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Second Quantization - Exercises

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1. Commutator algebra

Show that for any three operators A, B, C, the following relations hold (where $[A,B] = AB - BA$ and $\{A,B\} = AB + BA$:

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

$$[A,BC] = [A,B]C + B[A,C] = \{A,B\}C - B\{A,C\} \tag{2}$$

2. Eigenstates of Diagonal Hamiltonian

Consider the diagonal Hamiltonian $H = \sum_k \varepsilon_k b_k^\dagger b_k$, where k is a discrete index, ε_k is a corresponding discrete energy, and b_k and $b_k^\dagger$ are creation and annihilation operators satisfying either bosonic or fermionic canonical commutation relations:

$$\text{bosonic}: \quad [b_k, b_{k'}^\dagger] = \delta_{kk'}, \quad [b_k, b_{k'}] = 0, \quad [b_k^\dagger, b_{k'}^\dagger] = 0, \tag{3}$$

$$\text{fermionic}: \quad \{b_k, b_{k'}^\dagger\} = \delta_{kk'}, \quad \{b_k, b_{k'}\} = 0, \quad \{b_k^\dagger, b_{k'}^\dagger\} = 0. \tag{4}$$

(i) Show that $[H, b_k^\dagger] = \varepsilon_k b_k^\dagger$.

(ii) Show that if $|E\rangle$ is an eigenstate of H with eigenenergy E, then $b_k^\dagger|E\rangle$ is also an eigenstate, with energy $E + \varepsilon_k$.

(iii) Let $|0\rangle$ be the "vacuum state", defined by the condition that $b_k|0\rangle = 0$ for all k. Write down a general expression for the eigenstates of H, expressed in terms of products of creation operators acting on $|0\rangle$. What is the corresponding eigenenergy?

3. Tight-binding chain

The Hamiltonian for a periodic tight-binding chain of length L is given by

$$H_{\text{chain}} = -t \sum_{n=1}^{L} \left(a_n^\dagger a_{n+1} + a_{n+1}^\dagger a_n \right) \tag{5}$$

where t is the hopping matrix element t between neighboring sites n and $n+1$, and $a_n^\dagger$ creates a fermion on site n, and the set of operators $\{a_n^\dagger, a_n; n = 1, \ldots, L\}$ satisfies canonical anticommutation relations of the form of Eq. (4). We assume periodic boundary conditions, i.e. we make the identification $a_{L+n}^\dagger \equiv a_n^\dagger$.

The purpose of this excerise is to show that this Hamiltonian can be diagonalized by a linear transformation having the form of a discrete Fourier transformation:

$$b_k^\dagger = \frac{1}{\sqrt{L}} \sum_{n=1}^{L} e^{ikn} a_n^\dagger \tag{6}$$

(i) Let us require that $b_k^\dagger$ remains invariant under an arbitrary a shift of the summation index, $n \to n + n'$ ("translational invariance"). Show that this implies that the index k is quantized, and determine the set of allowed k-values. How many independent $b_k^\dagger$ operators are there?

(ii) Check that the set of b_k and $b_k^\dagger$ operators satisfies canonical anticommutation relations [Eq. (4)]. Hint: use the identity $\sum_{m=1}^{L} e^{i2\pi m/L} = 0$.

(iii) Show that the inverse of the transformation (6) has the form

$$a_n^\dagger = \frac{1}{\sqrt{L}} \sum_{k} e^{-ikn} b_k^\dagger \,, \tag{7}$$

where the sum is over the set of allowed k-values determined in (i).

(iv) Show that $b_k^\dagger$ actually is a creation operator for a 1-particle *eigenstate* of H, by showing that its commutator with the Hamiltonian H_{chain} has the form $[H_{\mathrm{chain}}, b_k^\dagger] = \varepsilon_k b_k^\dagger$. Give an explicit expression for the corresponding eigenenergy ε_k.

(v) The result of (iv) implies that the Hamiltonian can be written in the form $H = \sum_k \varepsilon_k b_k^\dagger b_k$. Verify this explicitly, by inserting Eq. (7) into Eq. (5) for H_{chain}, and simplifying. Show that $\varepsilon_k = -2t\cos(k)$.

(vi) Give a formula for the ground state of a half-filled chain (total particle number $= L/2$).

4. Fermionic representation of spin operators

Let $c_{n\mu}^\dagger$ be the creation operators for a set of spinful fermions labeled by a discrete index n (for sites on a chain) and a spin index $\mu = +1$ or -1. The total spin of these fermions is described by the set of three spin operators

$$S_i \equiv \frac{\hbar}{2} \sum_{n\mu} c_{n\mu}^\dagger \sigma_{\mu\mu'}^i c_{n\mu'} \qquad (i = \{x, y, z\}\,)$$

where the Pauli matrices σ^i, obeying $[\sigma_i, \sigma_j] = i2\sum_k \varepsilon_{ijk}\sigma_k$, are defined as

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Show that the operators S_i fulfill the standard spin commutor relations

$$[S_i, S_j] = \hbar i \sum_k \varepsilon_{ijk} S_k.$$