Loengu 10-13

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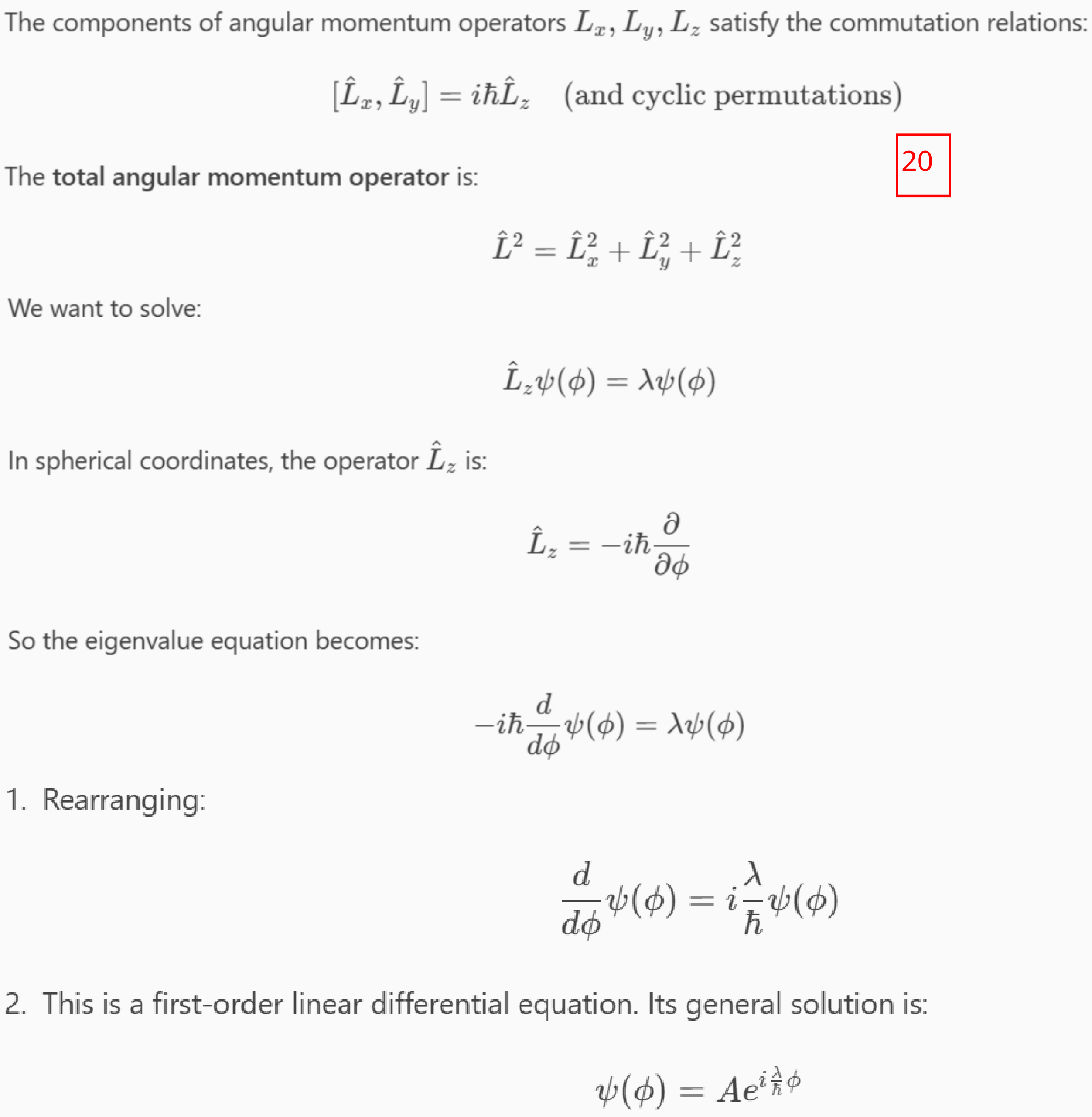

The components of angular momentum operators L_x, L_y, L_z satisfy the commutation relations:

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z \quad \text{(and cyclic permutations)}$$

