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1. Derive that relation between orbital and magnetic quantum numbers m=l ,. . . , 0 ,...+l .

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Step 1: Definitions

We begin by defining the relevant quantum numbers:

- l: orbital quantum number - determines the *magnitude* of orbital angular momentum.
- m: magnetic quantum number - determines the *z-component* of angular momentum.

Step 2: Orbital Angular Momentum Magnitude

The magnitude of orbital angular momentum is given by:

$$|\vec{L}| = \hbar\sqrt{l(l+1)}$$

Step 3: Angular Momentum z-Component

Only the z-component of angular momentum is directly observable:

$$L_z = m\hbar$$

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where m must be an integer.

Step 4: Physical Constraint on m

From quantum mechanics, the z-component cannot exceed the total angular momentum:

$$|L_z| \leq |\vec{L}| \Rightarrow |m\hbar| \leq \hbar\sqrt{l(l+1)}$$

$$\Rightarrow |m| \leq \sqrt{l(l+1)}$$

However, this only limits m's range in magnitude, not the actual discrete values it can take.

Step 5: Quantum Mechanical Restriction

From solving the Schrödinger equation in spherical coordinates, we know that m must be an integer satisfying:

$$m = -l, -(l-1), \ldots, 0, \ldots, +(l-1), +l$$

Hence, for a given l, the magnetic quantum number m takes $(2l+1)$ possible integer values.

m = -l, -(l-1), . . . , 0, . . . , +(l-1), +l

16: Angle Between Angular Momentum Vector and z-axis

Problem: How in quantum mechanics can the angle between the angular momentum vector $\vec{L}$ and the z-axis be calculated? Calculate this angle for **magnetic quantum numbers** $m = -2$ and $+1$ for **3d orbitals**.

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Step 1: General Formula
In quantum mechanics, we have:

$$|\vec{L}| = \hbar\sqrt{l(l+1)} \qquad \text{and} \qquad L_z = m\hbar$$

The angle θ between $\vec{L}$ and the z-axis is given by the projection:

$$\cos\theta = \frac{L_z}{|\vec{L}|} = \frac{m\hbar}{\hbar\sqrt{l(l+1)}} = \frac{m}{\sqrt{l(l+1)}}$$

Step 2: For 3d orbitals

$$l = 2 \Rightarrow \sqrt{l(l+1)} = \sqrt{2 \cdot 3} = \sqrt{6}$$

Case 1: $m = -2$

$$\cos\theta = \frac{-2}{\sqrt{6}} = -\frac{\sqrt{6}}{3}$$

$$\theta = \cos^{-1}\left(-\frac{\sqrt{6}}{3}\right) \approx \cos^{-1}(-0.8165) \approx 144.7^\circ$$

Case 2: $m = +1$

$$\cos\theta = \frac{1}{\sqrt{6}} = \frac{\sqrt{6}}{6}$$

$$\theta = \cos^{-1}\left(\frac{\sqrt{6}}{6}\right) \approx \cos^{-1}(0.4082) \approx 66.4^\circ$$

$$\text{For } m = -2, \quad \theta \approx 144.7^\circ$$
$$\text{For } m = +1, \quad \theta \approx 66.4^\circ$$

21: Radial wave function for an uncharged electron

Question: What does the equation for the radial wave function look like if we assume that the electron is an uncharged particle?

Step 1: Start from the radial Schrödinger equation
In spherical coordinates, the time-independent Schrödinger equation for the radial wave function is:

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left[\frac{2\mu}{\hbar^2}\left(E - V(r)\right) - \frac{l(l+1)}{r^2}\right]R = 0$$

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For the hydrogen atom, the potential is Coulombic:

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$$

Step 2: Assume the electron is uncharged
If the electron has no electric charge, it does not interact with the proton. Hence:

$$V(r) = 0$$

Substituting this into the radial equation gives:

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left(\frac{2\mu E}{\hbar^2} - \frac{l(l+1)}{r^2}\right)R = 0$$

$$\boxed{\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} - \left(\frac{l(l+1)}{r^2} + \frac{2\mu|E|}{\hbar^2}\right)R = 0}$$

Step 3: Physical Interpretation

- The equation now describes a **free particle** in spherical coordinates.
- The only remaining potential term is the **centrifugal barrier** $\frac{l(l+1)}{r^2}$, due to angular momentum.
- Without the Coulomb potential, the particle is **no longer bound** to the nucleus.
- The solutions are not hydrogen-like orbitals, but resemble **spherical Bessel functions**.
- The energy spectrum is **continuous**, and all energies are allowed ($E > 0$). There are no quantized (bound state) energy levels.

Conclusion: Assuming the electron is uncharged removes the Coulomb interaction, resulting in a free-particle-like radial equation. The wavefunction no longer describes discrete bound states, and the system supports only scattering solutions.

