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Problem 7.1: Representation of the angular momentum **[Written] (5 pts.)**

↪ ID: ex_representation_of_the_angular_momentum:qm2122

> **Learning objective**
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> 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 6.

We start by defining the angular momentum operators

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

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

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 $N = N_x + N_y$ with the number operators $N_x = a_x^\dagger a_x$ und $N_y = a_y^\dagger a_y$.

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

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

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

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

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

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

d) Define

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

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 $a_x^\dagger$, $a_y^\dagger$, and the vacuum state $|0, 0\rangle$. Interpret the obtained result.

Problem 7.2: Symmetric top **[Oral] (2 pts.)**

↪ ID: ex_symmetric_top:qm2122

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 7.3: Asymmetric top **[Oral] (4 pts.)**

↪ ID: ex_asymmetric_top:qm2122

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.