Quantentheorie II Übung 7

– Sample solutions –

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2. **Creation and annihilation operators:**

3. **Number operator:** $\hat{N} \equiv \sum_i \hat{a}_i{}^\dagger \hat{a}_i$. Use

$$[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B} = \hat{A}\{\hat{B}, \hat{C}\} - \{\hat{A}, \hat{C}\}\hat{B} \tag{1}$$

(a) Bosons

$$[\hat{N}, \hat{a}_j{}^\dagger] = \sum_i \left(\hat{a}_i{}^\dagger [\hat{a}_i, \hat{a}_j{}^\dagger] + [\hat{a}_i{}^\dagger, \hat{a}_j{}^\dagger] \hat{a}_i \right) = \hat{a}_j{}^\dagger, \tag{2}$$

$$[\hat{N}, \hat{a}_j] = \sum_i \left(\hat{a}_i{}^\dagger [\hat{a}_i, \hat{a}_j] + [\hat{a}_i{}^\dagger, \hat{a}_j] \hat{a}_i \right) = -\hat{a}_j. \tag{3}$$

Fermions

$$[\hat{N}, \hat{a}_j{}^\dagger] = \sum_i \left(\hat{a}_i{}^\dagger \{\hat{a}_i, \hat{a}_j{}^\dagger\} - \{\hat{a}_i{}^\dagger, \hat{a}_j{}^\dagger\} \hat{a}_i \right) = \hat{a}_j{}^\dagger, \tag{4}$$

$$[\hat{N}, \hat{a}_j] = \sum_i \left(\hat{a}_i{}^\dagger \{\hat{a}_i, \hat{a}_j\} - \{\hat{a}_i{}^\dagger, \hat{a}_j\} \hat{a}_i \right) = -\hat{a}_j. \tag{5}$$

(b) For the Hamiltonian

$$\hat{H} = \sum_{ij} T_{ij} [\hat{N}, \hat{a}_i{}^\dagger \hat{a}_j] + \frac{1}{2} \sum_{ijkl} V_{ijkl} [\hat{N}, \hat{a}_i{}^\dagger \hat{a}_j{}^\dagger \hat{a}_l \hat{a}_k] \tag{6}$$

the commutator is

$$\begin{aligned}
[\hat{N}, \hat{H}] &= \sum_{ij} T_{ij} [\hat{N}, \hat{a}_i{}^\dagger \hat{a}_j] + \frac{1}{2} \sum_{ijkl} [\hat{N}, \hat{a}_i{}^\dagger \hat{a}_j{}^\dagger \hat{a}_l \hat{a}_k] \\
&= \sum_{ij} T_{ij} \left([\hat{N}, \hat{a}_i{}^\dagger] \hat{a}_j + \hat{a}_i{}^\dagger [\hat{N}, \hat{a}_j] \right) \\
&+ \frac{1}{2} \sum_{ijkl} V_{ijkl} \left([\hat{N}, \hat{a}_i{}^\dagger] \hat{a}_j{}^\dagger + \hat{a}_i{}^\dagger [\hat{N}, \hat{a}_j{}^\dagger] \right) \hat{a}_l \hat{a}_k \\
&+ \frac{1}{2} \sum_{ijkl} V_{ijkl}\, \hat{a}_i{}^\dagger \hat{a}_j{}^\dagger \left([\hat{N}, \hat{a}_l] \hat{a}_k + \hat{a}_l [\hat{N}, \hat{a}_k] \right) \\
&= 0 \Longleftarrow \text{ See 3(a)}
\end{aligned} \tag{7}$$

$\Longrightarrow$ The total particle number is conserved. The numbers of creation and annihilation operators are equal.

4. **Second quantization I:** let $\hat{O}$ be $\hat{O} = \sum_i \hat{O}_i$, where $\hat{O}_i$ applies only to the ith particle among the N identical bosons, and all $\hat{O}_i$ are equal.

