\dagger\hat{a}_l\hat{a}_3^\dagger|0\rangle\\ &+ \delta_{m1}\delta_{l1}\,\langle 0|\hat{a}_j\hat{a}_k\hat{a}_3^\dagger\hat{a}_3^\dagger|0\rangle + \delta_{m1}\,\langle 0|\hat{a}_j\hat{a}_k\hat{a}_1^\dagger\hat{a}_l\hat{a}_3^\dagger\hat{a}_3^\dagger|0\rangle\\ &+ \delta_{m3}\,\langle 0|\hat{a}_j\hat{a}_k\hat{a}_l\hat{a}_1^\dagger\hat{a}_1^\dagger\hat{a}_3^\dagger|0\rangle + \langle 0|\hat{a}_j\hat{a}_k\hat{a}_l\hat{a}_1^\dagger\hat{a}_1^\dagger\hat{a}_3^\dagger\hat{a}_m\hat{a}_3^\dagger|0\rangle\\ &=\end{aligned}$$

For bosons,

$$\phi^B(x_1, x_2, x_3, x_4) = \frac{1}{\sqrt{4! \cdot 2! \cdot 2!}} \sum_{(\alpha)} \prod_{j=1}^{4} \varphi_{\alpha_j}(x_j).$$

2. Calculate the quantity $\langle \hat{n}(\mathbf{r}) \rangle$ where Ψ is a pure state in Fock-space:

$$\Psi = |n_1, n_2, \ldots\rangle .$$

Compare the result (obtained at the practice) for fermions, given by a single Slater-determinant in first quantization.

Solution. The particle number density in second quantization (in the spin-independent case) is

$$\hat{n}(\mathbf{r}) = \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r}).$$

where

$$\hat{\Psi}^\dagger(\mathbf{r}) = \sum_{i=1}^{N} \varphi_i(\mathbf{r})^* \hat{a}_i^\dagger.$$
$$\hat{\Psi}(\mathbf{r}) = \sum_{i=1}^{N} \varphi_i(\mathbf{r}) \hat{a}_i.$$

We also know how the fermionic creation and annihillation operators act on the Fock-space:

$$\begin{aligned}
&\hat{a}_i^\dagger |n_1, \ldots, n_i, \ldots\rangle = \sqrt{1 - n_i}(-1)^{\Sigma_i} |n_1, \ldots, 1 + n_i, \ldots\rangle \\
&\hat{a}_i |n_1, \ldots, n_i, \ldots\rangle = \sqrt{n_i}(-1)^{\Sigma_i} |n_1, \ldots, 1 - n_i, \ldots\rangle \\
&\text{where } \Sigma_k = \sum_{j=1}^{k-1} n_j.
\end{aligned}$$

The expectation value of the particle number density operator in state $|\Psi\rangle$ is

$$\begin{aligned}
\langle \hat{n}(\mathbf{r}) \rangle &= \langle \Psi | \hat{n}(\mathbf{r}) | \Psi \rangle \\
&= \left\langle \Psi \middle| \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r}) \middle| \Psi \right\rangle \\
&= \left\langle \Psi \middle| \sum_{i=1}^{N} \varphi_i(\mathbf{r})^* \hat{a}_i^\dagger \sum_{j=1}^{N} \varphi_j(\mathbf{r}) \hat{a}_j \middle| \Psi \right\rangle \\
&= \sum_{i,j=1}^{N} \varphi_i(\mathbf{r})^* \varphi_j(\mathbf{r}) \langle \Psi | \hat{a}_i^\dagger \hat{a}_j | \Psi \rangle \\
&= \sum_{i,j=1}^{N} \varphi_i(\mathbf{r})^* \varphi_j(\mathbf{r}) \langle n_1, n_2 \ldots | \hat{a}_i^\dagger \hat{a}_j | n_1, n2, \ldots \rangle \\
&= \sum_{i,j=1}^{N} \varphi_i(\mathbf{r})^* \varphi_j(\mathbf{r}) \langle n_1, n_2 \ldots | \hat{a}_i^\dagger \sqrt{n_j}(-1)^{\Sigma_j} | n_1, \ldots 1 - n_j, \ldots \rangle \\
&= \sum_{i,j=1}^{N} \varphi_i(\mathbf{r})^* \varphi_j(\mathbf{r}) \sqrt{n_j}(-1)^{\Sigma_j} \langle n_1, n_2 \ldots | \hat{a}_i^\dagger | n_1, \ldots 1 - n_j, \ldots \rangle \\
&= \sum_{i,j=1}^{N} \varphi_i(\mathbf{r})^* \varphi_j(\mathbf{r}) \sqrt{n_j}(-1)^{\Sigma_j} \sqrt{1 - n_i}(-1)^{\Sigma_i} \langle n_1, n_2 \ldots | n_1, \ldots, 1 + n_i, \ldots 1 - n_j, \ldots \rangle
\end{aligned}$$

