Statistical Physics (MSc)
Homework 1.

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PROBLEM 1.

QUESTION

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

$$|2,0,2,0,0,\ldots\rangle$$

of four particles, and the fermionic wave function corresponding to

$$|1,0,1,1,1,0,0,\ldots\rangle\,.$$

SOLUTION

First, we're looking for the $\Psi^{B}_{1133}\left(x_1,\ldots,x_4\right)$ wavefunction at the bosonic (symmetric) case. The many-body wavefunction of this case could be written as follows:

$$\Psi^{B}_{\alpha}\left(x_1,\ldots,x_n\right)=\langle x_1,\ldots,x_N|n_1,\ldots,n_N\rangle=\sqrt{\frac{\prod_j n_j!}{N!}}\sum_p \psi_{p(1)}\left(x_1\right)\psi_{p(2)}\left(x_2\right)\ldots\psi_{p(N)}\left(x_N\right) \tag{1}$$

Here, the sum is taken over all different states under permutations p acting on N elements. Since we only have 4 particles, we can write the following:

$$\Psi^{B}_{1133}\left(x_1,x_2,x_3,x_4\right)=\sqrt{\frac{2!\cdot 0!\cdot 2!\cdot 0!\cdot\cdots\cdot 0!}{4!}}\sum_p \psi_{p(1)}\left(x_1\right)\psi_{p(2)}\left(x_2\right)\psi_{p(3)}\left(x_3\right)\psi_{p(4)}\left(x_4\right) \tag{2}$$

$$\Psi^{B}_{1133}\left(x_1,x_2,x_3,x_4\right)=\sqrt{\frac{1}{6}}\sum_p \psi_{p(1)}\left(x_1\right)\psi_{p(2)}\left(x_2\right)\psi_{p(3)}\left(x_3\right)\psi_{p(4)}\left(x_4\right) \tag{3}$$

Second, the $\Psi^{F}_{1345}\left(x_1,\ldots,x_4\right)$ fermionic wavefunction could be written as a Slater determinant in the following form:

$$\Psi^{F}_{\alpha}\left(x_1,\ldots,x_n\right)=\frac{1}{\sqrt{N!}}\begin{vmatrix}\psi_{n_1}\left(x_1\right) & \psi_{n_1}\left(x_2\right) & \ldots & \psi_{n_1}\left(x_N\right)\\ \psi_{n_2}\left(x_1\right) & \psi_{n_2}\left(x_2\right) & \ldots & \psi_{n_2}\left(x_N\right)\\ \vdots & \vdots & \ddots & \vdots\\ \psi_{n_N}\left(x_1\right) & \psi_{n_N}\left(x_2\right) & \ldots & \psi_{n_N}\left(x_N\right)\end{vmatrix} \tag{4}$$

In our case, it is the following:

$$\Psi^{F}_{1345}\left(x_1,x_2,x_3,x_4\right)=\frac{1}{\sqrt{4!}}\begin{vmatrix}\psi_1\left(x_1\right) & \psi_1\left(x_2\right) & \psi_1\left(x_3\right) & \psi_1\left(x_4\right)\\ \psi_0\left(x_1\right) & \psi_0\left(x_2\right) & \psi_0\left(x_3\right) & \psi_0\left(x_4\right)\\ \psi_1\left(x_1\right) & \psi_1\left(x_2\right) & \psi_1\left(x_3\right) & \psi_1\left(x_4\right)\\ \psi_1\left(x_1\right) & \psi_1\left(x_2\right) & \psi_1\left(x_3\right) & \psi_1\left(x_4\right)\end{vmatrix} \tag{5}$$

PROBLEM 2.

QUESTION

Calculate the quantity $\langle \hat{\varrho}(\boldsymbol{r}, s) \rangle_\Psi$, where Ψ is a pure state in Fock-space

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

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

SOLUTION

The expectation value of the density operator $\hat{\varrho}(\boldsymbol{r}, s)$ could be derived as follows:

$$\langle \hat{\varrho}(\boldsymbol{r}, s) \rangle_\Psi = \langle \Psi \mid \hat{\varrho}(\boldsymbol{r}, s) \mid \Psi \rangle \tag{6}$$

Where the density operator is

$$\hat{\varrho}(\boldsymbol{r}, s) = \sum_{i\,=\,1}^{N} \delta(\boldsymbol{r} - \boldsymbol{r}_i)\, \delta_{s,s_i} \tag{7}$$

Thus the equation could be reorganized into the following form:

$$\langle \hat{\varrho}(\boldsymbol{r}, s) \rangle_\Psi = \left\langle \Psi \,\middle|\, \sum_{i\,=\,1}^{N} \delta(\boldsymbol{r} - \boldsymbol{r}_i)\, \delta_{s,s_i} \,\middle|\, \Psi \right\rangle = \left\langle n_1, n_2, \ldots, n_N \,\middle|\, \sum_{i\,=\,1}^{N} \delta(\boldsymbol{r} - \boldsymbol{r}_i)\, \delta_{s,s_i} \,\middle|\, n_1, n_2, \ldots, n_N \right\rangle \tag{8}$$

