Kvantmehaanika ja spektroskoopia

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7. Is it possible measure simultaneously absolute value of angular momentum $|\vec{L}|$ and its x projection? Why? Proof.

Angular momentum operator in quantum mechanics is $\hat{\vec{L}} = \vec{r} \times \hat{\vec{p}}$.
In rectangular coordinates it has x component as:

$$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial y} - z\frac{\partial}{\partial z}\right), \text{with relation to y and z as } \left[\hat{L}_y, \hat{L}_z\right] = i\hbar\hat{L}_x$$

The components do not commute and are not simultaneously measureable. Only one componenet is exactly measurable and other are then arbitrary.

Squere of angular momentum can be simultaneosusly measured with one component as: $\hat{\vec{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$

With $\left[\hat{\vec{L}}^2, \hat{L}_x\right] = 0$, meaning that it is possible to mesure absolute value of angular momentum and it's x projecton.

Proof.

$$\left[\hat{\vec{L}}^2, \hat{L}_x\right] = \left[\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_x\right]$$

$$\left[\hat{L}_x^2, \hat{L}_x\right] = 0, \text{reduces it to} \left[\hat{L}_y^2, \hat{L}_x\right] + \left[\hat{L}_z^2, \hat{L}_x\right]$$

$$\text{with using} \quad [A^2, B] = A[A, B] + [A, B]A \quad \text{identity, we get:}$$

$$[L_y^2, L_x] = L_y[L_y, L_x] + [L_y, L_x]L_y = L_y(i\hbar L_z) + (i\hbar L_z)L_y = i\hbar(L_yL_z + L_zL_y),$$

$$[L_z^2, L_x] = L_z[L_z, L_x] + [L_z, L_x]L_z = L_z(-i\hbar L_y) + (-i\hbar L_y)L_z = -i\hbar(L_zL_y + L_yL_z).$$

$$i\hbar(L_yL_z + L_zL_y) - i\hbar(L_zL_y + L_yL_z) = 0 \quad \text{gives us} \left[\hat{\vec{L}}^2, \hat{L}_x\right] = 0$$

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19. How to calculate in quantum mechanics the kinetic energy of a rotating body with the moment of inertia I ? If body is an electron moving around nucleus in orbit with radius 10^{-10} m. Calculate the minimum possible non zero value of velocity of an electron (NB! Electron is a point particle). 20

For a rotating body the kinetic energy is:

$$T = \frac{1}{2} I \omega^2 \quad \text{The angular momentum } L \text{ is :} \quad L = I\omega$$

Giving us the kinetic energy as:

$$T = \frac{L^2}{2I}$$

In quantum mechanics, the angular momentum is:

$$L = \hbar \sqrt{\ell(\ell + 1)}$$

where ℓ is the orbital angular momentum quantum number ($\ell = 0, 1, 2, \ldots$).

The smallest non-zero angular momentum occurs when $\ell = 1$:

$$L = \hbar \sqrt{2}$$

For an electron (point particle) orbiting at radius $r = 10^{-10}$ m:

$$I = m_e r^2$$

where m_e is the electron mass.

Using the orbital quantum number $\ell = 1$

$$T = \frac{L^2}{2I} = \frac{(\hbar\sqrt{2})^2}{2m_e r^2} = \frac{2\hbar^2}{2m_e r^2} = \frac{\hbar^2}{m_e r^2}$$

The linear velocity v from angular velocity is: $v = \omega r$ and $L = I\omega$, using these we can get the velocity of the electron:

$$v = \omega r = \frac{L}{I} r = \frac{\hbar\sqrt{2}}{m_e r}$$

Given:

$$\hbar \approx 1.05 \times 10^{-34} \text{ J·s},$$
$$m_e \approx 9.11 \times 10^{-31} \text{ kg},$$
$$r = 10^{-10} \text{ m}.$$

The velocity is:

$$v = \frac{(1.05 \times 10^{-34})\sqrt{2}}{(9.11 \times 10^{-31})(10^{-10})} \approx 1.63 \times 10^6 \text{m/s}$$

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20. Obtain the equation for radial part of wave function: 20

$$-\frac{\hbar^2}{2M}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right)\right]+\left[\frac{\hbar^2 l(l+1)}{2Mr^2}+U(r)\right]R_{nl}(r)=ER_{nl}(r)$$

from the general Schrödinger equation for hydrogen atom

$$-\frac{\hbar^2}{2M}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)-\frac{1}{\hbar^2 r^2}\hat{\vec{L}}^2_{\theta\phi}-\frac{2M}{\hbar^2}U(r)\right]\psi_{nlm}(\vec{r})=E\psi_{nlm}(\vec{r})$$

here $\psi_{nlm}=R_{nl}(r)Y_{lm}(\theta,\phi)$

Start with the general Schrödinger equation for the hydrogen atom:

$$\hat{H}\psi_{nlm}(\vec{r})=-\frac{\hbar^2}{2M}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)-\frac{1}{\hbar^2 r^2}\hat{\vec{L}}^2_{\theta\phi}-\frac{2M}{\hbar^2}U(r)\right]\psi_{nlm}(\vec{r})=E\psi_{nlm}(\vec{r})$$

