Quantentheorie II Übung 7

Besprechung: 2021WE23 (KW23)

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1. **Questions**

   (a) In the lecture some remarks were made on the normalization of symmetrized states (see e.g. section 2.2.2 on states obtained via the symmetrization operators). Discuss the different options for normalization for the example states $|nn\rangle^{(+)}$ and $|nm\rangle^{(+)}$ for $n \neq m$.

   (b) Discuss simple examples how you can experimentally determine whether two particles are distinguishable bosons/fermions. (see e.g. lecture 2.3.2)

   (c) What is the difference between the occupation number formalism and the "multi-particle-state" formalism?

2. **Creation and annihilation operators:** What are the resulting states of the following expressions for bosons and fermions respectively?

   (a) $a_5^\dagger a_3^\dagger a_4^\dagger a_2^\dagger a_7^\dagger |0\rangle$

   (b) $a_4^\dagger a_8^\dagger a_5 a_1 a_3^\dagger a_5^\dagger a_6^\dagger |0\rangle$

   (c) $a_4^\dagger a_7^\dagger a_5 a_1 a_1^\dagger a_3^\dagger a_5^\dagger a_8^\dagger |0\rangle$

   (d) $a_5^\dagger a_3^\dagger a_8^\dagger a_1 a_3^\dagger a_2^\dagger a_1^\dagger a_7^\dagger |0\rangle$

3. **Number operator:**

   (a) The number operator is defined as

   $$\hat{N} \equiv \sum_i a_i^\dagger a_i \,.$$

   Prove that the following commutation relations are valid for both bosons and fermions:

   $$[\hat{N}, a_j^\dagger] = a_j^\dagger \,, \qquad [\hat{N}, a_j] = -a_j \,.$$

   Use the identity

   $$[\hat{A}\hat{B}, \hat{C}] = \hat{A}\{\hat{B}, \hat{C}\} - \{\hat{A}, \hat{C}\}\hat{B} \,.$$

   (b) Show that the general Hamiltonian

   $$\hat{H} = \sum_{ij} T_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k$$

   commutes with the number operator $\hat{N}$, i.e. $[\hat{N}, \hat{H}] = 0$. What is the physical meaning of this?

4. **Second quantization I:** consider a system of N identical bosons and let $\hat{\mathcal{O}}_i$ be an operator which operates on the variables of the ith particle only.

   (a) Find the expression for an operator of the form $\hat{\mathcal{O}} = \sum_{i=1}^{N} \hat{\mathcal{O}}_i$ in second quantization. Assume the discrete basis for the one-particle states.

   (b) Repeat this to find the second quantization expression for the total momentum operator of the system:

   $$\hat{P} = \sum_{i=1}^{N} p_i \,.$$

   Use as basis the continuous 1-dimensional momentum eigenstates normalized as $\langle p'|p\rangle = \delta(p' - p)$.

5. **Second quantization II:** similarly to the previous task consider an operator of the form

$$\hat{\mathcal{O}} = \frac{1}{2} \sum_{i,j=1(i\neq j)}^{N} \hat{\mathcal{O}}_{ij} \,, \tag{1}$$

where $\hat{\mathcal{O}}_{ij}$ acts simultaneously on the ith and on the jth particles.

   (a) Rewrite $\hat{\mathcal{O}}$ in Eq. (1) in the second quantization formalism.

   (b) Consider a particular Hamiltonian $\hat{H}$ written in terms of the variables ξ_i (the position and spin of the ith particle) in the form

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

   As one-particle basis states use the eigenstates $|\psi_k\rangle$, where $\hat{H}_i|\psi_k\rangle = E_k|\psi_k\rangle$.

6. N **bosons in a cube of edge length** L**:** consider a system of bosons whose Hamiltonian is of the form

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

where $V(|\vec{r}_i - \vec{r}_j|)$ is the two-particle interaction energy, and depends only on the distance between the particles.

Choose as one-particle basis states the eigenstates of momentum with eigenvalue $\vec{p}$ with wave function

$$\psi_{\vec{p}}(\vec{r}) = L^{-\frac{3}{2}} e^{i\vec{p}\cdot\vec{r}} \,,$$

which are periodic and normalized in a cube of edge length L, and show that the Hamiltonian $\hat{H}$ in Eq. (2) can be written in second quantization in the form

$$\hat{H} = \sum_k \frac{p_k^2}{2m} a_{\vec{p}_k}^\dagger a_{\vec{p}_k} + \frac{1}{2} \sum \frac{1}{L^3} \omega(\vec{p}_l - \vec{p}_i) a_{\vec{p}_l}^\dagger a_{\vec{p}_m}^\dagger a_{\vec{p}_i} a_{\vec{p}_k} \,, \tag{3}$$

where $\omega(\vec{p}) \equiv \int d\vec{q} V(|\vec{q}|) e^{-i\vec{p}\cdot\vec{q}}$, and the second summation in Eq. (3) is carried out subject to the condition $\vec{p}_l + \vec{p}_m = \vec{p}_i + \vec{p}_k$.