The wavefunction Ψ could be expressed as we've learned on the lecture for Fermions:

$$\Psi = \frac{1}{\sqrt{N!}} \sum_{i_1=1}^{N} \cdots \sum_{i_N=1}^{N} \epsilon_{i_1,i_2,\ldots,i_N} \varphi_{i_1}(\boldsymbol{r}_1, s_1)\, \varphi_{i_2}(\boldsymbol{r}_2, s_2) \ldots \varphi_{i_N}(\boldsymbol{r}_N, s_N) \tag{9}$$

Since $\hat{\rho}(\boldsymbol{r}, s)$ is Hermitian, we can reorganize the equations:

$$\langle \hat{\varrho}(\boldsymbol{r}, s) \rangle_\Psi = \sum_{i\,=\,1}^{N} \delta(\boldsymbol{r} - \boldsymbol{r}_i)\, \delta_{s,s_i} \langle \Psi \mid \Psi \rangle = \sum_{i\,=\,1}^{N} \delta(\boldsymbol{r} - \boldsymbol{r}_i)\, \delta_{s,s_i} \langle n_1, n_2, \ldots, n_N \mid n_1, n_2, \ldots, n_N \rangle \tag{10}$$

The second part could be expressed as follows:

$$\langle \Psi \mid \Psi \rangle = \sum_{s_1} \cdots \sum_{s_N} \int \cdots \int dr_1^3 \ldots dr_N^3 \Psi^* \Psi \tag{11}$$

Using the identity

$$\sum_{i_1=1}^{N} \cdots \sum_{i_N=1}^{N} \epsilon_{i_1,i_2,\ldots,i_N} \cdot \epsilon_{i_1,i_2,\ldots,i_N} = N! \tag{12}$$

we can simplify $\Psi^*\Psi$:

$$\Psi^* \Psi = \frac{1}{\sqrt{N!}} \frac{1}{\sqrt{N!}} \sum_{i_1=1}^{N} \cdots \sum_{i_N=1}^{N} \epsilon_{i_1,i_2,\ldots,i_N} \epsilon_{i_1,i_2,\ldots,i_N} \left| \varphi_{i_1}(\boldsymbol{r}_1, s_1) \right|^2 \ldots \left| \varphi_{i_N}(\boldsymbol{r}_N, s_N) \right|^2 \tag{13}$$

$$\Psi^* \Psi = \frac{\cancel{N!}}{\cancel{N!}} \left| \varphi(\boldsymbol{r}_1, s_1) \right|^2 \ldots \left| \varphi(\boldsymbol{r}_N, s_N) \right|^2 \tag{14}$$

Substituting back into the equation (11):

$$\langle \Psi \mid \Psi \rangle = \sum_{s_1} \cdots \sum_{s_N} \int \cdots \int dr_1^3 \ldots dr_N^3 \left| \varphi \left(\boldsymbol{r}_1, s_1 \right) \right|^2 \ldots \left| \varphi \left(\boldsymbol{r}_N, s_N \right) \right|^2 \tag{15}$$

Summing all deltas in equation (10), we get the following form:

$$\langle \hat{\varrho} \left(\boldsymbol{r}, s \right) \rangle_\Psi = \sum_{i\,=\,1}^{N} \delta \left(\boldsymbol{r} - \boldsymbol{r}_i \right) \delta_{s,s_i} \sum_{s_1} \cdots \sum_{s_N} \int \cdots \int dr_1^3 \ldots dr_N^3 \left| \varphi \left(\boldsymbol{r}_1, s_1 \right) \right|^2 \ldots \left| \varphi \left(\boldsymbol{r}_N, s_N \right) \right|^2 \tag{16}$$

$$\langle \hat{\varrho} \left(\boldsymbol{r}, s \right) \rangle_\Psi = N \cdot \sum_{s_2} \cdots \sum_{s_N} \int \cdots \int dr_2^3 \ldots dr_N^3 \left| \varphi \left(\boldsymbol{r}, s \right) \right|^2 \left| \varphi \left(\boldsymbol{r}_2, s_2 \right) \right|^2 \ldots \left| \varphi \left(\boldsymbol{r}_N, s_N \right) \right|^2 \tag{17}$$

Which is really the same form, we've derived on the practice.

PROBLEM 3.

QUESTION

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

$$P\left(\boldsymbol{r}, s, \boldsymbol{r'}, s'\right) = \varrho\left(\boldsymbol{r}, s\right) \cdot \varrho\left(\boldsymbol{r'}, s'\right) - \left|\varrho\left(\boldsymbol{r}, s, \boldsymbol{r'}, s'\right)\right|^2 \tag{18}$$

where $\varrho\left(\boldsymbol{r}, s\right)$ is the spin dependent density and $\varrho\left(\boldsymbol{r}, s, \boldsymbol{r'}, s'\right)$ is the density matrix.

