

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

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

of four particles, and the fermionic wave function corresponding to

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

SOLUTION

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

$$\Psi_{\alpha}^B(x_1, \dots, x_n) = \langle x_1, \dots, x_n | n_1, \dots, n_N \rangle = \sqrt{\frac{\prod_j n_j!}{N!}} \sum_p \psi_{p(1)}(x_1) \psi_{p(2)}(x_2) \dots \psi_{p(N)}(x_N) \quad (1)$$

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:

$$\Psi_{1133}^B(x_1, x_2, x_3, x_4) = \sqrt{\frac{2! \cdot 0! \cdot 2! \cdot 0! \cdot \dots \cdot 0!}{4!}} \sum_p \psi_{p(1)}(x_1) \psi_{p(2)}(x_2) \psi_{p(3)}(x_3) \psi_{p(4)}(x_4) \quad (2)$$

$$\Psi_{1133}^B(x_1, x_2, x_3, x_4) = \sqrt{\frac{1}{6}} \sum_p \psi_{p(1)}(x_1) \psi_{p(2)}(x_2) \psi_{p(3)}(x_3) \psi_{p(4)}(x_4) \quad (3)$$

Second, the $\Psi_{1345}^F(x_1, \dots, x_4)$ fermionic wavefunction could be written as a Slater determinant in the following form:

$$\Psi_{\alpha}^F(x_1, \dots, x_n) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_{n_1}(x_1) & \psi_{n_1}(x_2) & \dots & \psi_{n_1}(x_N) \\ \psi_{n_2}(x_1) & \psi_{n_2}(x_2) & \dots & \psi_{n_2}(x_N) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_{n_N}(x_1) & \psi_{n_N}(x_2) & \dots & \psi_{n_N}(x_N) \end{vmatrix} \quad (4)$$

In our case, it is the following:

$$\Psi_{1345}^F(x_1, x_2, x_3, x_4) = \frac{1}{\sqrt{4!}} \begin{vmatrix} \psi_1(x_1) & \psi_1(x_2) & \psi_1(x_3) & \psi_1(x_4) \\ \psi_0(x_1) & \psi_0(x_2) & \psi_0(x_3) & \psi_0(x_4) \\ \psi_1(x_1) & \psi_1(x_2) & \psi_1(x_3) & \psi_1(x_4) \\ \psi_1(x_1) & \psi_1(x_2) & \psi_1(x_3) & \psi_1(x_4) \end{vmatrix} \quad (5)$$

PROBLEM 2.

QUESTION

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

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

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 $\hat{\rho}(\mathbf{r}, s)$ could be derived as follows:

$$\langle \hat{\rho}(\mathbf{r}, s) \rangle_{\Psi} = \langle \Psi | \hat{\rho}(\mathbf{r}, s) | \Psi \rangle \quad (6)$$

Where the density operator is

$$\hat{\rho}(\mathbf{r}, s) = \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i) \delta_{s, s_i} \quad (7)$$

Thus the equation could be reorganized into the following form:

$$\langle \hat{\rho}(\mathbf{r}, s) \rangle_{\Psi} = \left\langle \Psi \left| \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i) \delta_{s, s_i} \right| \Psi \right\rangle = \left\langle n_1, n_2, \dots, n_N \left| \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i) \delta_{s, s_i} \right| n_1, n_2, \dots, n_N \right\rangle \quad (8)$$

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

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

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

$$\langle \hat{\rho}(\mathbf{r}, s) \rangle_{\Psi} = \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i) \delta_{s, s_i} \langle \Psi | \Psi \rangle = \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i) \delta_{s, s_i} \langle n_1, n_2, \dots, n_N | n_1, n_2, \dots, n_N \rangle \quad (10)$$

The second part could be expressed as follows:

$$\langle \Psi | \Psi \rangle = \sum_{s_1} \cdots \sum_{s_N} \int \cdots \int d\mathbf{r}_1^3 \cdots d\mathbf{r}_N^3 \Psi^* \Psi \quad (11)$$

Using the identity

$$\sum_{i_1=1}^N \cdots \sum_{i_N=1}^N \epsilon_{i_1, i_2, \dots, i_N} \cdot \epsilon_{i_1, i_2, \dots, i_N} = N! \quad (12)$$