Note: this exercise is useful in describing superfluidity.

1. **Questions**

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   (b) Discuss simple examples how you can experimentally determine whether two particles are distinguishable bosons/fermions. (see e.g. lecture 2.3.2)

   (c) What is the difference between the occupation number formalism and the "multi-particle-state" formalism?

a)

Nolting, Vorlesung

$\mathbb{1}_{\mathcal{H}_N^{(\pm)}} = \sum\!\!\!\!\!\!\int_{n_1..n_N} |n_1..n_N\rangle^{(\pm)(\pm)}\langle n_1..n_N|$

$|n_1, n_2, ...\rangle = (a_1^+)^{n_1} (a_2^+)^{n_2} ... |0\rangle$

$S^{(\pm)2} = S^{(\pm)}$

gemeinsamer Vorfaktor

$|n_1..n_N\rangle^{(\pm)} = S_N^{(\pm)} |n_1^{(1)}..n_N^{(N)}\rangle$

Carsten Timm

Zustände Norm $=1$

$|n_1, n_2, ...\rangle = \frac{1}{\sqrt{n_1!\, n_2! ..}} (a_1^+)^{n_1} (a_2^+)^{n_2} ... |0\rangle$

$$|n_1 .. n_N\rangle^{(\pm)} = \frac{1}{N!} \sum_{\mathcal{P}} (\pm 1)^p \, \mathcal{P}\left(|n_1^{(1)}\rangle .. |n_N^{(N)}\rangle\right)$$

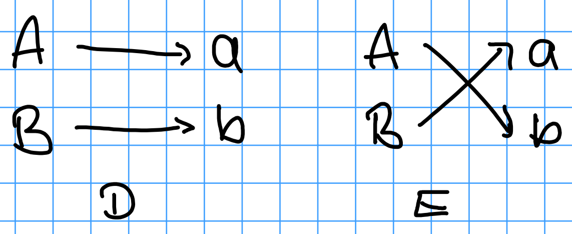
$N = \#$ Teil

$N=2$

$\frac{1}{2!}\left(|nm\rangle + |mn\rangle\right)$	$|nm\rangle^{(+)}$	$\frac{1}{\sqrt{2}}\left(|nm\rangle + |mn\rangle\right)$
$\frac{1}{2!}|nn\rangle$	$|nn\rangle^{(+)}$	$|nn\rangle$

b)

- Bose-Einstein-Kondensation
- Atomspektren



$$P = \begin{cases} |A^D + A^E|^2 & \text{(Bosonen)} \\ |A^D - A^E|^2 & \text{(Fermion)} \end{cases}$$

c)

Besetzungszahl	Anderer	
✗	✓	Fixed N
✓	✗	nur symm./antisymm
✓	✗	diskrete Basis

2. **Creation and annihilation operators:** What are the resulting states of the following expressions for bosons and fermions respectively?

   (a) $a_5^\dagger a_3^\dagger a_4^\dagger a_2^\dagger a_7^\dagger |0\rangle$

   (b) $a_4^\dagger a_8^\dagger a_5 a_1 a_3^\dagger a_5^\dagger a_6^\dagger |0\rangle$

   (c) $a_4^\dagger a_7^\dagger a_5 a_1 a_1^\dagger a_3^\dagger a_5^\dagger a_8^\dagger |0\rangle$

   (d) $a_5^\dagger a_3^\dagger a_8^\dagger a_1 a_3^\dagger a_2^\dagger a_1^\dagger a_7^\dagger |0\rangle$

$a^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$

$a|n\rangle = \sqrt{n}\,|n-1\rangle$

Bosonen | Fermionen

(a) $a_2^+ a_3^+ a_4^+ a_5^+ a_7^+ |0\rangle$ $\qquad (-1)^5\, a_2^+ a_3^+ a_4^+ a_5^+ a_7^+ |0\rangle$

$= |0,1,1,1,1,0,1,\ldots\rangle \qquad = -|0,1,1,1,1,0,1\ldots\rangle$

b) $a_5 \underline{a_1} a_3^+ a_4^+ a_5^+ a_6^+ a_8^+ \underline{|0\rangle}$ $\qquad (-1)^8 \ldots |0\rangle$