   (a) To compute the matrix element $\langle n_1', n_2', \cdots |\hat{O}| n_1, n_2, \cdots\rangle$, first consider $\langle n_1', n_2', \cdots |\hat{O}_i| n_1, n_2, \cdots\rangle$. The state with occupation numbers can be written as $|n_1, n_2, \cdots\rangle = \sqrt{\frac{n_1!n_2!\cdots}{N!}} \sum |\psi_{p_1}^{(1)} \psi_{p_2}^{(2)} \cdots \psi_{p_N}^{(N)}\rangle$ in eigenstates of $\hat{O}_i$ basis ψ_k, which is an eigenstate with eigenvalue p_k momentum. The operator $\hat{O}_i$ applies to the ith particle only

$$\hat{O}_i|n_1, n_2, \cdots\rangle = \sqrt{\frac{n_1!n_2!\cdots}{N!}} \sum |\psi_{p_1}^{(1)} \psi_{p_2}^{(2)} \cdots, \hat{O}_i|\psi_{p_i}^{(i)}\rangle, \cdots \psi_{p_N}^{(N)}\rangle. \tag{8}$$

   As all other particles except the ith particle stay unchanged the mateix element represents the transition of the ith particle to change from the initial $p_i = p_k$-state to the final $p_i = p_l$-state, and also all $\hat{O}_i$ are equivalent. Therefore we define $T_{lk} \equiv (\hat{O}_i)_{lk} = \langle \psi_{p_l}^{(i)} | \hat{O}_i | \psi_{p_k}^{(i)}\rangle$. As a consequence the number of particles in the k-state is *decreased* by one, and the number in the l-state is *increased* by one

$$\begin{aligned}
&\langle \cdots n_k - 1, \cdots, n_l, \cdots |\hat{O}_i| \cdots, n_k, \cdots, n_l - 1, \cdots\rangle \\
&= \left(\frac{n_1! \cdots (n_k-1)! \cdots n_l! \cdots}{N!}\right)^{\frac{1}{2}} \left(\frac{n_1! \cdots n_k! \cdots (n_l-1)! \cdots}{N!}\right)^{\frac{1}{2}} \frac{(N-1)!}{n_1! \cdots (n_k-1)! \cdots (n_l-1)!} (\hat{O}_i)_{lk} \\
&= \frac{\sqrt{n_l n_k}}{N} (\hat{O}_i)_{lk},
\end{aligned} \tag{9}$$

   and

$$\begin{aligned}
&\langle \cdots, n_k - 1, \cdots, n_l, \cdots | \sum_i^N \hat{O}_i | \cdots, n_k, \cdots, n_l - 1, \cdots\rangle \\
&= \langle \cdots, n_k - 1, \cdots, n_l, \cdots | \sum_{l,k} \sum_i^N \frac{\sqrt{n_l n_k}}{N} (\hat{O}_i)_{lk} | \cdots, n_k, \cdots, n_l - 1, \cdots\rangle \\
&= \langle \cdots, n_k - 1, \cdots, n_l, \cdots | \sum_{l,k} \sqrt{n_l n_k} (\hat{O}_i)_{lk} | \cdots, n_k, \cdots, n_l - 1, \cdots\rangle \\
&= \langle \cdots, n_k - 1, \cdots, n_l, \cdots | \sum_{l,k} T_{lk} \hat{a}_l^\dagger \hat{a}_k | \cdots, n_k, \cdots, n_l - 1, \cdots\rangle
\end{aligned} \tag{10}$$

$$\begin{aligned}
&\Longleftarrow \ \hat{a}_k | \cdots n_k \cdots\rangle = \sqrt{n_k} | \cdots n_k - 1 \cdots\rangle \\
&\qquad T_{lk} \equiv (\hat{O}_i)_{lk} = \langle \psi_{p_l}^{(i)} | \hat{O}_i | \psi_{p_k}^{(i)}\rangle
\end{aligned}$$

$$\therefore \hat{O} = \sum_i^N \hat{o}_i = \sum_{lk} T_{lk} \hat{a}_l^\dagger \hat{a}_k. \tag{11}$$

   (b) We choose momentum eigenstates $|\vec{p}\rangle$ as basis

$$\hat{p}|\vec{p}\rangle = \vec{p}|\vec{p}\rangle, \quad \langle \vec{p}'|\vec{p}\rangle = \delta^{(3)}(\vec{p}' - \vec{p}), \tag{12}$$

   and the total momentum operator of a system is $\hat{P} = \sum_i \hat{p}_i$. Using Eq. (11) we obtain

$$T_{lk} = (\hat{p})_{\vec{p}-l\vec{p}-k} = \langle \vec{p}_l | \hat{p} | \vec{p}_k \rangle = \vec{p}_k \delta^{(3)}(\vec{p}_l - \vec{p}_k), \text{ and} \tag{13}$$

$$\sum_{lk} T_{lk} \hat{a}_l^\dagger \hat{a}_k \xrightarrow{\text{continuous}} \int dk dl T_{lk} \hat{a}_l^\dagger \hat{a}_k. \tag{14}$$