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

$$\Psi^* \Psi = \frac{1}{\sqrt{N!}} \frac{1}{\sqrt{N!}} \sum_{i_1=1}^N \cdots \sum_{i_N=1}^N \epsilon_{i_1, i_2, \dots, i_N} \epsilon_{i_1, i_2, \dots, i_N} |\varphi_{i_1}(\mathbf{r}_1, s_1)|^2 \cdots |\varphi_{i_N}(\mathbf{r}_N, s_N)|^2 \quad (13)$$

$$\Psi^* \Psi = \frac{N!}{N!} |\varphi(\mathbf{r}_1, s_1)|^2 \cdots |\varphi(\mathbf{r}_N, s_N)|^2 \quad (14)$$

Substituting back into the equation (11):

$$\langle \Psi | \Psi \rangle = \sum_{s_1} \cdots \sum_{s_N} \int \cdots \int d\mathbf{r}_1^3 \cdots d\mathbf{r}_N^3 |\varphi(\mathbf{r}_1, s_1)|^2 \cdots |\varphi(\mathbf{r}_N, s_N)|^2 \quad (15)$$

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

$$\langle \hat{\rho}(\mathbf{r}, s) \rangle_{\Psi} = \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i) \delta_{s, s_i} \sum_{s_1} \cdots \sum_{s_N} \int \cdots \int d\mathbf{r}_1^3 \cdots d\mathbf{r}_N^3 |\varphi(\mathbf{r}_1, s_1)|^2 \cdots |\varphi(\mathbf{r}_N, s_N)|^2 \quad (16)$$

$$\langle \hat{\rho}(\mathbf{r}, s) \rangle_{\Psi} = N \cdot \sum_{s_2} \cdots \sum_{s_N} \int \cdots \int d\mathbf{r}_2^3 \cdots d\mathbf{r}_N^3 |\varphi(\mathbf{r}, s)|^2 |\varphi(\mathbf{r}_2, s_2)|^2 \cdots |\varphi(\mathbf{r}_N, s_N)|^2 \quad (17)$$

Which is really the same form, we 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)

$$P(\mathbf{r}, s, \mathbf{r}', s') = \varrho(\mathbf{r}, s) \cdot \varrho(\mathbf{r}', s') - |\varrho(\mathbf{r}, s, \mathbf{r}', s')|^2 \quad (18)$$

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

SOLUTION

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

$$P(\mathbf{r}, s, \mathbf{r}', s') = \Psi^\dagger(\mathbf{r}, s) \Psi^\dagger(\mathbf{r}', s') \Psi(\mathbf{r}, s) \Psi(\mathbf{r}', s') \quad (19)$$

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

$$\varrho(\mathbf{r}, s) = \Psi^\dagger(\mathbf{r}, s) \Psi(\mathbf{r}, s) \quad (20)$$

$$\varrho(\mathbf{r}', s') = \Psi^\dagger(\mathbf{r}', s') \Psi(\mathbf{r}', s') \quad (21)$$

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

$$\varrho(\mathbf{r}, s, \mathbf{r}', s') = N \sum_{s_2} \cdots \sum_{s_n} \int d^3r_2 \dots d^3r_n \Psi^*(\mathbf{r}_1, s_1, \dots) \cdot \Psi(\mathbf{r}_1, s_1, \dots) \quad (22)$$

$$\text{diag} [\varrho(\mathbf{r}, s, \mathbf{r}', s')] = \varrho(\mathbf{r}, s, \mathbf{r}' = \mathbf{r}, s' = s) = \varrho(\mathbf{r}, s) \quad (23)$$

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

$$|\varrho(\mathbf{r}, s, \mathbf{r}', s')| = \sqrt{\varrho(\mathbf{r}, s, \mathbf{r}', s') \cdot \varrho(\mathbf{r}, s, \mathbf{r}', s')} \quad (24)$$

which positive square root exist.

PROBLEM 4.

QUESTION

Prove that the particle number operator

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

and the Hamiltonian

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

commute:

$$[\hat{H}, \hat{N}] = 0 \quad (27)$$

both for bosons and for fermions.

SOLUTION

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

$$[\hat{H}, \Psi^\dagger \Psi] \quad (28)$$

commutes. Using the identity, learned on the lecture:

$$[\hat{O}_1, \hat{O}_2 \hat{O}_3] = [\hat{O}_1, \hat{O}_2] \cdot \hat{O}_3 - \hat{O}_2 \cdot [\hat{O}_1, \hat{O}_3] \quad (29)$$

We can expand the above commutator as follows:

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

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

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