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Problem 2.1: Angular momentum and rotations

[**Oral** | 8 pt(s)]

ID: ex_angular_momentum:aqt2425

> **Learning objective**
>
> Although we already investigated the angular momentum commutation relations in the first problem list, here we will do this from a different perspective, i.e., by seeing angular momentum operators as the generators of infinitesimal rotations.

Consider the angular momentum operator $\mathbf{L} = \mathbf{r} \times \mathbf{p}$. In the lecture it was shown that $\mathbf{L}$ is the infinitesimal generator of rotations such that rotations around some axis $\mathbf{n}$ with $\mathbf{n}^2 = 1$ about some angle ω can be written as $U_{\boldsymbol{\omega}} = \exp\left(-i\omega \mathbf{L} \cdot \mathbf{n}/\hbar\right)$. If $U_{\boldsymbol{\omega}}$ is the operator performing a rotation around some axis $\boldsymbol{\omega} = \omega\mathbf{n}$ in the Hilbert space, i.e. $|\phi_{\boldsymbol{\omega}}\rangle = U_{\boldsymbol{\omega}}|\phi\rangle$; a *scalar* operator S transforms like

$$U_{\boldsymbol{\omega}}^\dagger \, S \, U_{\boldsymbol{\omega}} = S \,, \tag{1}$$

and a *vector* operator $\mathbf{X}$ transforms like

$$U_{\boldsymbol{\omega}}^\dagger \, \mathbf{X} \, U_{\boldsymbol{\omega}} = R_{\boldsymbol{\omega}} \, \mathbf{X} \,, \tag{2}$$

where $R_{\boldsymbol{\omega}}$ is the usual rotation matrix in three dimensions around some axis $\boldsymbol{\omega}$.

a) Show that for a scalar operator S, $[\mathbf{L}, S] = 0$. **2**pt(s)

b) Show that for a vector operator $\mathbf{X}$ it is $[L_i, X_j] = i\hbar\varepsilon_{ijk}X_k$. **2**pt(s)
Hint: Use the representation $(\mathcal{R}_{\boldsymbol{\omega}})_{ij} = [1 - \cos(\omega)]\hat{\omega}_i\hat{\omega}_j + \cos(\omega)\,\delta_{ij} - \sin(\omega)\,\varepsilon_{ijk}\hat{\omega}_k$ for the rotation matrix and linearize (2) for small ω.

c) Using that $\mathbf{r}$ and $\mathbf{p}$ are vector operators, show that $\mathbf{L}$ is also a vector operator. **2**pt(s)
Hint: Consider the components of $U_{\boldsymbol{\omega}}^\dagger \, \mathbf{r} \times \mathbf{p} \, U_{\boldsymbol{\omega}}$ and show that $U_{\boldsymbol{\omega}}^\dagger \, \mathbf{r} \times \mathbf{p} \, U_{\boldsymbol{\omega}} = U_{\boldsymbol{\omega}}^\dagger \, \mathbf{r} \, U_{\boldsymbol{\omega}} \times U_{\boldsymbol{\omega}}^\dagger \, \mathbf{p} \, U_{\boldsymbol{\omega}}$.

d) Show that $[\mathbf{L}, \mathbf{p} \cdot \mathbf{r}] = 0$ on the one hand by explicitely calculating the commutator and on the other hand by showing that $\mathbf{p} \cdot \mathbf{r}$ is a scalar operator. **2**pt(s)

Problem 2.2: Pauli Matrices

[**Written** | 4 pt(s)]

ID: ex_pauli_matrices:aqt2425

> **Learning objective**
>
> The Pauli matrices are very important for the description of two-level systems. In this exercise you will derive some useful properties of the Pauli matrices.

The Pauli matrices are

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3}$$

a) Prove that the Pauli matrices fulfill the following commutation relation: 1pt(s)

$$[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k. \tag{4}$$

b) Show that 1pt(s)

$$\sigma_i\sigma_j = \delta_{ij}\mathbb{1} + i\epsilon_{ijk}\sigma_k. \tag{5}$$

Use this relation to prove that

$$(\mathbf{r}\cdot\boldsymbol{\sigma})^2 = |\mathbf{r}|^2\mathbb{1}, \tag{6}$$

with $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)^T$.

c) For spin 1/2 the spin operator $\mathbf{S} = (S_x, S_y, S_z)^T$ can be written in terms of Pauli matrices $\mathbf{S} = \hbar/2\boldsymbol{\sigma}$. Show that the representation of the rotation takes the form 1pt(s)

$$U_{\theta\hat{\mathbf{n}}} = \exp\left(-\frac{i}{\hbar}\theta\,\mathbf{S}\cdot\hat{\mathbf{n}}\right) = \mathbb{1}\cos\frac{\theta}{2} - i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\sin\frac{\theta}{2}, \tag{7}$$

where $\hat{\mathbf{n}}$ is the rotation axis and θ the rotation angle.
Consider the state $|\uparrow\rangle = (1,0)^T$. What is the expectation value of the spin operator after rotation by $\pi/2$ and π around the y axis?

d) Show that the spin operator **S** transforms like a vector under rotation. 1pt(s)
Hint: Refer to subtask b of problem 2.1.

Problem 2.3: Hydrogen Atom – Lowest States

[**Written** | 4 pt(s)]

ID: ex_hydrogen_atom_lowest_states:aqt2425

> **Learning objective**
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> In this exercise, we will revisit the hydrogen atom problem and determine the size of the atoms where electrons occupy the lower states.

Consider the wave functions of the Hydrogen atom $\psi_{n,\ell,m}$,

$$\psi_{n,l,m}(r,\theta,\varphi) = R_{n,l}(r)Y_{lm}(\theta,\varphi), \tag{8}$$

$$R_{nl}(r) = -N_{nl}(2\kappa r)^l e^{-\kappa r}L^{2l+1}_{n-l-1}(2\kappa r), \tag{9}$$

$$N_{nl} = \left(\frac{1}{a}\right)^{3/2}\frac{2}{n^2(n+l)!}\sqrt{\frac{(n-l-1)!}{(n+l)!}}, \tag{10}$$

where $\kappa = 1/an$, and a refers to the Bohr radius, and L^k_p are the Laguerre polynomials.

a) Write explicitly the $1s$, $2s$, and $2p_z$ wave functions, which correspond to the set of quantum numbers $\{n,\ell,m\} = \{1,0,0\}$, $\{2,0,0\}$, and $\{2,1,0\}$, respectively. 2pt(s)

b) Determine the expectation value of the radial components r, r^2 and $1/r$ in the ground state (i.e. the $1s$ state) and the $2p_z$ state. Deduce the size of the atom in each of these states. 2pt(s)