Particle in a box

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- Schrödinger equation

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Q & A

Review

Schrödinger equation

- **Helmholz wave equation**

$$\nabla^2\psi = -k^2\psi, \qquad (k = \frac{\omega}{c} = \frac{2\pi}{\lambda})$$

- **de Brogile's matter wave**

$$\lambda = \frac{h}{p} \quad , \qquad k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h} = \frac{p}{\hbar}$$

- **Schrödinger equation**

$$\nabla^2\psi = -k^2\psi \quad \rightarrow \quad \nabla^2\psi = -\frac{p^2}{\hbar^2}\psi$$

$$-\frac{\hbar^2}{2m_0}\nabla^2\psi = \frac{p^2}{2m_0}\psi \quad \rightarrow \quad -\frac{\hbar^2}{2m_0}\nabla^2\psi = (E - V(r))\psi \rightarrow \quad -\frac{\hbar^2}{2m_0}\nabla^2\psi + V(r)\psi = E\psi$$

Particle in a box

Max Born's postulate

- **Probability density function**

- The probability density function : $P(r)$

The probability of finding the particle : $P(r)d^3r \;\rightarrow\; \int P(r)d^3r = 1$

- Max Born's postulate

$\rightarrow$ The probability $P(r)$ of finding a particle near a point **r** is $\propto |\psi(r)|^2$

So, the probability of finding a particle at the point **r** is

$$\boxed{|\psi(r)|^2 d^3r} \rightarrow \int |\psi(r)|^2 d^3r = 1$$

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Max Born's postulate

- **Normalization of the wavefunction**

- For general case, the integral gives some other number

$$\int |\psi(r)|^2 d^3 r = \frac{1}{|a|^2}$$

- Linearity of Schrödinger equation, $a\psi(r)$ is also a solution.

$$\psi_N(r) = a\psi(r) \quad \rightarrow \quad \int |\psi_N(r)|^2 d^3 r = 1$$

$\psi_N(r) \rightarrow$ Normalized wavefunction

Particle in a box

Schrödinger equation of a particle in a box

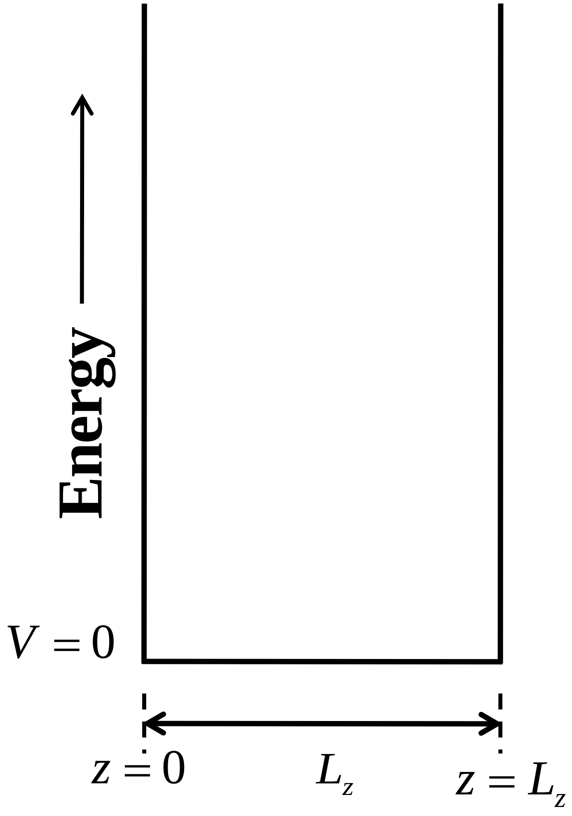
- **Schrödinger equation**

  - Assume a particle of mass ***m*** with potential in the ***z*** direction

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(z)}{dz^2}+V(z)\psi(z)=E\psi(z)$$

- **Boundary condition**

  - Suppose the potential energy is a rectangular well
  - Potential energy inside the well $V=0$
  - Potential energy at the wall rises to infinity
  - A particle is confined within $0<z<L_z$



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Schrödinger equation of a particle in a box

- **Schrödinger equation outside the box**

- From the assumption, there is no possibility of finding the particle outside.

