80

20

5: Is it possible to measure simultaneously the square of angular momentum and its z-projection (i.e., $\hat{L}^2$ and $\hat{L}_z$)? Why? Provide a proof.

Yes, it is possible to simultaneously measure the square of the angular momentum operator $\hat{L}^2$ and its z-component $\hat{L}_z$. This is because these two operators commute with each other.

Proof:
We use the commutation relations for the components of the angular momentum operator:

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z, \quad [\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x, \quad [\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$$

The total angular momentum squared operator is defined as:

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

We want to evaluate the commutator $[\hat{L}^2, \hat{L}_z]$:

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

We know that $[\hat{L}_z^2, \hat{L}_z] = 0$. We compute the others using the identity:

$$[\hat{A}^2, \hat{B}] = \hat{A}[\hat{A}, \hat{B}] + [\hat{A}, \hat{B}]\hat{A}$$

Thus:

$$[\hat{L}_x^2, \hat{L}_z] = \hat{L}_x[\hat{L}_x, \hat{L}_z] + [\hat{L}_x, \hat{L}_z]\hat{L}_x = \hat{L}_x(-i\hbar\hat{L}_y) + (-i\hbar\hat{L}_y)\hat{L}_x = -i\hbar(\hat{L}_x\hat{L}_y + \hat{L}_y\hat{L}_x)$$

$$[\hat{L}_y^2, \hat{L}_z] = \hat{L}_y[\hat{L}_y, \hat{L}_z] + [\hat{L}_y, \hat{L}_z]\hat{L}_y = \hat{L}_y(i\hbar\hat{L}_x) + (i\hbar\hat{L}_x)\hat{L}_y = i\hbar(\hat{L}_y\hat{L}_x + \hat{L}_x\hat{L}_y)$$

Adding the two:

$$[\hat{L}_x^2, \hat{L}_z] + [\hat{L}_y^2, \hat{L}_z] = -i\hbar(\hat{L}_x\hat{L}_y + \hat{L}_y\hat{L}_x) + i\hbar(\hat{L}_y\hat{L}_x + \hat{L}_x\hat{L}_y) = 0$$

Therefore:

$$[\hat{L}^2, \hat{L}_z] = 0$$

Since $\hat{L}^2$ and $\hat{L}_z$ commute, they share a common set of eigenstates, and can be simultaneously measured.

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

20

The kinetic energy of a rotating object is given by:

$$E_{\text{kin}} = \frac{L^2}{2I}$$

where:

- L is the angular momentum,
- I is the moment of inertia.

Angular momentum is quantized:

$$L^2 = \hbar^2 \cdot l(l+1), \quad \text{with } l = 1, 2, 3, \ldots$$

For the **minimum non-zero** angular momentum, we take $l = 1$:

$$L^2 = \hbar^2 \cdot 1(1+1) = 2\hbar^2$$

The moment of inertia for a point particle in a circular orbit is:

$$I = mr^2$$

where:

- $m = 9.11 \times 10^{-31}$ kg is the mass of the electron,
- $r = 1.0 \times 10^{-10}$ m is the radius of the orbit.

So:

$$I = 9.11 \times 10^{-31} \cdot (1.0 \times 10^{-10})^2 = 9.11 \times 10^{-51} \text{ kg} \cdot \text{m}^2$$

Now we calculate the kinetic energy:

$$E_{\text{kin}} = \frac{2\hbar^2}{2I} = \frac{\hbar^2}{I}$$

Using $\hbar = 1.055 \times 10^{-34}$ J $\cdot$ s:

$$E_{\text{kin}} = \frac{(1.055 \times 10^{-34})^2}{9.11 \times 10^{-51}} \approx 1.22 \times 10^{-18} \text{ J}$$

The classical relation between angular momentum and velocity is:

$$L = mvr \Rightarrow v = \frac{L}{mr}$$

We use $L = \sqrt{2}\hbar$:

$$v = \frac{\sqrt{2}\hbar}{mr}$$

Substituting the values:

$$v = \frac{\sqrt{2} \cdot 1.055 \times 10^{-34}}{9.11 \times 10^{-31} \cdot 1.0 \times 10^{-10}} \approx 1.63 \times 10^{6} \text{ m/s}$$

