Quantum theory of angular momentum

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1 Orbital angular momentum in real space

A rotation $\mathcal{D}$ transforms an arbitrary function $f(\mathbf{r})$ (such as a potential or a wave function) into a new function $\tilde{f}(\mathbf{r})$. In order to construct $\tilde{f}(\mathbf{r})$, we consider the rotation of space, where $\mathcal{D}(\mathbf{r}) = \tilde{\mathbf{r}}$ can be described by an orthogonal matrix. Now $\tilde{f}(\tilde{\mathbf{r}}) = f(\mathbf{r})$ holds, which implies

$$\tilde{f}(\mathbf{r}) = f(\mathcal{D}^{-1}(\mathbf{r}))$$

In particular we consider an infinitesimal rotation with angle $\delta\boldsymbol{\phi}$, where the vector denotes the direction of the axis of rotation (right-hand rule). We find $\mathcal{D}(\mathbf{r}) = \mathbf{r} + \delta\boldsymbol{\phi} \times \mathbf{r}$ and

$$\begin{aligned}\tilde{\Psi}(\mathbf{r}) =&\Psi(\mathbf{r} - \delta\boldsymbol{\phi} \times \mathbf{r}) \approx \Psi(\mathbf{r}) - (\delta\boldsymbol{\phi} \times \mathbf{r}) \cdot \nabla\Psi(\mathbf{r}) \\ =&\Psi(\mathbf{r}) - \frac{\mathrm{i}}{\hbar}\delta\boldsymbol{\phi} \cdot \left(\mathbf{r} \times \frac{\hbar}{\mathrm{i}}\nabla\right)\Psi(\mathbf{r}) = \left(1 - \frac{\mathrm{i}}{\hbar}\delta\boldsymbol{\phi} \cdot \hat{\mathbf{L}}\right)\Psi(\mathbf{r})\end{aligned}$$

The operator of the orbital angular momentum $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$ generates infinitesimal rotations in the three-dimensional space.

Defining $\hat{\mathbf{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ we find the commutator relations

$$[\hat{\mathbf{L}}^2, \hat{L}_j] = 0 \quad \text{und} \quad [\hat{L}_j, \hat{L}_k] = \mathrm{i}\hbar\sum_l \epsilon_{jkl}\hat{L}_l\,,$$

which have the following interpretation: Consider a sequence of two infinitesimal rotations around the x and y axis:

$$\begin{aligned}\mathcal{D}_x\mathcal{D}_y =& \left(1 - \frac{\mathrm{i}}{\hbar}\delta\phi_x\hat{L}_x\right)\left(1 - \frac{\mathrm{i}}{\hbar}\delta\phi_y\hat{L}_y\right) \\ =&1 - \frac{\mathrm{i}}{\hbar}\delta\phi_x\hat{L}_x - \frac{\mathrm{i}}{\hbar}\delta\phi_y\hat{L}_y - \frac{1}{\hbar^2}\delta\phi_x\delta\phi_y\hat{L}_x\hat{L}_y \\ =&\mathcal{D}_y\mathcal{D}_x - \frac{1}{\hbar^2}\delta\phi_x\delta\phi_y\left(\hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x\right) = \mathcal{D}_y\mathcal{D}_x - \frac{\mathrm{i}}{\hbar}\delta\phi_x\delta\phi_y\hat{L}_z \\ \approx&\mathcal{D}_y\mathcal{D}_x\left(1 - \frac{\mathrm{i}}{\hbar}\delta\phi_x\delta\phi_y\hat{L}_z\right)\end{aligned}$$

The fact that the commutator between $\hat{L}_x$ and $\hat{L}_y$ is finite, relates to the geometrical observation, that rotations around the x and y axis do not commute.