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The **total angular momentum operator** is:

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

We want to solve:

$$\hat{L}_z\psi(\phi) = \lambda\psi(\phi)$$

In spherical coordinates, the operator $\hat{L}_z$ is:

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$$

So the eigenvalue equation becomes:

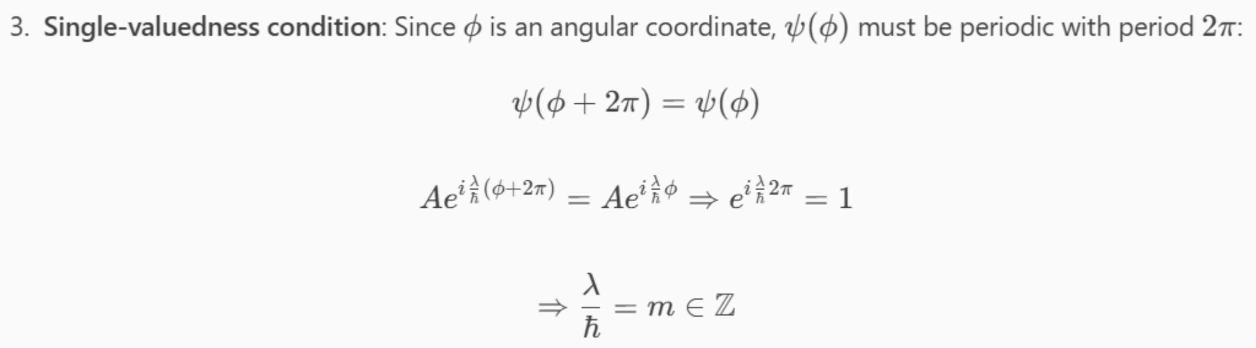
$$-i\hbar\frac{d}{d\phi}\psi(\phi) = \lambda\psi(\phi)$$

1. Rearranging:

$$\frac{d}{d\phi}\psi(\phi) = i\frac{\lambda}{\hbar}\psi(\phi)$$

2. This is a first-order linear differential equation. Its general solution is:

$$\psi(\phi) = Ae^{i\frac{\lambda}{\hbar}\phi}$$



3. **Single-valuedness condition**: Since ϕ is an angular coordinate, $\psi(\phi)$ must be periodic with period 2π:

$$\psi(\phi + 2\pi) = \psi(\phi)$$

$$Ae^{i\frac{\lambda}{\hbar}(\phi+2\pi)} = Ae^{i\frac{\lambda}{\hbar}\phi} \Rightarrow e^{i\frac{\lambda}{\hbar}2\pi} = 1$$

$$\Rightarrow \frac{\lambda}{\hbar} = m \in \mathbb{Z}$$

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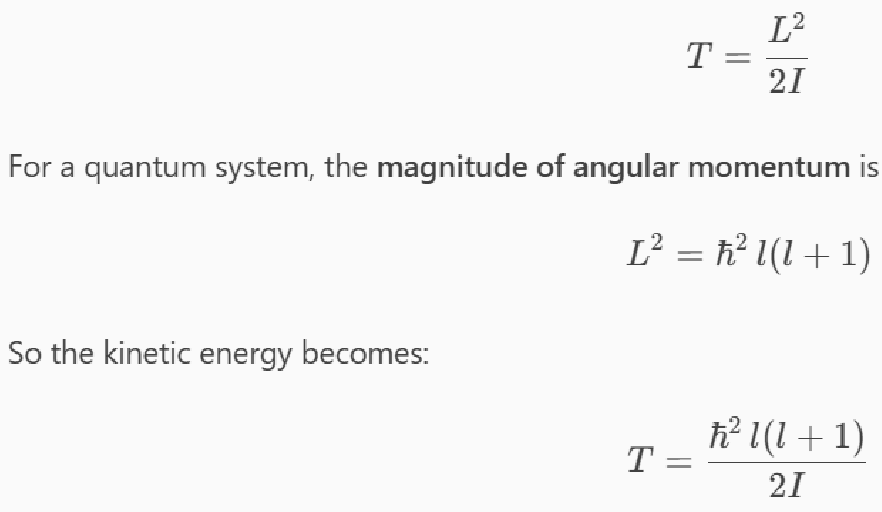