So, $z < 0$ or $z > L_z$, $\psi \to 0$

- **Schrödinger equation inside the box**

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(z)}{dz^2} + V(z)\psi(z) = E\psi(z) \quad \to \quad -\frac{\hbar^2}{2m}\frac{d^2\psi(z)}{dz^2} = E\psi(z)$$

with the boundary conditions

$$\psi(0) = 0 \quad \text{and} \quad \psi(L_z) = 0$$

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Schrödinger equation of a particle in a box

- **Solution of Schrödinger equation inside the box**

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(z)}{dz^2} = E\psi(z)$$

- The general solution to the equation is

$$\psi(z) = A\sin(kz) + B\cos(kz) \quad \text{when} \quad k = \sqrt{2mE/\hbar^2}$$

- From the boundary condition :

1. $\psi(0) = 0 \rightarrow B = 0 \rightarrow \psi(z) = A\sin(kz)$

2. $\psi(L_z) = 0 \rightarrow kL_z = n\pi \,, \quad k = \sqrt{2mE/\hbar^2} = n\pi / L_z$

$$\rightarrow \boxed{\psi_n(z) = A_n \sin\left(\frac{n\pi z}{L_z}\right) \quad \textbf{with} \quad E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L_z}\right)^2}$$

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Normalization of solution

- **Solution of Schrödinger equation inside the box**

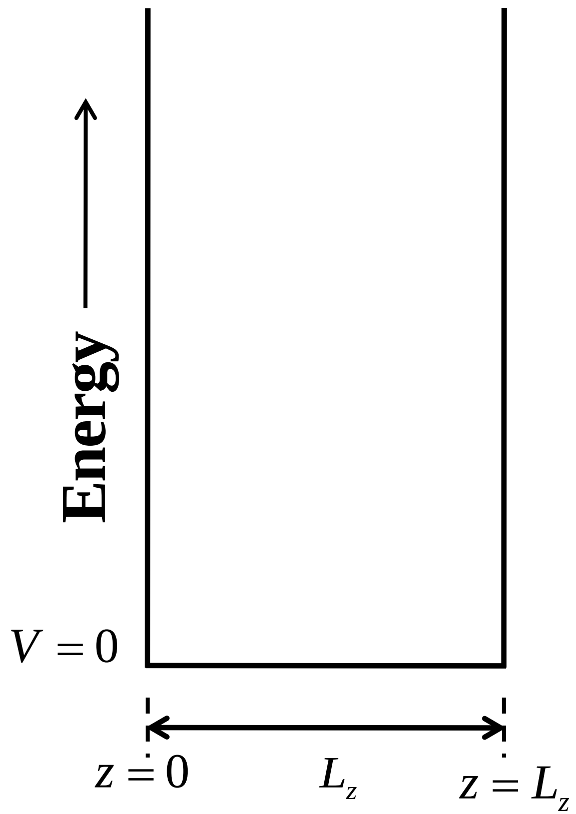
$$\psi_n(z) = A_n \sin\left(\frac{n\pi z}{L_z}\right)$$

- **Normalization of wavefunction**

$$\int_0^{L_z} |A_n|^2 \sin^2\left(\frac{n\pi z}{L_z}\right) dz = |A_n|^2 \frac{L_z}{2} = 1 \longrightarrow |A_n| = \sqrt{2/L_z}$$

- **Complete solution of a particle in a box**

$$\begin{cases} \psi_n(z) = \sqrt{\dfrac{2}{L_z}} \sin\left(\dfrac{n\pi z}{L_z}\right) & \textbf{for } 0 < z < L_z \\ \psi(z) = 0 & \textbf{for } z < 0\,, \quad z > L_z \end{cases}$$



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Summary

- **Particle in a box**

$$\psi_n(z) = \sqrt{\frac{2}{L_z}}\sin(\frac{n\pi z}{L_z})$$

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L_z}\right)^2$$

$$n = 1, 2, \ldots$$