After combining all together

$$
\begin{aligned}
\hat{P} = \sum_i^N \hat{p}_i &= \int d^3p_k d^3p_l T_{p_l p_k} \hat{a}_{p_l}{}^\dagger \hat{a}_{p_k} \\
&= \int d^3p_k d^3p_l \delta^{(3)}(\vec{p}_k - \vec{p}_l)\vec{p}_k \hat{a}_{p_l}{}^\dagger \hat{a}_{p_k} \\
&= \int d^3p\, \vec{p}\, \hat{a}_p{}^\dagger \hat{a}_p. \Longleftarrow \; p_k = p
\end{aligned} \tag{15}
$$

5. **Second quantization II:**

   (a) Likewise (see 4-a) define

$$
V_{mn,kl} \equiv (\hat{o}_{ij})_{mn,kl} = \langle \cdots \phi_m^{(i)} \cdots \phi_n^{(i)} \cdots |\hat{o}_{ij}| \cdots \phi_k^{(i)} \cdots \phi_l^{(j)} \cdots \rangle, \tag{16}
$$

   and

$$
\begin{aligned}
&\langle \cdots n_k - 1, \cdots, n_l - 1, \cdots, n_m, \cdots, n_n, \cdots |\hat{o}_{ij}| \cdots n_k, \cdots, n_l, \cdots, n_m - 1, \cdots, n_n - 1, \cdots \rangle \\
&= \sqrt{n_m n_n n_k n_l}(\hat{o}_{ij})_{nm,kl} \\
&\Longrightarrow (\hat{o}_{ij})_{nm,kl} \hat{a}_n{}^\dagger \hat{a}_m{}^\dagger \hat{a}_l \hat{a}_k
\end{aligned} \tag{17}
$$

$$
\hat{O} = \frac{1}{2}\sum_{i,j=1(i\neq j)}^N \hat{o}_{ij} \hat{a}_n{}^\dagger \hat{a}_m{}^\dagger \hat{a}_l \hat{a}_k \Longrightarrow \frac{1}{2}\sum_{klmn} V_{mn,kl} \hat{a}_n{}^\dagger \hat{a}_m{}^\dagger \hat{a}_l \hat{a}_k \tag{18}
$$

   (b) The Hamiltonian $\hat{H}$ is given as

$$
\hat{H} = \sum_{i=1}^N \left(-\frac{1}{2}\nabla_i^2 + V(\xi_i) \right) + \frac{1}{2}\sum_{i,j(i\neq j)}^N W(\xi_i, \xi_j) = \sum_{i=1}^N \hat{H}_i + \frac{1}{2}\sum_{i,j(i\neq j)}^N W(\xi_i, \xi_j). \tag{19}
$$

   $|\psi_k\rangle$ are eigenstates of $\hat{H}_i$, $\hat{H}_i|\psi_k\rangle = E_k|\psi_k\rangle$. The matrix elements for 1-particle and 2-particle parts are

$$
\langle \psi_k|\hat{H}_i|\psi_l\rangle = E_k \delta_{kl}, \tag{20}
$$

$$
\langle \psi_{k_2}\psi_{l_2}|W|\psi_{k_1}\psi_{l_1}\rangle \equiv W_{k_2,l_2,k_1l_1}, \tag{21}
$$

   and we can express the Hamiltonian as

$$
\hat{H} = \sum_k E_k \hat{a}_k{}^\dagger \hat{a}_k + \frac{1}{2}\sum_{k_1,l_1,k_2,l_2} W_{k_2l_2,k_1l_1} \hat{a}_{k_2}{}^\dagger \hat{a}_{l_2}{}^\dagger \hat{a}_{k_1} \hat{a}_{l_1} \tag{22}
$$

6. The Hamiltonian of N bosons in a cube of edge lengen L is given as

$$
\hat{H} = \sum_{i=1}^N \left(-\frac{1}{2m}\nabla_i^2 + \frac{1}{2}\sum_{j=1(i\neq j)}^N V(|\vec{r}_i - \vec{r}_j|). \right) \tag{23}
$$