From the orthogonality, we know that

$$\langle n_1, n_2 \ldots | n_1, \ldots, 1 + n_i, \ldots 1 - n_j, \ldots \rangle = \delta_{n_i, 1+n_i} \delta_{n_j, 1-n_j},$$

so,

$$\begin{aligned}
\langle \hat{n}(\mathbf{r}) \rangle &= \sum_{i,j=1}^{N} \varphi_i(\mathbf{r})^* \varphi_j(\mathbf{r}) \sqrt{n_j} (-1)^{\Sigma_j} \sqrt{1 - n_i} (-1)^{\Sigma_i} \delta_{n_i, 1+n_i} \delta_{n_j, 1-n_j} \\
&= \sum_{i,j=1}^{N} \varphi_i(\mathbf{r})^* \varphi_j(\mathbf{r}) \sqrt{n_j (1 - n_i)} (-1)^{\Sigma_i + \Sigma_j} \delta_{n_i, 1+n_i} \delta_{n_j, 1-n_j}
\end{aligned}$$

3. Show that for a pure n-particle fermionic state (given by a single Slater-determinant in first quantization)

$$P(\mathbf{r}, s, \mathbf{r}', s') = n(\mathbf{r}, s) n(\mathbf{r}', s') - |n(\mathbf{r}, s, \mathbf{r}', s')|^2,$$

where $n(\mathbf{r}, s)$ is the spin dependent density and $n(\mathbf{r}, s, \mathbf{r}', s')$ is the density matrix. The particle density operator in second quantization is

$$\hat{n}(\mathbf{r}, s) = \hat{\Psi}^\dagger(\mathbf{r}, s) \hat{\Psi}(\mathbf{r}, s)$$

and the pair correlation operator is

$$\hat{P}(\mathbf{r}, s, \mathbf{r}', s') = \hat{\Psi}^\dagger(\mathbf{r}, s) \hat{\Psi}^\dagger(\mathbf{r}', s') \hat{\Psi}(\mathbf{r}, s) \hat{\Psi}(\mathbf{r}', s')$$

For fermions, the field operators satisfy the anticommutation relations:

$$\left\{ \hat{\Psi}(\mathbf{r}, s), \hat{\Psi}^\dagger(\mathbf{r}', s') \right\} = \delta(\mathbf{r} - \mathbf{r}') \delta_{ss'}.$$

Thus,

$$\begin{aligned}
\hat{n}(\mathbf{r}, s) \hat{n}(\mathbf{r}', s') &= \hat{\Psi}^\dagger(\mathbf{r}, s) \hat{\Psi}(\mathbf{r}, s) \hat{\Psi}^\dagger(\mathbf{r}', s') \hat{\Psi}(\mathbf{r}', s') \\
&= \hat{\Psi}^\dagger(\mathbf{r}, s) \left(\delta(\mathbf{r} - \mathbf{r}') \delta_{ss'} - \hat{\Psi}^\dagger(\mathbf{r}', s') \hat{\Psi}(\mathbf{r}, s) \right) \hat{\Psi}(\mathbf{r}', s') \\
&= \delta(\mathbf{r} - \mathbf{r}') \delta_{ss'} \hat{\Psi}^\dagger(\mathbf{r}, s) \hat{\Psi}(\mathbf{r}', s') - \hat{\Psi}^\dagger(\mathbf{r}, s) \hat{\Psi}^\dagger(\mathbf{r}', s') \hat{\Psi}(\mathbf{r}, s) \hat{\Psi}(\mathbf{r}', s') \\
&= \delta(\mathbf{r} - \mathbf{r}') \delta_{ss'} \hat{\Psi}^\dagger(\mathbf{r}, s) \hat{\Psi}(\mathbf{r}', s') - \hat{P}(\mathbf{r}, s, \mathbf{r}', s').
\end{aligned}$$

