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6. Is it possible measure simultaneously square of angular momentum and its x projection?

Total angular-momentum operator

$$L^{2} = L_{x}^{2} + L_{y}^{2} + L_{z}^{2}$$

Two observables A and B can be measured simultaneously with definite values if and only if

$$[A, B] = 0$$

 $[L^2, L_x] = 0$

Starting from $L^2 = L_x^2 + L_y^2 + L_z^2$, we have

$$[L^2, L_x] = [L_x^2, L_x] + [L_y^2, L_x] + [L_z^2, L_x].$$

 $[L_x^2, L_x] = L_x[L_x, L_x] + [L_x, L_x]L_x = 0 + 0 = 0.$

Using the identity $[A^2, B] = A[A, B] + [A, B]A$:

$$[L_y^2, L_x] = L_y[L_y, L_x] + [L_y, L_x] L_y$$

From $[L_y, L_x] = i\hbar \varepsilon_{yxk} L_k = -i\hbar L_z$, it follows that

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

Similarly,

$$[L_z^2, L_x] = L_z[L_z, L_x] + [L_z, L_x] L_z$$

and since $[L_z, L_x] = i\hbar \varepsilon_{zxk} L_k = i\hbar L_y$, we get

$$[L_z^2, L_x] = +i\hbar \left(L_z L_y + L_y L_z\right).$$

Adding these contributions,

$$[L^{2}, L_{x}] = 0 - i\hbar (L_{y}L_{z} + L_{z}L_{y}) + i\hbar (L_{z}L_{y} + L_{y}L_{z}) = 0.$$

Since $[L^2, L_x] = 0$, the operators L^2 and L_x commute and therefore can be measured simultaneously. A common set of eigenstates $\{|l, m_x\rangle\}$ satisfies

$$L^{2} |l, m_{x}\rangle = \hbar^{2} l(l+1) |l, m_{x}\rangle, \quad L_{x} |l, m_{x}\rangle = \hbar m_{x} |l, m_{x}\rangle,$$

where $l = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$ and $m_x = -l, -l + 1, \ldots, +l.$ poole täisarvu väärtused?

19. How to calculate in quantum mechanics the kinetic energy of a rotating body with the moment of inertia I ?

Kinetic Energy of a Quantum Rigid Rotor

In quantum mechanics, a $rigid \ rotor$ of moment of inertia I has kinetic-energy operator

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

where

• $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ is the total angular-momentum operator,

• *I* is the moment of inertia about the rotation axis.

The eigenvalues of \hat{L}^2 are

$$\hat{L}^2 |l,m\rangle = \hbar^2 l(l+1) |l,m\rangle, \quad l = 0, 1, 2, \dots, \quad m = -l, -l+1, \dots, +l.$$

Hence the energy levels of the rigid rotor are

$$E_l = \frac{\hbar^2 l(l+1)}{2I}.$$

For a point mass m constrained to move on a circle of radius r, the moment of inertia about the center is

$$I = m r^2.$$

Substituting $I = mr^2$ into the expression for E_l gives

$$E_l = \frac{\hbar^2 \, l(l+1)}{2 \, m \, r^2}.$$

The ground state (l = 0) has $E_0 = 0$. The first excited state (l = 1) has

$$E_1 = \frac{\hbar^2 \cdot 1 \cdot 2}{2 \, m \, r^2} = \frac{\hbar^2}{m \, r^2}.$$

Classically,

$$T = \frac{1}{2} m_e v^2.$$

Equate this to E_1 :

$$\frac{1}{2} m_e v^2 = \frac{\hbar^2}{m_e r^2} \implies v = \sqrt{\frac{2 \hbar^2}{m_e^2 r^2}} = \sqrt{2} \frac{\hbar}{m_e r}.$$

Substituting numerical values:

$$\hbar = 1.054 \times 10^{-34} \,\mathrm{J\,s}, \quad m_e = 9.109 \times 10^{-31} \,\mathrm{kg}, \quad r = 1.0 \times 10^{-10} \,\mathrm{m},$$

we find

$$v \approx \sqrt{2} \frac{1.054 \times 10^{-34}}{(9.109 \times 10^{-31}) (1.0 \times 10^{-10})} \approx 1.6 \times 10^6 \,\mathrm{m/s}.$$

23. Write the radial part of wave function Rnl for quantum numbers n=3 and l=2

In a hydrogen-like atom the radial part of the bound-state wavefunction can be written in the form

$$R_{n\ell}(r) = N_{n\ell} \,\rho^{\,\ell} \,e^{-\rho/2} \,L_{n-\ell-1}^{\,2\ell+1}(\rho), \qquad \rho = \frac{2r}{n \,r_0},$$

 $n = 3, \ \ell = 2$

Here

$$n - \ell - 1 = 3 - 2 - 1 = 0 \implies L_0^5(\rho) = 1.$$

Hence the *unnormalized* radial part is

$$R_{3,2}(r) \propto \rho^2 e^{-\rho/2} = \left(\frac{2r}{3r_0}\right)^2 \exp\left(-\frac{r}{3r_0}\right).$$

therefore set

$$R_{3,2}(r) = C\left(\frac{r}{r_0}\right)^2 \exp\left(-\frac{r}{3r_0}\right),$$

with C to be determined.