1-particle basis states are $\psi_{\vec{p}}(\vec{r}) = L^{-\frac{3}{2}} e^{i\vec{p}\cdot\vec{r}}$ and the eigenvalues for momenta are $p_i = \frac{2\pi}{L} n_i$ where $i \in \{x, y, z\}$ and n_x, n_y and n_z are integers. We need to calcute the matrix elements

$$\langle \vec{p}'| \frac{-\nabla_i^2}{2m} |\vec{p}\rangle = \frac{\vec{p}^2}{2m} \delta_{\vec{p}\vec{p}'} \qquad : \text{ transition from } \vec{p} \text{ to } \vec{p}', \tag{24}$$

$$\langle \vec{p}_1'\vec{p}_2'|V(|\vec{x}_1 - \vec{x}_2|)|\vec{p}_1\vec{p}_2\rangle = V_{\vec{p}_1'\vec{p}_2'\,\vec{p}_1\vec{p}_2} \qquad : \text{ transition from } \vec{p}_1,\, \vec{p}_2 \text{ to } \vec{p}_1',\, \vec{p}_2', \tag{25}$$

and the explicit calculation of $V_{\vec{p}_1'\vec{p}_2'\,\vec{p}_1\vec{p}_2}$ is

$$\begin{aligned}
V_{\vec{p}_1'\vec{p}_2'\,\vec{p}_1\vec{p}_2} &= \int d^3x_1 d^3x_2 \langle \vec{p}_1'\vec{p}_2'|V(|\vec{x}_1 - \vec{x}_2|)|\vec{x}_1\rangle\langle\vec{x}_2|\vec{p}_1\vec{p}_2\rangle \\
&= \int d^3x_1 d^3x_2 \langle \vec{p}_1'\vec{p}_2'|\vec{x}_1\vec{x}_2\rangle V(|\vec{x}_1 - \vec{x}_2|)\langle\vec{x}_1\vec{x}_2|\vec{p}_1\vec{p}_2\rangle \\
&= \int d^3x_1 d^3x_2 V(|\vec{x}_1 - \vec{x}_2|) L^{-6} e^{-i\vec{x}_1\cdot(\vec{p}_1' - \vec{p}_1)} e^{-i\vec{x}_2\cdot(\vec{p}_2' - \vec{p}_2)} \\
&= \frac{1}{L^6} \int d^3x_1 d^3y V(|\vec{y}|) e^{i\vec{x}_1\cdot(\vec{p}_1 - \vec{p}_1' + \vec{p}_2 - \vec{p}_2')} e^{-i\vec{y}\cdot(\vec{p}_2' - \vec{p}_2)} \quad \Longleftarrow \; \vec{y} \equiv \vec{x}_1 - \vec{x}_2 \\
&= \begin{cases} \frac{1}{L^3} \int d^3y V(|\vec{y}|) e^{-i\vec{y}\cdot(\vec{p}_2' - \vec{p}_2)} & \text{for } \vec{p}_1 + \vec{p}_2 = \vec{p}_1' + \vec{p}_2' \\ 0 & \text{for } \vec{p}_1 + \vec{p}_2 \neq \vec{p}_1' + \vec{p}_2'. \end{cases}
\end{aligned} \tag{26}$$

The Hamiltonian in second quantization expression is

$$\hat{H} = \sum_{\vec{p}_k} \frac{\vec{p}_k^2}{2m} \hat{a}_{\vec{p}_k}{}^{\dagger} \hat{a}_{\vec{p}_k} + \frac{1}{2} \sum_{\vec{p}_l\vec{p}_m\vec{p}_k\vec{p}_i} \frac{1}{L^3} \omega(|\vec{p}_2' - \vec{p}_2|) \hat{a}_{\vec{p}_l}{}^{\dagger} \hat{a}_{\vec{p}_m}{}^{\dagger} \hat{a}_{\vec{p}_k} \hat{a}_{\vec{p}_i}, \tag{27}$$

where $\omega(|\vec{p}_2' - \vec{p}_2|) \equiv \int d^3y V(|\vec{y}|) e^{-i\vec{q}\cdot(\vec{p}_2' - \vec{p}_2)}$.