

Advanced Quantum Theory (WS 24/25)
 Homework no. 11 (December 18, 2024): Christmas edition!
Please hand in your solution by Monday, January 6!

1 Totally (Anti-)Symmetric N -Particle State

We saw in class that

$$\hat{S}_{\pm}|i_1, i_2, \dots, i_N\rangle = \frac{1}{\sqrt{N!}} \sum_{\hat{P}} (-1)^P \hat{P}|i_1, i_2, \dots, i_N\rangle \quad (1)$$

is a totally (anti-)symmetric N -particle state, if $|i_1, i_2, \dots, i_N\rangle = |i_1\rangle_1 |i_2\rangle_2 \dots |i_N\rangle_N$ is a product of one-particle states, in which particle no. α is in state $|i_\alpha\rangle$, for $\alpha = 1, 2, \dots, N$.

1. As a warm-up exercise, explicitly construct the three-particle states $\hat{S}_{\pm}|3, 1, 2\rangle = \hat{S}_{\pm}|3\rangle_1 |1\rangle_2 |2\rangle_3$, i.e. starting from a state where particle 1 is in state number 3, particle 2 is in state 1, and particle 3 is in state 2. What happens if one instead starts from the state $|1\rangle_1 |3\rangle_2 |2\rangle_3$? What happens if the single-particle states $|1\rangle$ and $|2\rangle$ are identical, $|1\rangle = |2\rangle$? What happens if all three states are identical, $|1\rangle = |2\rangle = |3\rangle$? **[5P]**
2. Show that the squared norm of the totally symmetric N -particle state is given by

$$\left\| \hat{S}_+ |i_1, i_2, \dots, i_N\rangle \right\|^2 = n_1! n_2! \dots n_n! \quad (2)$$

where n_i is the number of particles in state $|i\rangle$, with $\sum_{i=1}^n n_i = N$. Assume that the single-particle states are normalized, $\langle i|k\rangle = \delta_{ik}$. *Hint:* Use the fact that there are $n!$ permutations of n objects, and carefully distinguish between the permutations in \hat{S}_+ that do not change anything (since they exchange identical states $|i\rangle$) and permutations that do change something. How many different permutations of the latter kind are there altogether? **[5P]**

2 Two-Particle Operators in Second Quantization

Consider an operator \hat{F} that can be written as a sum of two-particle operators \hat{f} :

$$\hat{F} = \frac{1}{2} \sum_{\alpha \neq \beta} \hat{f}(\vec{x}_\alpha, \vec{x}_\beta). \quad (3)$$

Here α, β label identical particles.

1. Show that \hat{F} can be written as

$$\hat{F} = \frac{1}{2} \sum_{\alpha \neq \beta} \sum_{i,j,k,l} \langle i, j | \hat{f} | k, l \rangle |i\rangle_\alpha |j\rangle_\beta \langle k|_\alpha \langle l|_\beta, \quad (4)$$

where

$$\langle i, j | \hat{f} | k, l \rangle = \int d^3x d^3y \psi_i^*(\vec{x}) \psi_j^*(\vec{y}) \hat{f}(\vec{x}, \vec{y}) \psi_k(\vec{x}) \psi_l(\vec{y}). \quad (5)$$

Here $|i\rangle_\alpha$ again means that particle α is in the single-particle state $|i\rangle$, etc. *Hint:* Compute the matrix element of \hat{F} between two-particle states that can be written as products of single-particle states; this is sufficient, since all two-particle states can be written as linear superpositions of such products. **[2P]**

- Now assume that the particles in question are fermions (the first part of this problem holds equally for bosons and fermions). Show that \hat{F} can be written in terms of fermionic creation and annihilation operators:

$$\hat{F} = \frac{1}{2} \sum_{i,j,k,l} \langle i, j | \hat{f} | k, l \rangle \hat{b}_i^\dagger \hat{b}_j^\dagger \hat{b}_l \hat{b}_k. \quad (6)$$

Hint: First, show that

$$\sum_{\mathcal{P}} (-1)^P \hat{\mathcal{P}} |i_1\rangle_1 |i_2\rangle_2 \dots |i_N\rangle_N = (-1)^{\sum_{k < j} n_k} \sum_{\alpha} (-1)^{\alpha-1} |j\rangle_\alpha \sum_{\mathcal{P}} (-1)^P \hat{\mathcal{P}} |i_1\rangle_1 |i_2\rangle_2 \dots |i_{N-1}\rangle_{N-1},$$

where on the rhs the permutation is only over $N-1$ elements, and it has been assumed that one of the original $|i_\alpha\rangle = |j\rangle$. Following the corresponding derivation for bosonic operators shown in class, use this relation to prove

$$\sum_{\alpha} |i\rangle_\alpha \langle j|_\alpha = \hat{b}_i^\dagger \hat{b}_j, \quad (7)$$

which in turn can be used to prove eq.(6). **[5P]**

3 Field Operators in Momentum Space

In this homework we repeat the construction of the Hamiltonian in terms of field operators, done in class for coordinate space operators, for operators defined in momentum space.