2 Generalized angular momentum

The commutation relations of the angle momentum have their origin in the transformation of objects under rotations. This suggests

We define general self-adjoint operators $\hat{J}_x, \hat{J}_y, \hat{J}_z$ for angular momentum via the relations

$$[\hat{\mathbf{J}}^2, \hat{J}_j] = 0 \quad \text{and} \quad [\hat{J}_j, \hat{J}_k] = \mathrm{i}\hbar \sum_l \epsilon_{jkl} \hat{J}_l \tag{1}$$

where $\mathbf{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$. Furthermore we define the shift operators

$$\hat{J}_\pm = \hat{J}_x \pm \mathrm{i}\hat{J}_y \quad \text{with} \left(\hat{J}_\pm\right)^\dagger = \hat{J}_\mp$$

Then there exists a basis of the Hilbert space consisting of common eigenstates of the operators $\hat{\mathbf{J}}^2$ and $\hat{J}_z$. Let $|\Psi\rangle$ be such a normalized state. In the following we will determine the properties of the corresponding eigenvalues.

1. The eigenvalues of $\hat{\mathbf{J}}^2$ are not negative.

   Proof: Let $\hat{\mathbf{J}}^2|\Psi\rangle = \alpha|\Psi\rangle$. Then

   $$\alpha = \langle\Psi|\hat{\mathbf{J}}^2|\Psi\rangle = \langle\Psi_x|\Psi_x\rangle + \langle\Psi_y|\Psi_y\rangle + \langle\Psi_z|\Psi_z\rangle \geq 0$$

   where $|\Psi_i\rangle := \hat{J}_i|\Psi\rangle$ and thus $\langle\Psi_i| = \langle\Psi|\hat{J}_i$, as $\hat{J}_i$ is self-adjoint. □

   Therefore we can write the eigenvalues as

   $$\hat{\mathbf{J}}^2|\Psi\rangle = j(j+1)\hbar^2|\Psi\rangle \quad \text{and} \quad \hat{J}_z|\Psi\rangle = m\hbar|\Psi\rangle$$

   where we temporarily allow $j \in \mathbb{R}^+$ and $m \in \mathbb{R}$ (they will turn out to be half-integer numbers later).

2. Consider $|\Psi_+\rangle = \hat{J}_+|\Psi\rangle$. We find

   $$\begin{aligned}\langle\Psi_+|\Psi_+\rangle = \langle\Psi|\hat{J}_-\hat{J}_+|\Psi\rangle = \langle\Psi|\hat{J}_x^2 + \hat{J}_y^2 + \mathrm{i}[\hat{J}_x, \hat{J}_y]|\Psi\rangle = \langle\Psi|\mathbf{J}^2 - \hat{J}_z^2 - \hbar\hat{J}_z|\Psi\rangle \\ = [j(j+1) - m^2 - m]\hbar^2\end{aligned}$$

   Thus

   (a) $|\Psi_+\rangle = 0 \Leftrightarrow m = j \quad \text{or} \quad m = -j-1$

   (b) For $m > j$ or $m < -j-1$ we would find $\langle\Psi_+|\Psi_+\rangle < 0$. Thus $-j-1 \leq m \leq j$ is required.

   (c) $|\Psi_+\rangle$ is also eigenstate of $\hat{\mathbf{J}}^2$ and $\hat{J}_z$ with the eigenvalues $j(j+1)\hbar^2$ and $(m+1)\hbar$.
   Proof:

   $$\hat{\mathbf{J}}^2|\Psi_+\rangle = \hat{\mathbf{J}}^2\hat{J}_+|\Psi\rangle = \hat{J}_+\hat{\mathbf{J}}^2|\Psi\rangle = \hat{J}_+ j(j+1)\hbar^2|\Psi\rangle = j(j+1)\hbar^2|\Psi_+\rangle$$

   $$\begin{aligned}\hat{J}_z|\Psi_+\rangle = \hat{J}_z(\hat{J}_x + \mathrm{i}\hat{J}_y)|\Psi\rangle = (\hat{J}_x + \mathrm{i}\hat{J}_y)\hat{J}_z|\Psi\rangle + \left([\hat{J}_z, \hat{J}_x] + \mathrm{i}[\hat{J}_z, \hat{J}_y]\right)|\Psi\rangle \\ = (\hat{J}_x + \mathrm{i}\hat{J}_y)m\hbar|\Psi\rangle + \hbar\left(\mathrm{i}\hat{J}_y + \hat{J}_x\right)\Psi\rangle = (m+1)\hbar|\Psi_+\rangle \qquad \square\end{aligned}$$