The full three-dimensional normalization requires

$$\int_0^\infty R_{3,2}^2(r) \, r^2 \, dr = 1.$$

Substituting $r = r_0 x$, so $dr = r_0 dx$ and $r^2 dr = r_0^3 x^2 dx$. Then

$$\int_0^\infty \left| C \, x^2 e^{-x/3} \right|^2 \, r_0^3 x^2 \, dx = 1 \implies |C|^2 \, r_0^3 \int_0^\infty x^6 \, e^{-2x/3} \, dx = 1.$$

The remaining integral is evaluated via the Gamma function:

$$\int_0^\infty x^6 \, e^{-2x/3} \, dx = 6! \left(\frac{3}{2}\right)^7 = \frac{98415}{8}.$$

Hence

$$|C|^2 r_0^3 \frac{16}{81} \frac{98415}{8} = 1 \implies |C|^2 = \frac{1}{2430 r_0^3}$$

Taking the positive square root,

$$C = \frac{2\sqrt{2}}{81\sqrt{15}r_0^3}.$$
$$R_{3,2}(r) = \frac{2\sqrt{2}}{81\sqrt{15}r_0^3} \left(\frac{r}{r_0}\right)^2 \exp\left(-\frac{r}{3r_0}\right).$$

39.What does the eigenvalue problem look like for the operator of square of the orbital magnetic moment of an electron in a hydrogen atom?

In a hydrogen-like atom the orbital magnetic moment operator of the electron is defined by

$$\hat{\boldsymbol{\mu}}_{\ell} = -\frac{e}{2m}\,\hat{\mathbf{L}},$$

where

- e > 0 is the elementary charge,
- m is the electron mass,
- $\hat{\mathbf{L}} = (\hat{L}_x, \hat{L}_y, \hat{L}_z)$ is the orbital angular-momentum operator.

We are interested in the square of this operator,

$$\hat{\mu}_{\ell}^{2} = \hat{\mu}_{\ell} \cdot \hat{\mu}_{\ell} = \left(-\frac{e}{2m}\right)^{2} \hat{L}^{2} = \frac{e^{2}}{4m^{2}} \hat{L}^{2} = \frac{\mu_{B}^{2}}{\hbar^{2}} \hat{L}^{2},$$

where

$$\mu_B = \frac{e\hbar}{2m}$$
 (Bohr magneton).

The eigenvalue problem for $\hat{\mu}_{\ell}^2$ is

$$\hat{\mu}_{\ell}^2 \Psi(\mathbf{r}) = \lambda \Psi(\mathbf{r}).$$

Substituting $\hat{\mu}_{\ell}^2 = (\mu_B^2/\hbar^2)\,\hat{L}^2$ gives

$$\frac{\mu_B^2}{\hbar^2} \, \hat{L}^2 \, \Psi = \lambda \, \Psi \implies \hat{L}^2 \, \Psi = \frac{\hbar^2}{\mu_B^2} \, \lambda \, \Psi.$$

We know that \hat{L}^2 and \hat{L}_z admit a common basis of eigenfunctions, the spherical harmonics $Y_{\ell m}(\theta, \phi)$, which satisfy

$$\hat{L}^2 Y_{\ell m} = \hbar^2 \,\ell(\ell+1) \,Y_{\ell m}, \quad \hat{L}_z \,Y_{\ell m} = \hbar \,m \,Y_{\ell m},$$

with quantum numbers

$$\ell = 0, 1, 2, \dots, \quad m = -\ell, -\ell + 1, \dots, +\ell.$$

The stationary eigenstates of the hydrogen atom separate in spherical coordinates as

$$\Psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r) Y_{\ell m}(\theta,\phi),$$

where $R_{n\ell}(r)$ is the well-known radial function (solution of the radial Schrödinger equation). Because $\hat{\mu}_{\ell}^2$ acts only on the angular variables, we have

$$\hat{\mu}_{\ell}^{2} \Psi_{n\ell m} = \frac{\mu_{B}^{2}}{\hbar^{2}} \hat{L}^{2} \left[R_{n\ell}(r) Y_{\ell m}(\theta, \phi) \right] = \frac{\mu_{B}^{2}}{\hbar^{2}} \left(\hbar^{2} \ell(\ell+1) \right) R_{n\ell}(r) Y_{\ell m}(\theta, \phi).$$