SOLUTION

On the course we've seen, that the pair distribution function is the following:

$$P\left(\boldsymbol{r}, s, \boldsymbol{r'}, s'\right) = \Psi^{\dagger}\left(\boldsymbol{r}, s\right) \Psi^{\dagger}\left(\boldsymbol{r'}, s'\right) \Psi\left(\boldsymbol{r}, s\right) \Psi\left(\boldsymbol{r'}, s'\right) \tag{19}$$

We also derived, the spin-dependent density operator is the following:

$$\varrho\left(\boldsymbol{r}, s\right) = \Psi^{\dagger}\left(\boldsymbol{r}, s\right) \Psi\left(\boldsymbol{r}, s\right) \tag{20}$$

$$\varrho\left(\boldsymbol{r'}, s'\right) = \Psi^{\dagger}\left(\boldsymbol{r'}, s'\right) \Psi\left(\boldsymbol{r'}, s'\right) \tag{21}$$

It is also the diagonal of the density matrix which could be written in the following form:

$$\varrho\left(\boldsymbol{r}, s, \boldsymbol{r'}, s'\right) = N \sum_{s_2} \cdots \sum_{s_n} \int d^3 r_2 \dots d^3 r_n \Psi^{*}\left(\boldsymbol{r_1}, s_1, \dots\right) \cdot \Psi\left(\boldsymbol{r_1}, s_1, \dots\right) \tag{22}$$

$$\operatorname{diag}\left[\varrho\left(\boldsymbol{r}, s, \boldsymbol{r'}, s'\right)\right] = \varrho\left(\boldsymbol{r}, s, \boldsymbol{r'} = \boldsymbol{r}, s' = s\right) = \varrho\left(\boldsymbol{r}, s\right) \tag{23}$$

The absolute value of a positive operator, like $\varrho\left(\boldsymbol{r}, s, \boldsymbol{r'}, s'\right)$ is well-defined and is the following:

$$\left|\varrho\left(\boldsymbol{r}, s, \boldsymbol{r'}, s'\right)\right| = \sqrt{\varrho\left(\boldsymbol{r}, s, \boldsymbol{r'}, s'\right) \cdot \varrho\left(\boldsymbol{r}, s, \boldsymbol{r'}, s'\right)} \tag{24}$$

which positive square root exist.

PROBLEM 4.

QUESTION

Prove that the particle number operator

$$\hat{N} = \sum_s \int d^3r \hat{\Psi}^\dagger(\boldsymbol{r}, s)\, \hat{\Psi}(\boldsymbol{r}, s) \tag{25}$$

and the Hamiltonian

$$\begin{aligned}\hat{H} = \sum_s \int d^3r \hat{\Psi}^\dagger(\boldsymbol{r}, s) \left(-\frac{\hbar^2}{2m}\nabla - V(\boldsymbol{r})\right) \hat{\Psi}(\boldsymbol{r}, s) + \\ + \frac{1}{2}\sum_s \sum_{s'} \int d^3r \int d^3r' \hat{\Psi}^\dagger(\boldsymbol{r}, s)\, \hat{\Psi}^\dagger(\boldsymbol{r'}, s')\, v\left(|\boldsymbol{r} - \boldsymbol{r'}|\right) \hat{\Psi}(\boldsymbol{r'}, s')\, \hat{\Psi}(\boldsymbol{r}, s)\end{aligned} \tag{26}$$

commute:

$$\left[\hat{H}, \hat{N}\right] = 0 \tag{27}$$

both for bosons and for fermions.

SOLUTION

To solve the problem, we exactly need to prove, that the two expressions

$$\left[\hat{H}, \Psi^\dagger\Psi\right] \tag{28}$$

commutes. Using the identity, learned on the lecture:

$$\left[\hat{O}_1, \hat{O}_2\hat{O}_3\right] = \left[\hat{O}_1, \hat{O}_2\right] \cdot \hat{O}_3 - \hat{O}_2 \cdot \left[\hat{O}_1, \hat{O}_3\right] \tag{29}$$

We can expand the above commutator as follows:

$$\left[\hat{H}, \Psi^\dagger\Psi\right] = \left[\hat{H}, \Psi^\dagger\right] \cdot \Psi - \Psi^\dagger \cdot \left[\hat{H}, \Psi\right] = \left(\hat{H}\Psi^\dagger\Psi - \Psi^\dagger\hat{H}\Psi\right) - \left(\Psi^\dagger\hat{H}\Psi - \Psi^\dagger\Psi\hat{H}\right) \tag{30}$$

Since $\hat{H}$, the Hamiltonian is a Hermitian operator, we can reorganize the above equation:

$$\left[\hat{H}, \Psi^\dagger\Psi\right] = \left(\Psi^\dagger\hat{H}\Psi - \Psi^\dagger\hat{H}\Psi\right) - \left(\Psi^\dagger\hat{H}\Psi - \Psi^\dagger\hat{H}\Psi\right) = 0 \tag{31}$$