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Exercise 1: Properties of bosonic operators (Oral)

In the harmonic oscillator, the creation and annihilation operators can be introduced, their commutation satisfies the following relation

$$[b, b^\dagger] = 1 \tag{1}$$

Then the occupation operator can be written as $\hat{n} = b^\dagger b$. The states $|n\rangle$, $n \in \mathbb{N}$, indicate the eigenstates of occupation operator.

a) With the commutation (1), show that $b|n\rangle$ und $b^\dagger|n\rangle$ are the eigenstates of the operator $\hat{n}$.

b) Show the following relations

$$\begin{aligned} b|n\rangle &= \sqrt{n}\,|n-1\rangle\,, \\ b^\dagger|n\rangle &= \sqrt{n+1}\,|n+1\rangle\,. \end{aligned}$$

c) Show that for the case $n = 0$ there is

$$b|0\rangle = 0$$

d) Prove the following relation for eigenstates in bosonic Fock space

$$\left[b_i\,,\,b_j^\dagger\right] = \delta_{ij}\;,\;[b_i\,,\,b_j] = \left[b_i^\dagger\,,\,b_j^\dagger\right] = 0\,;$$

- $b_i|n_1,...,n_i,...\rangle = \sqrt{n_i}\,|n_1,...,n_i-1,...\rangle$,
- $b_i^\dagger|n_1,...,n_i,...\rangle = \sqrt{n_i+1}\,|n_1,...,n_i+1,...\rangle$.

Exercise 2: Properties of fermionic operators (written, 5 points)

In order to deepen the understanding of eigenproblems for fermionic operators, consider the BCS-state (BSC: Bardeen Cooper Schriefer) in the form of

$$|\Omega\rangle = \prod_{k>0}\left(u_k + v_k\, c^\dagger_{k,\uparrow}\, c^\dagger_{-k,\downarrow}\right)\,|0\rangle, \tag{2}$$

here u_k and v_k are the parameters, they can be fixed through $|u_k|^2 + |v_k|^2 = 1$. The fermionic operator $c^\dagger_{\pm k,\sigma}$ creates a fermion with $\pm k$ and spin σ out of the vacuum $|0\rangle$.

a) Show that the BCS-state is normalized.

b) Calculate the expectation value within the BCS-state
   i. $\langle\Omega|c^{\dagger}_{k,\uparrow}\, c^{\dagger}_{-k,\downarrow}|\Omega\rangle$
   ii. $\langle\Omega|c^{\dagger}_{k,\sigma}\, c_{k,\sigma}|\Omega\rangle$

c) now we define the BCS-operators $\alpha_{k,\uparrow,\downarrow}$ and $\alpha^{\dagger}_{k,\uparrow,\downarrow}$ via

$$\alpha_{k,\uparrow} = u_k\, c_{k,\uparrow} - v_k\, c^{\dagger}_{-k,\downarrow}\,, \qquad \alpha^{\dagger}_{k,\uparrow} = u^*_k\, c^{\dagger}_{k,\uparrow} - v^*_k\, c_{-k,\downarrow}\,, \tag{3}$$

$$\alpha_{k,\downarrow} = u_k\, c_{-k,\downarrow} + v_k\, c^{\dagger}_{k,\uparrow}\,, \qquad \alpha^{\dagger}_{k,\downarrow} = u^*_k\, c^{\dagger}_{-k,\downarrow} + v^*_k\, c_{k,\uparrow}\,. \tag{4}$$

Explicitly show that the BCS-operators obey the fermionic anticommutation relations i.e. calculate $\{\alpha_{k,\uparrow,\downarrow}\,,\, \alpha^{\dagger}_{k,\uparrow,\downarrow}\}$. Prove that $\alpha_{k,\uparrow,\downarrow}|\Omega\rangle = 0$. Which consequence is for $|\Omega\rangle$?

d) To describe the ground state for free fermions, how do you choose u_k and v_k?

e) The Hamiltonian of free fermion is given by

$$\mathrm{H} = \sum_k \left(\frac{\hbar^2 k^2}{2m} - \varepsilon_F\right) \left(c^{\dagger}_{k,\uparrow}\, c_{k,\uparrow} + c^{\dagger}_{-k,\downarrow}\, c_{-k,\downarrow}\right)\,, \tag{5}$$

where ε_F is the Fermi energy. Express this Hamiltonian with the BCS-operators obtained from question c). Calculate the expectation value of the Hamiltonian $\langle\Omega|\mathrm{H}|\Omega\rangle$. What does $\alpha^{\dagger}_{k,\sigma}$ describe for $k > k_F$? What does $\alpha^{\dagger}_{k,\sigma}$ describe for $k < k_F$?

Exercise 3: Hund's Rules (oral)

The electronic configurations indicate the occupation of electrons in different atomic orbits. The state of one electron is determined through four quantum numbers: principal quantum number $n(1, 2, 3, ...)$, angular momentum quantum number $l(0, 1, ..., n-1)$, magnetic angular momentum quantum number $m_l(-l, ..., +l)$ and the spin quantum number $m_s(1/2, -1/2)$. The principle quantum number indicates the shell and the angular momentum quantum number indicates the subshell ($l = 0 = s, 1 = p, 2 = d$ and so on). Starting from the shell with the lowest energy, in one atom the shells are filled by available electrons. It should be noted that according to Pauli's principle, no state can be doubly occupied and each state can only be occupied singly. The angular momentum and spin of all electrons in a closed shell add up to **0**. However, if a shell is not completely filled, then the orbital angular momenta and the spins of the electrons add up to a total angular momentum $\mathbf{J}$. Depending on the state, several degenerate combinations with different angular momentum and spin are possible for a given principle quantum number n. The degeneracy of the energy in a shell can be removed by spin-orbit coupling and electron-electron interaction. The electronic configurations for angular momentum in the ground state can be found with the Hund's rules.

i) Full shells give no contribution to the orbit / spin angular momentum L and S.
ii) The LS-multiplicity with largest S has the lowest energy.
iii) For the same S, the state with the largest L has the lowest energy.

iv) When the shell is half filled or less, the configuration with the smallest value for $J = |L - S|$ is the lowest in energy; when the shell is more than half-filled, the maximal $J = L + S$ corresponds to the lowest energy.

Now consider carbon C in the electronic configuration $1s^2 2s^2 2p^2$

a) Determine the product basis of the electronic system in the non-fully-filled subshell. Which states do fall out the consideration due to Pauli's principle? What is the degeneracy?

b) Determine **all** the combinations of orbital and spin angular momentum (LS-multiplicity) and indicate each state with the symbol $^{2S+1}L_J$.

c) Now consider the LS combinations which are allowed by the Pauli principle.
(**Tip:** Note that the total wave function must be antisymmetric. Separate the total wave function into the parts of spin and orbit. With these reduced separated parts, the combination of symmetries can be finally fingured out: $(\mathbf{s}_1 \otimes \mathbf{s}_2) \otimes (\mathbf{l}_1 \otimes \mathbf{l}_2)$.)

d) With the Hund's rules determine the ground state.