The wave function into radial and angular parts:

$$\psi_{nlm}(\vec{r})=R_{nl}(r)Y_{lm}(\theta,\varphi)$$

Substitute $\psi_{nlm}(\vec{r})$ into the Schrödinger equation:

$$-\frac{\hbar^2}{2M}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)-\frac{1}{\hbar^2 r^2}\hat{\vec{L}}^2_{\theta\phi}-\frac{2M}{\hbar^2}U(r)\right]R_{nl}(r)Y_{lm}(\theta,\varphi)=ER_{nl}(r)Y_{lm}(\theta,\varphi)$$

Since $\hat{\vec{L}}^2Y_{lm}=\hbar^2 l(l+1)Y_{lm}$, the angular momentum simplifies:

$$-\frac{\hbar^2}{2M}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)-\frac{l(l+1)}{r^2}-\frac{2M}{\hbar^2}U(r)\right]R_{nl}(r)Y_{lm}(\theta,\varphi)=ER_{nl}(r)Y_{lm}(\theta,\varphi)$$

Divide both sides by $Y_{lm}(\theta,\phi)$:

$$-\frac{\hbar^2}{2M}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_{nl}(r)}{dr}\right)-\frac{l(l+1)}{r^2}R_{nl}(r)\right]+U(r)R_{nl}(r)=ER_{nl}(r)$$

Rearrange to get:

$$-\frac{\hbar^2}{2M}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_{nl}(r)}{dr}\right)\right]+\left[\frac{\hbar^2 l(l+1)}{2Mr^2}+U(r)\right]R_{nl}(r)=ER_{nl}(r)$$

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38. Why the vector of angular momentum and magnetic moment of electron are have an opposite directions?

electron's magnetic moment $\vec{\mu}$ and its angular momentum $\vec{L}$ have opposite directions due to the negative charge of the electron. This can be expressed as:

$$\vec{\mu} = -\left(\frac{e}{2m_e}\right)\vec{L}$$

where: e is the elementary charge (magnitude) and m_e is the electron mass.

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40. Write the Schrodinger equation for third order approximation of perturbation theory.

Consider an unperturbed Hamiltonian H_0 with known eigenstates $|n^{(0)}\rangle$ and eigenvalues $E_n^{(0)}$, and a perturbation H'. The perturbed eigenstates $|n\rangle$ and eigenvalues E_n can be expanded up to third order in perturbation theory.

The third-order corrections to the energy and wave function are derived from the perturbation expansion.

The Schrödinger equation is:

$$(\hat{H}_0+\lambda\hat{H}')(\psi_n^0+\lambda\psi_n^1+\lambda^2\psi_n^2+\lambda^3\psi_n^3+\dots) = (E_n^0+\lambda E_n^1+\lambda^2 E_n^2+\lambda^3 E_n^3+\dots)(\psi_n^0+\lambda\psi_n^1+\lambda^2\psi_n^2+\lambda^3\psi_n^3+\dots).$$

Collecting terms of order λ^3:

$$\hat{H}_0\psi_n^3 + \hat{H}'\psi_n^2 = E_n^0\psi_n^3 + E_n^1\psi_n^2 + E_n^2\psi_n^1 + E_n^3\psi_n^0.$$

Rearranging:

$$(\hat{H}_0 - E_n^0)\psi_n^3 = (E_n^1 - \hat{H}')\psi_n^2 + E_n^2\psi_n^1 + E_n^3\psi_n^0.$$

The third-order wave function correction is expanded as:

$$\psi_n^3 = \sum_{m\neq n} a_m^{(3)}\psi_m^0.$$

Projecting onto ψ_k^0 $(k \neq n)$:

$$(E_k^0 - E_n^0)a_k^{(3)} = -\sum_{m\neq n} a_m^{(2)} H'_{km} + E_n^1 a_k^{(2)} + E_n^2 a_k^{(1)}.$$

The third-order energy correction is:

$$E_n^3 = \langle\psi_n^0|H'|\psi_n^2\rangle - E_n^1\langle\psi_n^0|\psi_n^2\rangle - E_n^2\langle\psi_n^0|\psi_n^1\rangle.$$

Substituting the lower-order corrections:

$$E_n^3 = \sum_{k\neq n}\sum_{m\neq n} \frac{H'_{nk}H'_{km}H'_{mn}}{(E_n^0 - E_k^0)(E_n^0 - E_m^0)} - E_n^1 \sum_{k\neq n} \frac{|H'_{nk}|^2}{(E_n^0 - E_k^0)^2}.$$