$= 0 \qquad = 0$

c) $a_5 a_1 a_1^+ a_3^+ a_4^+ a_5^+ a_7^+ a_8^+ |0\rangle$ $\qquad (-1)^9$

$= a_5 a_1 \; |1\,0\,1\,1\,1\,0\,1\,1\ldots\rangle$

$= \quad |1\,0\,0\,1\,1\,0\,0\,1\,1\ldots\rangle$

d) $a_1 a_1^+ a_2^+ (a_3^+)^2 a_5^+ \ldots |0\rangle$ $\qquad = 0 \qquad (-1)^{16}$ Pauli Prinzip

$= a_1 \sqrt{2}\,|1\,1\,2\,0\,1\,0\,1\,1\ldots\rangle$

$= \sqrt{2}\,|0\,1\,2\,0\,1\,0\,1\,1\ldots\rangle$

$a_3^+ a_3^+ |0\rangle = a_3^+|0\,0\,1\ldots\rangle$

$a_3^+|0\,0\,1\ldots\rangle = \sqrt{2}\;|0\,0\,2\rangle$

$a_5^+ a_3^+ a_4^+ a_2^+ a_7^+ |0\rangle$

5 3 2 4 7

5 2 3 4 7

2 5 3 4 7

$\Sigma 5$

$\{a_n^+, a_{n'}^+\} = 0 \qquad n \neq n'$

$a_n^+ a_{n'}^+ = -a_{n'}^+ a_n^+$

$\{a_n, a_{n'}^+\} = \delta_{nn'}$

4. **Second quantization I:** consider a system of N identical bosons and let $\hat{\mathcal{O}}_i$ be an operator which operates on the variables of the ith particle only.

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(b) Repeat this to find the second quantization expression for the total momentum operator of the system:

$$\hat{P} = \sum_{i=1}^{N} p_i \, .$$

Use as basis the continuous 1-dimensional momentum eigenstates normalized as $\langle p'|p\rangle = \delta(p'-p)$.

a) $\mathcal{O} = \sum_{k\ell} (\mathcal{O})_{\ell k} \, a^{+}_{\ell} a_k$

b)

$\sum_{k\ell} \longrightarrow \int dk \, d\ell$

$(\mathcal{O})_{\ell k} \longrightarrow \delta^{(3)}(\vec{p}_\ell - \vec{p}_k) \; \vec{p}_\ell$

$\langle p|\hat{P}|p'\rangle$

$= \underbrace{\langle p|p'\rangle}_{\delta^{(3)}(\dots)} p'$

$$\hat{P} = \sum_{i=1}^{N} \hat{p}_i = \int d^3p_k \, d^3p_\ell \, (p_i)_{k\ell} \, a^{+}_{p_\ell} a_{p_k}$$

$$= \int d^3p_k \, d^3p \; \delta^{(3)}(\vec{p}_k - \vec{p}_\ell) \; \vec{p}_\ell \; a^{+}_{\vec{p}_\ell} a_{\vec{p}_k}$$

$$\hat{\vec{P}} = \int d^3p \; \vec{p} \; a^{+}_{\vec{p}} a_{\vec{p}}$$

5. **Second quantization II:** similarly to the previous task consider an operator of the form

$$\hat{\mathcal{O}} = \frac{1}{2} \sum_{i,j=1(i\neq j)}^{N} \hat{\mathcal{O}}_{ij}\,, \tag{1}$$

where $\hat{\mathcal{O}}_{ij}$ acts simultaneously on the ith and on the jth particles.

(a) Rewrite $\hat{\mathcal{O}}$ in Eq. (1) in the second quantization formalism.

(b) Consider a particular Hamiltonian $\hat{H}$ written in terms of the variables ξ_i (the position and spin of the ith particle) in the form

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

As one-particle basis states use the eigenstates $|\psi_k\rangle$, where $\hat{H}_i|\psi_k\rangle = E_k|\psi_k\rangle$.

a)
$$\mathcal{O} = \frac{1}{2}\sum_{mnkl} (\mathcal{O}_{ij})_{mnkl}\, a_m^+ a_n^+ a_l a_k$$

$$\langle \varphi_m^{(i)} \varphi_n^{(j)} | \mathcal{O}_{ij} | \varphi_k^{(i)} \varphi_l^{(j)} \rangle = (\mathcal{O}_{ij})_{mn,kl}$$

$$\langle n_k - 1 \ldots, n_l - 1, \ldots n_m \ldots n_n | \mathcal{O}_{ij} | \ldots n_k \ldots n_l \ldots n_{m-1} \ldots n_{n-1} \rangle$$

$$a_k \quad a_l \quad a_m^+ \quad a_n^+$$

$$F = \frac{1}{2}\sum_{ijkm} \langle ij|f|km\rangle \underbrace{a_i^+ a_j^+ a_m a_k}$$