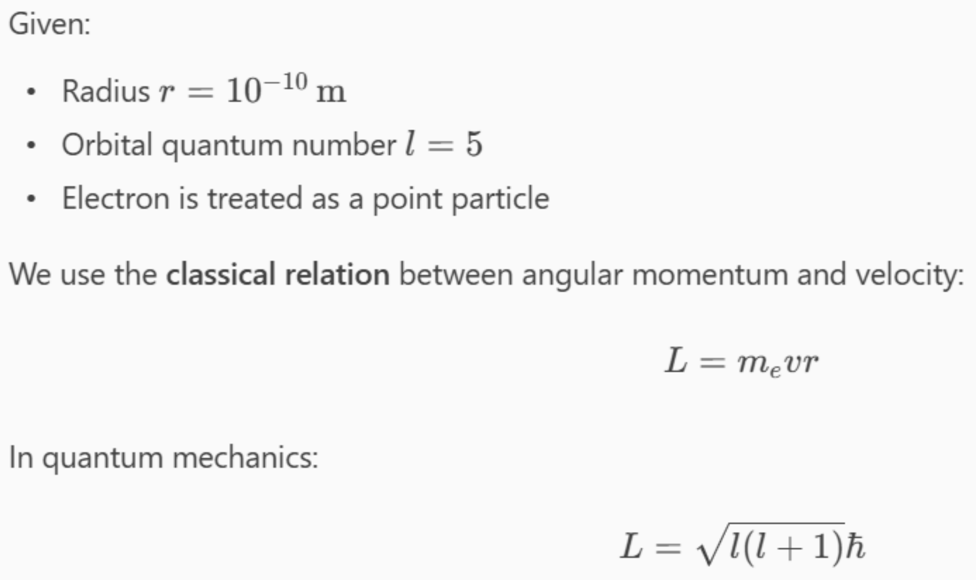
$$T = \frac{L^2}{2I}$$

For a quantum system, the **magnitude of angular momentum** is quantized:

$$L^2 = \hbar^2\, l(l+1)$$

So the kinetic energy becomes:

$$T = \frac{\hbar^2\, l(l+1)}{2I}$$



Given:

- Radius $r = 10^{-10}\,\mathrm{m}$
- Orbital quantum number $l = 5$
- Electron is treated as a point particle

We use the **classical relation** between angular momentum and velocity:

$$L = m_e v r$$

In quantum mechanics:

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

So:

$$v = \frac{\sqrt{l(l+1)}\hbar}{m_e r}$$

Where:

- $\hbar \approx 1.055 \times 10^{-34}\,\mathrm{J}$\cdotps
- $m_e \approx 9.109 \times 10^{-31}\,\mathrm{kg}$
- $r = 10^{-10}\,\mathrm{m}$
- $l = 5$

The **velocity of the electron** in an orbit of radius $10^{-10}\,\mathrm{m}$ with orbital quantum number $l = 5$ is approximately:

$$\boxed{6.34 \times 10^{6}\,\mathrm{m/s}}$$

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The full Schrödinger equation for a central potential $U(r)$ in spherical coordinates is:

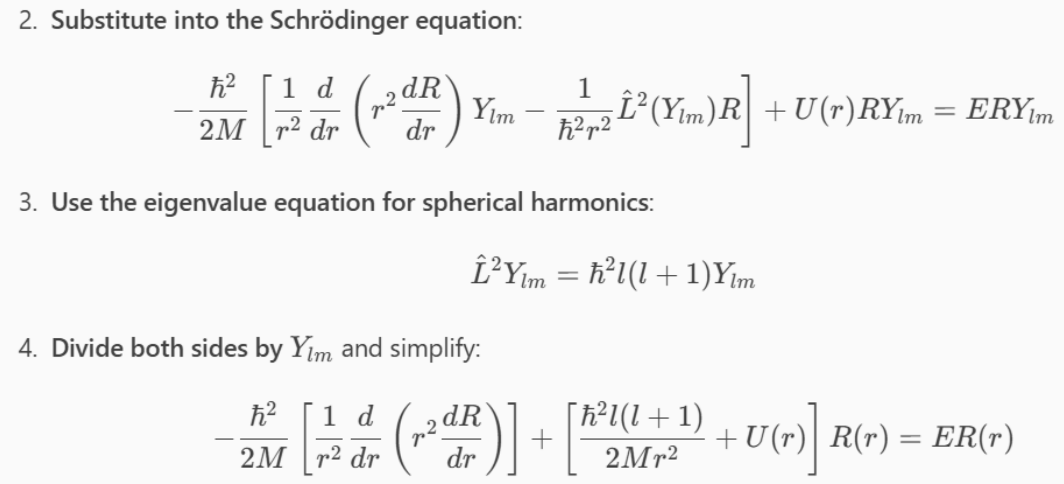
$$-\frac{\hbar^2}{2M}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{\hbar^2 r^2}\hat{L}^2\right]\psi_{nlm}(r,\theta,\phi) + U(r)\psi_{nlm}(r,\theta,\phi) = E\psi_{nlm}(r,\theta,\phi)$$

We use the **separation of variables**:

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

1. **Apply the Laplacian in spherical coordinates**:

$$\nabla^2 = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) - \frac{1}{r^2}\hat{L}^2/\hbar^2$$



2. **Substitute into the Schrödinger equation**:

$$-\frac{\hbar^2}{2M}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)Y_{lm}-\frac{1}{\hbar^2 r^2}\hat{L}^2(Y_{lm})R\right]+U(r)RY_{lm}=ERY_{lm}$$

3. **Use the eigenvalue equation for spherical harmonics**:

$$\hat{L}^2 Y_{lm}=\hbar^2 l(l+1)Y_{lm}$$

4. **Divide both sides by Y_{lm}** and simplify:

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

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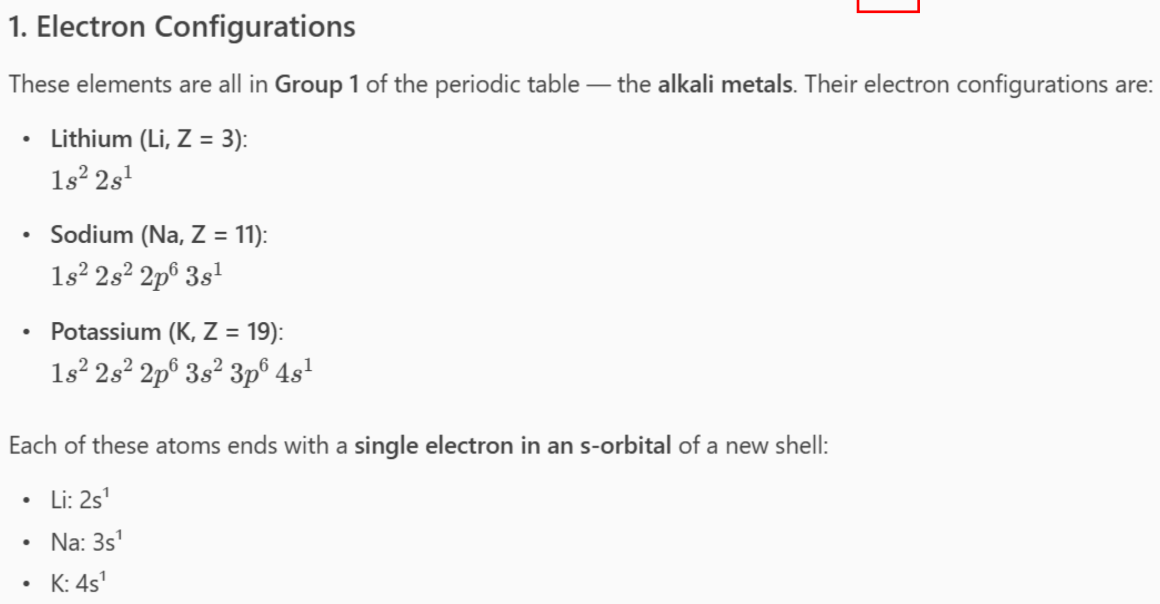