Now we write $|\Psi\rangle = |a, j, m\rangle$, where a denotes further quantum numbers, as there can be several states with equal j and m. Using (a) and (c) we define for $m \neq j$

$$|a, j, m+1\rangle = \frac{1}{\hbar\sqrt{j(j+1) - m(m+1)}} \hat{J}_+ |a, j, m\rangle \tag{2}$$

The repeated operation of $\hat{J}_+$ provides a sequence of states $|a, j, m\rangle$, $|a, j, m+1\rangle$, $|a, j, m+2\rangle, \ldots$. This sequence stops if $m + i_+ = j$, as in this case $\hat{J}_+|a, j, m + i_+\rangle = 0$. If the sequence does not terminate one reaches states contradicting (b) for $i > j - m$. The necessity to stop provides us with the condition that $m = j - i_+$ with $i_+ \in \mathbb{N}_0$ holds.

3. Consider $|\Psi_-\rangle = \hat{J}_-|\Psi\rangle$. Now we find $\langle\Psi_-|\Psi_-\rangle = \hbar^2[j(j+1) - m^2 + m]$ implying

   (a) $|\Psi_-\rangle = 0 \Leftrightarrow m = -j \quad \text{or} \quad m = j+1$

   (b) For $m < -j$ or $m > j+1$ we would find $\langle\Psi_-|\Psi_-\rangle < 0$. Thus $-j \leq m \leq j+1$ holds.

   (c) $|\Psi_-\rangle$ is also eigenstate of $\hat{\mathbf{J}}^2$ and $\hat{J}_z$ with eigenvalues $j(j+1)\hbar^2$ and $(m-1)\hbar$.

   For $m \neq -j$ we define

$$|a, j, m-1\rangle = \frac{1}{\hbar\sqrt{j(j+1) - m(m-1)}} \hat{J}_- |a, j, m\rangle \tag{3}$$

   Now the repeated operation of $\hat{J}_-$ provides a sequence of states $|a, j, m\rangle$, $|a, j, m-1\rangle$, $|a, j, m-2\rangle, \ldots$. This sequence stops if $m - i_- = -j$ holds, as $\hat{J}_-|a, j, m - i_-\rangle = 0$ in this case. Otherwise the state $|a, j, m - i\rangle$ contradicts (b) for $i > -j + m$. Thus $m = -j + i_-$ holds with $i_- \in \mathbb{N}_0$.

Summary of 2 and 3:

For each common eigenstate $|\Psi\rangle$ of $\hat{\mathbf{J}}^2$ and $\hat{J}_z$ with eigenvalues $j(j+1)\hbar^2$ and $m\hbar$ holds:

- There are $i_+, i_- \in \mathbb{N}_0$ with $m + i_+ = j$ and $m - i_- = -j$. $\Rightarrow \quad 2j = i_+ + i_- \in \mathbb{N}_0$
- Repeated operation of $\hat{J}_+$ and $\hat{J}_-$ creates a sequence of states $|a, j, m'\rangle$ with $m' = -j, -j+1, \ldots j$, which are all common eigenstates of $\hat{\mathbf{J}}^2$ and $\hat{J}_z$.