$$= \frac{1}{2}\sum_{\alpha\neq\beta}\sum_{ijkm} \langle ij|f|km\rangle \underbrace{|i\rangle_\alpha |j\rangle_\beta \langle k|_\alpha \langle m|_\beta}$$

$$= \sum_{\alpha\neq\beta} |i\rangle_\alpha \langle k|_\alpha |j\rangle_\beta \langle m|_\beta$$

$$T = \sum T_{ij}\, a_i^+ a_j$$

$$= \langle i|T|j\rangle\, |i\rangle\langle j|$$

$$= \sum_{\alpha\beta} |i\rangle_\alpha \langle k|_\alpha |j\rangle_\beta \langle m|_\beta - \delta_{kj}\sum_\alpha |i\rangle_\alpha \langle m|_\alpha$$

$$= a_i^+ a_k a_j^+ a_m - a_i^+ \underbrace{[a_k, a_j^+]_\mp}_{a_k a_j^+ \mp a_j^+ a_k} a_m$$

$$= \pm\, a_i^+ a_j^+ a_k a_m = a_i^+ a_j^+ a_m a_k$$

b) $$\hat{H} = \sum_i H_i + \frac{1}{2} \sum_{ij} W(\xi_i, \xi_j)$$

$$H|\varphi_i\rangle = E_i |\varphi_i\rangle$$

$$\hookrightarrow \langle \varphi_k | H_i | \varphi_l \rangle = E_k \, \delta_{kl}$$

$$H = \sum_k E_k a_k^\dagger a_k + \frac{1}{2} \sum_{\dots} W_{k_1 k_2 l_1 l_2} a^\dagger_{k_1} a^\dagger_{k_2} a_{l_2} a_{l_1}$$

3. **Number operator:**

(a) The number operator is defined as

$$\hat{N} \equiv \sum_i a_i^\dagger a_i \, .$$

Prove that the following commutation relations are valid for both bosons and fermions:

$$[\hat{N}, a_j^\dagger] = a_j^\dagger \, , \qquad [\hat{N}, a_j] = -a_j \, .$$

Use the identity

$$[\hat{A}\hat{B}, \hat{C}] = \hat{A}\{\hat{B}, \hat{C}\} - \{\hat{A}, \hat{C}\}\hat{B} \, . \quad = A[B,C] + [A,C]B$$

(b) Show that the general Hamiltonian

$$\hat{H} = \sum_{ij} T_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k$$

commutes with the number operator $\hat{N}$, i.e. $[\hat{N}, \hat{H}] = 0$. What is the physical meaning of this?

a) $$[N, a_j^\dagger] = \sum \left(a_i^\dagger \underbrace{[a_i, a_j^\dagger]}_{\delta_{ij}} + \cancel{[a_i^\dagger, a_j^\dagger]} a_i \right) = a_j^\dagger$$

Nr 3) $N = \sum_i a_i^+ a_i$

$$[N, a_j^+] = \sum [a_i^+ a_i, a_j^+] = \sum a_i^+ \{a_i, a_j^+\} - \{a_i^+, a_j^+\} a_i$$

$$= \sum a_i^+ a_i a_j^+ + \cancel{a_i^+ a_j^+ a_i} - \cancel{a_i^+ a_j^+ a_i} - a_j^+ a_i^+ a_i$$

$$= \sum a_i^+ a_i a_j^+ - a_j^+ a_i^+ a_i = \sum [n_i, a_j^+] = a_j^+$$

$[n_i, a_j] = \delta_{ij} a_j$

$$[N, a_j] = \sum [a_i^+ a_i, a_j] = \sum a_i^+ \{a_i, a_j\} - \{a_i^+, a_j\} a_i$$

$$= \sum a_i^+ a_i a_j + \cancel{a_i^+ a_j a_i} - \cancel{a_i^+ a_j a_i} - a_j a_i^+ a_i$$

$$= \sum a_i^+ a_i a_j - \underbrace{a_j a_i^+ a_i}_{\text{Kommutator}} = \sum a_i^+ a_i a_j - \delta_{ij} a_j + a_i^+ a_j a_i = -a_j$$

e) $$[N, H] = \Big[\underbrace{\sum a_n^+ a_n, \sum_{ij} T_{ij} a_i^+ a_j}_{[n_{ij}, n_i] = 0} + \frac{1}{2} \sum_{ijkl} V_{ijkl} a_i^+ a_j^+ a_k a_l\Big]$$

$$\frac{1}{2} \sum_{ijkl,n} V_{ijkl} [a_n^+ a_n, a_i^+ a_j^+ a_k a_l] = \ldots\ldots\ldots = 0$$