Comparing with the eigenvalue equation $\hat{\mu}_{\ell}^2 \Psi = \lambda \Psi$ gives

$$\lambda = \mu_B^2 \ell(\ell+1), \quad \ell = 0, 1, 2, \dots$$

Each eigenvalue $\lambda_{\ell} = \mu_B^2 \ell(\ell+1)$ is $(2\ell+1)$ -fold degenerate in the magnetic quantum number m.

42.Can you prove the following expression (page 127): "In the first order approximation of coefficient...

We consider a Hamiltonian of the form

$$\hat{H}(\lambda) = \hat{H}^{(0)} + \lambda \hat{H}',$$

and seek its eigenvalues and eigenfunctions expanded in powers of the small parameter λ :

$$E_n(\lambda) = E_n^{(0)} + \lambda E_n^{(1)} + \mathcal{O}(\lambda^2),$$

$$\Psi_n(\lambda) = \Psi_n^{(0)} + \lambda \Psi_n^{(1)} + \mathcal{O}(\lambda^2).$$

The unperturbed states $\{\Psi_m^{(0)}\}\$ form a complete orthonormal set: $\langle \Psi_m^{(0)} | \Psi_k^{(0)} \rangle = \delta_{mk}$.

Inserting these expansions into $\hat{H}(\lambda) \Psi_n(\lambda) = E_n(\lambda) \Psi_n(\lambda)$ and collecting terms of order λ^0 and λ^1 gives:

• Zeroth order (λ^0) :

$$\hat{H}^{(0)} \, \Psi_n^{(0)} = E_n^{(0)} \, \Psi_n^{(0)}.$$

• First order (λ^1) :

$$\left(\hat{H}^{(0)} - E_n^{(0)}\right)\Psi_n^{(1)} + \hat{H}'\Psi_n^{(0)} = E_n^{(1)}\Psi_n^{(0)}$$

We expand the first-order correction in the unperturbed basis:

$$\Psi_n^{(1)} = \sum_m a_m^{(1)} \, \Psi_m^{(0)}, \qquad a_m^{(1)} = \big\langle \Psi_m^{(0)} \ \big| \ \Psi_n^{(1)} \big\rangle.$$

Projecting the first-order equation onto $\langle \Psi_k^{(0)} |$. For k = n one finds

$$E_n^{(1)} = \left< \Psi_n^{(0)} \middle| \hat{H}' \middle| \Psi_n^{(0)} \right>,$$

the familiar diagonal energy shift. For $k \neq n$,

$$a_k^{(1)} \left(E_k^{(0)} - E_n^{(0)} \right) = \left\langle \Psi_k^{(0)} \middle| \hat{H}' \middle| \Psi_n^{(0)} \right\rangle,$$

hence

$$a_k^{(1)} = \frac{\langle \Psi_k^{(0)} | \hat{H}' | \Psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}}.$$

At all orders the perturbed state must remain normalized:

$$\langle \Psi_n(\lambda) \mid \Psi_n(\lambda) \rangle = 1.$$

Expanding to first order in λ :

$$\begin{split} 1 &= \left\langle \Psi_n^{(0)} + \lambda \, \Psi_n^{(1)} \mid \Psi_n^{(0)} + \lambda \, \Psi_n^{(1)} \right\rangle + \mathcal{O}(\lambda^2) \\ &= 1 + \lambda \Big[\left\langle \Psi_n^{(1)} | \Psi_n^{(0)} \right\rangle + \left\langle \Psi_n^{(0)} | \Psi_n^{(1)} \right\rangle \Big] + \mathcal{O}(\lambda^2). \end{split}$$

Since the λ^0 term already equals 1, the coefficient of λ must vanish:

$$\langle \Psi_n^{(1)} | \Psi_n^{(0)} \rangle \; + \; \langle \Psi_n^{(0)} | \Psi_n^{(1)} \rangle = 0.$$

But by definition $\langle \Psi_n^{(0)} | \Psi_n^{(1)} \rangle = a_n^{(1)}$ and its complex conjugate is $\langle \Psi_n^{(1)} | \Psi_n^{(0)} \rangle = (a_n^{(1)})^*$.

$$a_n^{(1)} + (a_n^{(1)})^* = 0,$$