The results of 1,2,3 can be summarized:

> The operator $\hat{\mathbf{J}}^2$ have the eigenvalues $j(j+1)\hbar^2$ with $j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}, \ldots$. The corresponding eigenstates form *multiplets* of $2j+1$ states $|a, j, m\rangle$ with $m = -j, -j+1, \ldots j$, which are eigenstates of $\hat{J}_z$ with the respective eigenvalue $m\hbar$ sind. I.e.,
>
> $$\hat{\mathbf{J}}^2|a, j, m\rangle = j(j+1)\hbar^2|a, j, m\rangle \quad \text{und} \quad \hat{J}_z|a, j, m\rangle = m\hbar|a, j, m\rangle \tag{4}$$

The Hamilton-operator $\hat{H}$ has rotational symmetry if it commutes with the operators $\hat{J}_i$ for the general angular momentum. Thus $[\hat{H}, \hat{J}_i] = 0$ for all $i = x, y, z$ and we also find $[\hat{H}, \hat{\mathbf{J}}^2] = 0$. Therefore there exists a system of common eigenstates for the operators $\hat{H}, \hat{\mathbf{J}}^2$ and $\hat{J}_z$ with respective eigenvalues E, $j(j+1)\hbar^2$ and $m\hbar$. For such an eigenstate $|\Psi\rangle$, we can construct $|\Psi_\pm\rangle = \hat{J}_\pm|\Psi\rangle$ and find $\hat{H}|\Psi_\pm\rangle = \hat{H}\hat{J}_\pm|\Psi\rangle = \hat{J}_\pm\hat{H}|\Psi\rangle = \hat{J}_\pm E|\Psi\rangle = E|\Psi_\pm\rangle$. Thus $|\Psi_\pm\rangle$ are eigenstates of $\hat{H}$ with the same energy. Repeating this procedure we find:

> In systems with rotational symmetry all states of a multiplet $|a, j, m\rangle$ with $m = -j, -j+1, \ldots j$ have the same energy. This provides a $(2j+1)$-fold degeneracy.

3 Spin of the electrons

Experimentally one observes a double degeneracy of the electron states. This degeneracy is lifted by a magnetic field as characteristic for angular momentum associated with a magnetic moment $\propto \mathbf{J}$. Such a doublet can be described by an internal angular momentum of the electron with $j = 0.5$, which is called *spin*, as postulated by Goudsmith and Uhlenbeck (1925). We denote the corresponding states with $m_j = \pm 1/2$ by $|+\rangle$ and $|-\rangle$. In this basis a general state can be written as a column (*Spinor*):

$$|a\rangle = a_+|+\rangle + a_-|-\rangle \to \begin{pmatrix} a_+ \\ a_- \end{pmatrix} \tag{5}$$

Let $\hat{S}_x, \hat{S}_y, \hat{S}_z$ be the angular momentum operators in spin space. From the general properties (2,3,4) we find

$$\begin{aligned} \hat{S}_z|+\rangle &= \frac{1}{2}\hbar|+\rangle & \hat{S}_z|-\rangle &= -\frac{1}{2}\hbar|-\rangle \\ \hat{S}_+|+\rangle &= 0 & \hat{S}_+|-\rangle &= \hbar|+\rangle \\ \hat{S}_-|+\rangle &= \hbar|-\rangle & \hat{S}_-|-\rangle &= 0 \end{aligned}$$

In the basis $|+\rangle$ and $|-\rangle$, the spin operators are therefore represented by the following matrices

$$\hat{S}_z \to \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \hat{S}_+ \to \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \hat{S}_- \to \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

As $\hat{S}_x = (\hat{S}_+ + \hat{S}_-)/2$ and $\hat{S}_y = (\hat{S}_+ - \hat{S}_-)/2i$ we obtain the representation

$$\hat{\mathbf{S}} = \hat{S}_x\mathbf{e}_x + \hat{S}_y\mathbf{e}_y + \hat{S}_z\mathbf{e}_z \to \frac{\hbar}{2}\boldsymbol{\sigma} \quad \text{with the Pauli matrices} \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \; \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \; \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Note that $\hat{\mathbf{S}}$ and $\boldsymbol{\sigma}$ are vectors in the conventional three-dimensional real space, with a direction pointing along the axis of rotation they generate. In contrast the columns in Eq. (5) and the Pauli matrices are elements of the two-dimensional complex spin space.