4. Prove that the particle number operator

$$\hat{N} = \sum_s \int \mathrm{d}^3 r \hat{\Psi}^\dagger(\mathbf{r}, s) \hat{\Psi}(\mathbf{r}, s)$$

and the Hamiltonian

$$\begin{aligned}
\hat{H} = &\sum_s \int \mathrm{d}^3 r \hat{\Psi}^\dagger(\mathbf{r}, s) \left(\frac{-\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right) \hat{\Psi}(\mathbf{r}, s) \\
&+ \frac{1}{2} \sum_{s,s'} \int \mathrm{d}^3 r \int \mathrm{d}^3 r' \hat{\Psi}^\dagger(\mathbf{r}, s) \hat{\Psi}^\dagger(\mathbf{r}', s') v(|\mathbf{r} - \mathbf{r}'|) \hat{\Psi}(\mathbf{r}', s') \hat{\Psi}(\mathbf{r}, s)
\end{aligned}$$

commute:

$$\left[\hat{H}, \hat{N} \right] = 0,$$

for both bosons and fermions.

Solution. Let's Introduce $\hat{K} = \frac{-\hbar^2}{2m} \nabla^2$. We know that the commutation is a linear operation, that is

$$\left[\int \mathrm{d}^3 r \hat{A}(r), \int \mathrm{d}^3 r' \hat{B}(r') \right] = \int \mathrm{d}^3 r \int \mathrm{d}^3 r' \left[\hat{A}(r), \hat{B}(r') \right].$$

Therefore,

$$\begin{aligned}
\left[\hat{H}, \hat{N}\right] &= \left[\sum_s \int \mathrm{d}^3 r \hat{\Psi}^\dagger(\mathbf{r}, s) \left(\hat{K} + V(\mathbf{r})\right) \hat{\Psi}(\mathbf{r}, s), \hat{N}\right] \\
&+ \left[\frac{1}{2}\sum_{s,s'} \int \mathrm{d}^3 r \int \mathrm{d}^3 r' \hat{\Psi}^\dagger(\mathbf{r}, s)\hat{\Psi}^\dagger(\mathbf{r}', s') v(|\mathbf{r}-\mathbf{r}'|)\hat{\Psi}(\mathbf{r}', s')\hat{\Psi}(\mathbf{r}, s), \hat{N}\right] \\
&= \sum_s \int \mathrm{d}^3 r \left[\hat{\Psi}^\dagger(\mathbf{r}, s)\hat{K}\hat{\Psi}(\mathbf{r}, s), \hat{N}\right] + \sum_s \int \mathrm{d}^3 r \left[\hat{\Psi}^\dagger(\mathbf{r}, s)V(\mathbf{r})\hat{\Psi}(\mathbf{r}, s), \hat{N}\right] \\
&+ \frac{1}{2}\sum_{s,s'} \int \mathrm{d}^3 r \int \mathrm{d}^3 r' \left[\hat{\Psi}^\dagger(\mathbf{r}, s)\hat{\Psi}^\dagger(\mathbf{r}', s') v(|\mathbf{r}-\mathbf{r}'|)\hat{\Psi}(\mathbf{r}', s')\hat{\Psi}(\mathbf{r}, s), \hat{N}\right].
\end{aligned}$$

Now, let's substitute $\hat{N}$, but change s to σ and $\mathbf{r}$ to $\mathbf{x}$in the sum:

$$\begin{aligned}
\left[\hat{H}, \hat{N}\right] &= \sum_s \int \mathrm{d}^3 r \left[\hat{\Psi}^\dagger(\mathbf{r}, s)\hat{K}\hat{\Psi}(\mathbf{r}, s), \sum_\sigma \int \mathrm{d}^3 x \hat{\Psi}^\dagger(\mathbf{x}, \sigma)\hat{\Psi}(\mathbf{x}, \sigma)\right] \\
&+ \sum_s \int \mathrm{d}^3 r \left[\hat{\Psi}^\dagger(\mathbf{r}, s)V(\mathbf{r})\hat{\Psi}(\mathbf{r}, s), \sum_\sigma \int \mathrm{d}^3 x \hat{\Psi}^\dagger(\mathbf{x}, \sigma)\hat{\Psi}(\mathbf{x}, \sigma)\right] \\
&+ \frac{1}{2}\sum_{s,s'} \int \mathrm{d}^3 r \int \mathrm{d}^3 r' \left[\hat{\Psi}^\dagger(\mathbf{r}, s)\hat{\Psi}^\dagger(\mathbf{r}', s') v(|\mathbf{r}-\mathbf{r}'|)\hat{\Psi}(\mathbf{r}', s')\hat{\Psi}(\mathbf{r}, s), \sum_\sigma \int \mathrm{d}^3 x \hat{\Psi}^\dagger(\mathbf{x}, \sigma)\hat{\Psi}(\mathbf{x}, \sigma)\right] \\
&= \sum_{s,\sigma} \int \mathrm{d}^3 r \mathrm{d}^3 x \left[\hat{\Psi}^\dagger(\mathbf{r}, s)\hat{K}\hat{\Psi}(\mathbf{r}, s), \hat{\Psi}^\dagger(\mathbf{x}, \sigma)\hat{\Psi}(\mathbf{x}, \sigma)\right] \\
&+ \sum_{s,\sigma} \int \mathrm{d}^3 r \mathrm{d}^3 x \left[\hat{\Psi}^\dagger(\mathbf{r}, s)V(\mathbf{r})\hat{\Psi}(\mathbf{r}, s), \hat{\Psi}^\dagger(\mathbf{x}, \sigma)\hat{\Psi}(\mathbf{x}, \sigma)\right] \\
&+ \frac{1}{2}\sum_{s,s',\sigma} \int \mathrm{d}^3 r \mathrm{d}^3 r' \mathrm{d}^3 x \left[\hat{\Psi}^\dagger(\mathbf{r}, s)\hat{\Psi}^\dagger(\mathbf{r}', s') v(|\mathbf{r}-\mathbf{r}'|)\hat{\Psi}(\mathbf{r}', s')\hat{\Psi}(\mathbf{r}, s), \hat{\Psi}^\dagger(\mathbf{x}, \sigma)\hat{\Psi}(\mathbf{x}, \sigma)\right]
\end{aligned}$$