We work in a cuboid volume

$$V_o = L_x L_y L_z, \quad (8)$$

hence the normalized eigenstates with fixed momentum $\hbar \vec{k}$ are

$$\phi_{\vec{k}}(\vec{x}) = \frac{1}{\sqrt{V_o}} e^{i\vec{k} \cdot \vec{x}}. \quad (9)$$

We impose periodic boundary conditions,

$$\phi_{\vec{k}}(x, y, z) = \phi_{\vec{k}}(x + L_x, y, z) = \phi_{\vec{k}}(x, y + L_y, z) = \phi_{\vec{k}}(x, y, z + L_z). \quad (10)$$

- Show that eq.(10) requires \vec{k} to be *quantized*, i.e.

$$\vec{k} = 2\pi \left(\frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z} \right), \quad (11)$$

where n_x, n_y, n_z are arbitrary integers. **[1P]**

2. Show that therefore the states $\phi_{\vec{k}}$ are orthonormal,

$$\int_{V_o} d^3x \phi_{\vec{k}}^*(\vec{x}) \phi_{\vec{k}'}(\vec{x}') = \delta_{n_x, n'_x} \delta_{n_y, n'_y} \delta_{n_z, n'_z} \equiv \delta_{\vec{k}, \vec{k}'} . \quad (12)$$

[1P]

3. Let $\hat{a}_{\vec{k}}^\dagger$ be the generators that create a single boson with wave vector \vec{k} . (The final result also holds for fermions, with commuting $\hat{a}_{\vec{k}}$ replaced by anticommuting $\hat{b}_{\vec{k}}$ as usual.) In order to express the Hamiltonian through these operators, we need three matrix elements. First, show that

$$\langle \vec{k}' | \hat{T} | \vec{k} \rangle = \frac{\hbar^2}{2m} \vec{k}^2 \delta_{\vec{k}, \vec{k}'}, \quad (13)$$

where \hat{T} is the operator of kinetic energy, and m is the mass of the particle under consideration. [2P]

4. Next, show that for arbitrary external potential $U(\vec{x})$,

$$\langle \vec{k}' | U | \vec{k} \rangle = \frac{1}{V_o} U_{\vec{k}' - \vec{k}} ; \quad (14)$$

the expression on the right is the Fourier transform of U with respect to the (discrete!) wave vector $\vec{k}' - \vec{k}$,

$$U_{\vec{q}} = \int_{V_o} d^3x U(\vec{x}) e^{-i\vec{q} \cdot \vec{x}} . \quad (15)$$

[1P]

5. Similarly, writing the two-particle interaction potential in terms of its Fourier components as

$$V(\vec{x} - \vec{x}') = \frac{1}{V_o} \sum_{\vec{q}} V_{\vec{q}} e^{i\vec{q} \cdot (\vec{x} - \vec{x}')} , \quad (16)$$

show that

$$\langle \vec{p}', \vec{k}' | V(\vec{x} - \vec{x}') | \vec{p}, \vec{k} \rangle = \frac{1}{V_o} \sum_{\vec{q}} V_{\vec{q}} \delta_{\vec{q}, \vec{p}' - \vec{p}} \delta_{\vec{q}, \vec{k} - \vec{k}'} . \quad (17)$$

[3P]

6. Finally, putting everything together, show that the Hamiltonian consisting of the sum of kinetic energy, external potential energy U and two-particle potential V , can be written as

$$\hat{H} = \sum_{\vec{k}} \frac{(\hbar \vec{k})^2}{2m} \hat{a}_{\vec{k}}^\dagger \hat{a}_{\vec{k}} + \frac{1}{V_o} \sum_{\vec{k}, \vec{k}'} U_{\vec{k} - \vec{k}'} \hat{a}_{\vec{k}'}^\dagger \hat{a}_{\vec{k}} + \frac{1}{2V_o} \sum_{\vec{k}, \vec{p}, \vec{q}} V_{\vec{q}} \hat{a}_{\vec{q} + \vec{p}}^\dagger \hat{a}_{\vec{k} - \vec{q}}^\dagger \hat{a}_{\vec{k}} \hat{a}_{\vec{p}} . \quad (18)$$

Interpret the interaction terms. Why are all combinations of \vec{k} and \vec{k}' allowed in the second term, whereas only specific combinations of wave vectors are allowed in the last term? [5P]

Merry Christmas and Happy New Year!