Answer:

- The kinetic energy of the rotating electron is approximately:

$$E_{\text{kin}} \approx 1.22 \times 10^{-18} \text{ J}$$

- The minimum possible non-zero velocity of the electron is approximately:

$$v_{\text{min}} \approx 1.63 \times 10^{6} \text{ m/s}$$

27: The total energy of electron in hydrogen atom can be calculated as follows: $E_n = -R\hbar\frac{1}{n^2}$. But how can we calculate separately the kinetic and potential energy of an electron in hydrogen atom for principal quantum number $n = 3$?
NB! The classical relation between the potential and kinetic energies for electron in hydrogen atom can be used.

20

The total energy of an electron in the hydrogen atom is:

$$E_n = -R\hbar \cdot \frac{1}{n^2}$$

Alternatively, it's often written using the Rydberg constant $R_H = 13.6$ eV:

$$E_n = -\frac{13.6 \text{ eV}}{n^2}$$

For $n = 3$:

$$E_3 = -\frac{13.6}{3^2} = -\frac{13.6}{9} \approx -1.51 \text{ eV}$$

Classical Relations Between Energies
In the hydrogen atom (based on the virial theorem or Bohr model):

$$E_{\text{total}} = E_{\text{kin}} + E_{\text{pot}}$$
$$E_{\text{kin}} = -E_{\text{total}}$$
$$E_{\text{pot}} = 2 \cdot E_{\text{total}}$$

Kinetic and Potential Energies for $n = 3$

$$E_{\text{kin}} = -E_3 = 1.51 \text{ eV}$$
$$E_{\text{pot}} = 2 \cdot E_3 = 2 \cdot (-1.51 \text{ eV}) = -3.02 \text{ eV}$$

Answer:

- Total energy: $E_3 = -1.51$ eV
- Kinetic energy: $E_{\text{kin}} = 1.51$ eV
- Potential energy: $E_{\text{pot}} = -3.02$ eV

35: How does the electron configuration look like for Cu atom and Cu^{2+} ion? Why?

Copper has atomic number 29, which means it has 29 electrons.

The expected configuration from the Aufbau principle would be:

$$\text{Cu: } [\text{Ar}]\, 4s^2\, 3d^9$$

?

10

However, the actual configuration is:

$$\text{Cu: } [\text{Ar}]\, 4s^1\, 3d^{10}$$

A fully filled $3d^{10}$ subshell provides extra stability due to exchange energy and symmetrical distribution, making this configuration more stable than the expected one.

Copper Ion (Cu^{2+})

To form a Cu^{2+} ion, copper loses two electrons. Electrons are lost first from the outermost shell — the 4s orbital — followed by the 3d orbital:

$$\text{Cu}^{2+} : [\text{Ar}]\, 3d^9$$

Even though the 3d orbital is filled after the 4s during electron configuration, the 4s electrons are higher in energy and are removed first during ionization. So:

- Cu loses the $4s^1$ electron and one $3d$ electron.
- Resulting configuration: $[\text{Ar}]\, 3d^9$

44: Can you prove that for harmonic oscillator in constant force field "...the first order energy correction is equal to zero

10

Consider a quantum harmonic oscillator subject to a constant force field F. The perturbing Hamiltonian is:

$$H' = -Fx$$

According to first-order perturbation theory, the first-order energy correction for the n-th state is:

$$E_n^{(1)} = \langle n|H'|n\rangle = \langle n|(-Fx)|n\rangle = -F\langle n|x|n\rangle$$

Now, in the harmonic oscillator, the position operator x can be expressed in terms of the ladder operators:

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$$

So we compute:

$$\langle n|x|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle n|(a + a^\dagger)|n\rangle$$

Using the properties of ladder operators:

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

Therefore:

$$\langle n|a|n\rangle = 0, \quad \langle n|a^\dagger|n\rangle = 0$$

Miks?
Kust see tuleb?

So:

$$\langle n|x|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}(0 + 0) = 0$$

Thus, the first-order energy correction is:

$$E_n^{(1)} = -F \cdot 0 = 0$$

Conclusion: The first-order energy correction for a harmonic oscillator in a constant force field is zero.