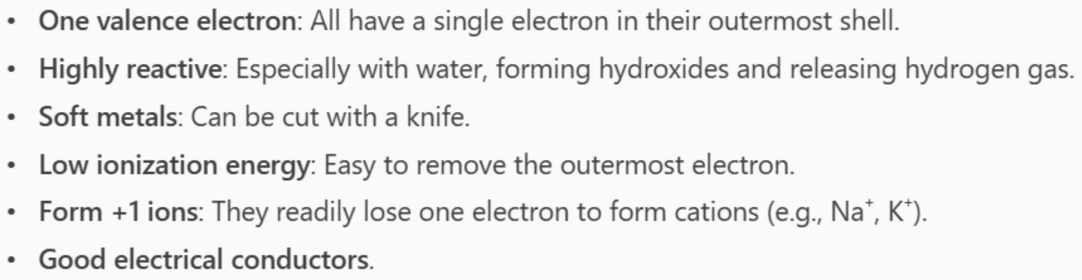
1. Electron Configurations

These elements are all in **Group 1** of the periodic table — the **alkali metals**. Their electron configurations are:

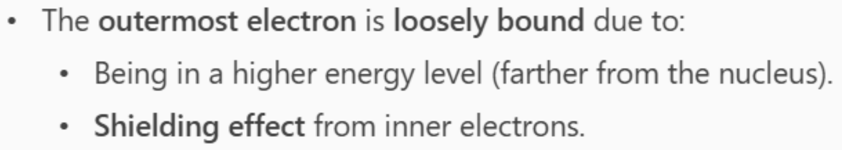
- **Lithium (Li, Z = 3)**:
  $1s^2\,2s^1$
- **Sodium (Na, Z = 11)**:
  $1s^2\,2s^2\,2p^6\,3s^1$
- **Potassium (K, Z = 19)**:
  $1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,4s^1$

Each of these atoms ends with a **single electron in an s-orbital** of a new shell:

- Li: $2s^1$
- Na: $3s^1$
- K: $4s^1$



- **One valence electron**: All have a single electron in their outermost shell.
- **Highly reactive**: Especially with water, forming hydroxides and releasing hydrogen gas.
- **Soft metals**: Can be cut with a knife.
- **Low ionization energy**: Easy to remove the outermost electron.
- **Form +1 ions**: They readily lose one electron to form cations (e.g., Na^+, K^+).
- **Good electrical conductors**.



- The **outermost electron** is **loosely bound** due to:
  - Being in a higher energy level (farther from the nucleus).
  - **Shielding effect** from inner electrons.

- This makes it **easy to ionize**, which explains their:
    - High reactivity.
    - Tendency to form ionic compounds.
    - Similar chemical behavior across the group.

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We consider a Hamiltonian:

$$\hat{H} = \hat{H}^{(0)} + \lambda \hat{H}^{(1)}$$

Where:

- $\hat{H}^{(0)}$: unperturbed Hamiltonian
- $\hat{H}^{(1)}$: perturbation
- λ: small parameter (set to 1 at the end)

We expand the energy and wavefunction as:

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \lambda^3 E_n^{(3)} + \cdots$$

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + \lambda |\psi_n^{(1)}\rangle + \lambda^2 |\psi_n^{(2)}\rangle + \lambda^3 |\psi_n^{(3)}\rangle + \cdots$$

Third-Order Schrödinger Equation

Substitute the expansions into the time-independent Schrödinger equation:

$$\hat{H} |\psi_n\rangle = E_n |\psi_n\rangle$$

Collecting terms of order λ^3, we get:

$$\hat{H}^{(0)} |\psi_n^{(3)}\rangle + \hat{H}^{(1)} |\psi_n^{(2)}\rangle = E_n^{(0)} |\psi_n^{(3)}\rangle + E_n^{(1)} |\psi_n^{(2)}\rangle + E_n^{(2)} |\psi_n^{(1)}\rangle + E_n^{(3)} |\psi_n^{(0)}\rangle$$