So, we have to calculate three commutators:

$$\begin{aligned}
&\left[\hat{\Psi}^\dagger(\mathbf{r}, s)\hat{K}\hat{\Psi}(\mathbf{r}, s), \hat{\Psi}^\dagger(\mathbf{x}, \sigma)\hat{\Psi}(\mathbf{x}, \sigma)\right] = ? \\
&\left[\hat{\Psi}^\dagger(\mathbf{r}, s)V(\mathbf{r})\hat{\Psi}(\mathbf{r}, s), \hat{\Psi}^\dagger(\mathbf{x}, \sigma)\hat{\Psi}(\mathbf{x}, \sigma)\right] = ? \\
&\left[\hat{\Psi}^\dagger(\mathbf{r}, s)\hat{\Psi}^\dagger(\mathbf{r}', s') v(|\mathbf{r}-\mathbf{r}'|)\hat{\Psi}(\mathbf{r}', s')\hat{\Psi}(\mathbf{r}, s), \hat{\Psi}^\dagger(\mathbf{x}, \sigma)\hat{\Psi}(\mathbf{x}, \sigma)\right] = ?
\end{aligned}$$

$$\begin{aligned}
\left[\hat{\Psi}^\dagger(\mathbf{r}, s)\hat{K}\hat{\Psi}(\mathbf{r}, s), \hat{\Psi}^\dagger(\mathbf{x}, \sigma)\hat{\Psi}(\mathbf{x}, \sigma)\right] &= \hat{\Psi}^\dagger(\mathbf{r}, s)\hat{K}\hat{\Psi}(\mathbf{r}, s)\hat{\Psi}^\dagger(\mathbf{x}, \sigma)\hat{\Psi}(\mathbf{x}, \sigma) - \hat{\Psi}^\dagger(\mathbf{x}, \sigma)\hat{\Psi}(\mathbf{x}, \sigma)\hat{\Psi}^\dagger(\mathbf{r}, s)\hat{K}\hat{\Psi}(\mathbf{r}, s) \\
&= \hat{K}\hat{\Psi}^\dagger(\mathbf{r}, s)\hat{\Psi}(\mathbf{r}, s)\hat{\Psi}^\dagger(\mathbf{x}, \sigma)\hat{\Psi}(\mathbf{x}, \sigma) + \left[\hat{\Psi}^\dagger(\mathbf{r}, s), \hat{K}\right]\hat{\Psi}(\mathbf{r}, s)\hat{\Psi}^\dagger(\mathbf{x}, \sigma)\hat{\Psi}(\mathbf{x}, \sigma) \\
&- \hat{\Psi}^\dagger(\mathbf{x}, \sigma)\hat{\Psi}(\mathbf{x}, \sigma)\hat{\Psi}^\dagger(\mathbf{r}, s)\hat{\Psi}(\mathbf{r}, s)\hat{K} - \hat{\Psi}^\dagger(\mathbf{x}, \sigma)\hat{\Psi}(\mathbf{x}, \sigma)\hat{\Psi}^\dagger(\mathbf{r}, s)\left[\hat{K}, \hat{\Psi}(\mathbf{r}, s)\right] \\
&=
\end{aligned}$$