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Problem 1: Representation of the angular momentum (Written, 5 points)

Learning objective

The purpose of this problem is to work out the connection between the algebra of angular momentum (see QM script chapter 4.3) and the algebra of the uncoupled two-dimensional harmonic oscillator which was discussed on problem set 5.

We start by defining the angular momentum operators

$$L_z = \frac{\hbar}{2}(a_+^\dagger a_+ - a_-^\dagger a_-) \qquad L_+ = \hbar a_+^\dagger a_- \qquad L_- = \hbar a_-^\dagger a_+ \tag{1}$$

in terms of creation and annihilation operators $a_+^\dagger$, $a_-^\dagger$ and a_+, a_- that fulfill the commutation relations $[a_\sigma, a_{\sigma'}^\dagger] = \delta_{\sigma,\sigma'}$ and $[a_\sigma^{(\dagger)}, a_{\sigma'}^{(\dagger)}] = 0$, with $\sigma \in \{+,-\}$.

a) Prove that the operators in (1) satisfy the commutation relations of angular momentum:

$$\big[L_z, L_\pm\big] = \pm\hbar L_\pm \qquad \big[L_+, L_-\big] = 2\hbar L_z \; . \tag{2}$$

b) Prove that

$$L^2 = L_z^2 + \frac{1}{2}L_+L_- + \frac{1}{2}L_-L_+ = \frac{\hbar^2}{2}N\left(\frac{N}{2}+1\right) \; , \tag{3}$$

where $N = N_+ + N_-$ with the number operators $N_+ = a_+^\dagger a_+$ und $N_- = a_-^\dagger a_-$.

c) Show that the operators L_+, L_-, L_z, and L^2 act on the eigenstates $|n_+, n_-\rangle$ of the operators N_+ and N_- as follows:

$$L_+ |n_+, n_-\rangle = \hbar\sqrt{n_-(n_+ + 1)}\, |n_+ + 1, n_- - 1\rangle \tag{4}$$

$$L_- |n_+, n_-\rangle = \hbar\sqrt{n_+(n_- + 1)}\, |n_+ - 1, n_- + 1\rangle \tag{5}$$

$$L_z |n_+, n_-\rangle = \frac{\hbar}{2}(n_+ - n_-)\, |n_+, n_-\rangle \tag{6}$$

$$L^2 |n_+, n_-\rangle = \frac{\hbar^2}{2}(n_+ + n_-)\left(\frac{n_+ + n_-}{2} + 1\right) |n_+, n_-\rangle \; . \tag{7}$$

Think of how the matrix representation of L_+, L_-, L_z, and L^2 in the basis $|n_+, n_-\rangle$ looks like. Which states $|n_+, n_-\rangle$ are coupled by the operators?

d) Define

$$l = \frac{1}{2}(n_+ + n_-) \qquad\qquad m = \frac{1}{2}(n_+ - n_-) \ . \tag{8}$$

and use these definitions to show that the equations (4)-(7) reduce to the familar expressions for the L_+, L_-, L_z, and L^2 operators:

$$L_+ |l, m\rangle = \hbar\sqrt{l(l+1) - m(m+1)}\, |l, m+1\rangle \tag{9}$$

$$L_- |l, m\rangle = \hbar\sqrt{l(l+1) - m(m-1)}\, |l, m-1\rangle \tag{10}$$

$$L_z |l, m\rangle = \hbar m\, |l, m\rangle \tag{11}$$

$$L^2 |l, m\rangle = \hbar^2 l(l+1)\, |l, m\rangle \ . \tag{12}$$

e) Write $|l, m\rangle$ in terms of $a_+^\dagger$, $a_-^\dagger$, and the vacuum state $|0, 0\rangle$. Interpret the obtained result.

Problem 2: Symmetric top (Oral, 2 points)

Learning objective

The rotational states of molecules can be very well described by employing the model of a quantum mechanical rigid rotor in which the distance of the atoms within the molecules is assumed to be fixed. In this problem, you consider the special case of a symmetric rotor (or symmetric top), which is analytically solvable, where two moments of inertia are equal and the third moment of inertia has a different value.

Consider a symmetric rigid rotor (symmetric top) where two moments of inertia are the same ($I_x = I_y \equiv I_\perp$) and the third moment of inertia has a different value ($I_z \equiv I_\parallel$).

a) Express the Hamiltonian of such a system in terms of the angular momentum operators L^2 and L_z. Provide examples for molecules whose rotation can be well described by this Hamiltonian.

b) Determine the eigenvalues and eigenstates of the Hamiltonian.

Problem 3: Asymmetric top (Oral, 4 points)

Learning objective

In this problem, we consider asymmetric rigid rotors (asymmetric tops) where all three moments of inertia (I_x, I_y, and I_z) have different values. You will approach the determination of eigenstates and eigenenergies by a successive splitting of the infinite-dimensional Hilbert space into finite-dimensional subspaces, which eventually can be diagonalized more easily. Note that unlike the symmetric top, the asymmetric top does not allow for a full analytical solution.

Consider the Hamiltonian of an asymmetric top given by

$$H = \frac{L_x^2}{2I_x} + \frac{L_y^2}{2I_y} + \frac{L_z^2}{2I_z} \ , \tag{13}$$

where all moments of inertia, I_j, are different from each other.

a) Show that the Hamiltonian commutes with L^2. Express the Hamiltonian in terms of L_z and the ladder operators $L_\pm = L_x \pm iL_y$.

b) We split the Hilbert space $\mathcal{H}$ of the system into subspaces $\mathcal{H}'_l$ and $\mathcal{H}''_l$, so that the sum $\bigoplus_l(\mathcal{H}'_l \oplus \mathcal{H}''_l)$ is the full Hilbert space again. The subspace $\mathcal{H}'_l$ contains the eigenstates $|l, m\rangle$ of L^2 and L_z with $m = l, l-2, \ldots, -l+2, -l$. The subspace $\mathcal{H}''_l$ contains the eigenstates $|l, m\rangle$ with $m = l-1, l-3, \ldots, -l+3, -l+1$.

   Show that the Hamiltonian leaves the subspaces invariant, i.e. if the Hamiltonian acts on a state of a certain subspace, the resulting state belongs to the same subspace.

c) Consider the operator $U = \exp(-i\pi L_y/\hbar)$. Make use of $[U, H] = 0$ and $U|l, m\rangle = (-1)^{l-m}|l, -m\rangle$ in order to show that the full Hilbert space $\mathcal{H}$ can be partioned as

$$\mathcal{H} = \bigoplus_l \mathcal{H}_l \quad \text{with} \quad \mathcal{H}_l = \mathcal{H}'_{l+} \oplus \mathcal{H}'_{l-} \oplus \mathcal{H}''_{l+} \oplus \mathcal{H}''_{l-}\ , \tag{14}$$

   where all of the subspaces are invariant under the Hamiltonian.

   Hint: At first, convince yourself that the operator U commutes with L^2 and that the operator U leaves the subspaces $\mathcal{H}'_l$ and $\mathcal{H}''_l$ invariant. Then, consider that the operator U couples the state $|l, m\rangle$ to the state $|l, -m\rangle$. The stated partition into subspaces follows from the diagonalization of the corresponding 2×2 matrices.

   Supplementary question: What is the physical meaning of the operator U?

d) Determine the eigenvalues and eigenstates of the Hamiltonian for $l = 1$. Compare the results with problem 2.