30: maximum number of electrons in 1p and 3f orbitals for hydrogen atom

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Question: Calculate the possible maximum number of electrons in **1p** and **3f** orbitals for the hydrogen atom.

Important Clarification: By quantum number rules, for an orbital to physically exist, the orbital quantum number l must satisfy:

$$l = 0, 1, \ldots, n-1$$

Hence:

- **1p:** $n = 1, l = 1 \Rightarrow l \not< n$ **Does not exist physically**
- **3f:** $n = 3, l = 3 \Rightarrow l \not< n$ **Does not exist physically**

However, for the sake of calculation, we can still compute the *hypothetical maximum number of electrons* assuming these orbitals did exist:

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Calculation Formula:

Each orbital is defined by quantum numbers (n, l, m_l, m_s). - For given l, there are $2l + 1$ values of m_l - Each m_l orbital can hold 2 electrons (with $m_s = \pm\frac{1}{2}$)

$$\text{Max electrons} = (2l + 1) \times 2$$

Hypothetical Calculations:

- **1p:** $l = 1 \Rightarrow m_l = -1, 0, +1 \Rightarrow 3$ orbitals Each orbital holds 2 electrons

$$\text{Max electrons} = 3 \times 2 = \boxed{6}$$

- **3f:** $l = 3 \Rightarrow m_l = -3, -2, -1, 0, +1, +2, +3 \Rightarrow 7$ orbitals Each orbital holds 2 electrons

$$\text{Max electrons} = 7 \times 2 = \boxed{14}$$

Summary Table:

Orbital	Physically Allowed?	Hypothetical Max Electrons	Reason
1p	No	6	$l = 1 \not< n = 1$
3f	No	14	$l = 3 \not< n = 3$

If 1p and 3f orbitals existed, they would accommodate up to: 6 electrons in 1p, 14 electrons in 3f

45: why only terms $n+1$ and $n-1$ contribute in second-order energy correction

We consider a quantum harmonic oscillator under a constant force F, leading to a perturbation of the form:

$$H' = -Fx$$

The second-order correction to the energy of the n-th state is given by:

$$E_n^{(2)} = \sum_{k \neq n} \frac{|\langle k|H'|n\rangle|^2}{E_n^{(0)} - E_k^{(0)}}$$

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Substituting the perturbation $H' = -Fx$:

$$E_n^{(2)} = \sum_{k \neq n} \frac{F^2 |\langle k|x|n\rangle|^2}{E_n^{(0)} - E_k^{(0)}}$$

Step 1: Matrix Elements of x in Harmonic Oscillator Basis

The position operator in terms of ladder operators is:

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

Hence, only transitions $k = n \pm 1$ give non-zero matrix elements:

$$\langle n+1|x|n\rangle = \sqrt{\frac{\hbar}{2M\omega}}\sqrt{n+1} \qquad \langle n-1|x|n\rangle = \sqrt{\frac{\hbar}{2M\omega}}\sqrt{n}$$

Therefore:

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$$|\langle n+1|x|n\rangle|^2 = \frac{\hbar}{2M\omega}(n+1) \qquad |\langle n-1|x|n\rangle|^2 = \frac{\hbar}{2M\omega}n$$

Step 2: Energy Denominators

For the harmonic oscillator:

$$E_n^{(0)} = \hbar\omega\left(n + \frac{1}{2}\right) \Rightarrow \begin{cases} E_n^{(0)} - E_{n+1}^{(0)} = -\hbar\omega \\ E_n^{(0)} - E_{n-1}^{(0)} = +\hbar\omega \end{cases}$$

Step 3: Plug into the Energy Correction Formula

$$E_n^{(2)} = F^2 \left[\frac{\frac{\hbar}{2M\omega}(n+1)}{-\hbar\omega} + \frac{\frac{\hbar}{2M\omega}n}{\hbar\omega} \right]$$

$$= F^2 \cdot \frac{\hbar}{2M\omega}\left(\frac{-1}{\hbar\omega} \cdot (n+1) + \frac{1}{\hbar\omega} \cdot n\right) = F^2 \cdot \frac{\hbar}{2M\omega} \cdot \left(\frac{n-(n+1)}{\hbar\omega}\right)$$

$$= F^2 \cdot \frac{\hbar}{2M\omega} \cdot \left(\frac{-1}{\hbar\omega}\right) = -\frac{F^2}{2M\omega^2}$$

$$\boxed{E_n^{(2)} = -\frac{F^2}{2M\omega^2}}$$

Conclusion

Only the $n+1$ and $n-1$ terms contribute to the second-order energy correction because the position operator x only connects adjacent harmonic oscillator eigenstates:

$$\langle k|x|n\rangle = 0 \quad \text{unless } k = n \pm 1$$