

Infinite Potential Well

$$V(x) = \begin{cases} 0 & \forall x \in [0, a] \\ \infty & \text{elsewhere} \end{cases}$$

Schrodinger: $-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi = E\psi$



→ In well: $-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E\psi \rightarrow \frac{\partial^2 \psi}{\partial x^2} = -\frac{2mE}{\hbar^2} \psi$

let $k = \sqrt{2mE}/\hbar$

↳ $\psi'' = -k^2 \psi$

general solution: $\psi(x) = A \sin kx + B \cos kx$

BC

$\psi(0) = \psi(a) = 0$

$\psi(0) = 0$: $\psi(0) = A \sin(0) + B \cos(0) = 0$
 $= B = 0$

$\psi(a) = 0$: $\psi(a) = A \sin(ka) = 0$

$\sin(ka) = 0$

$ka = n\pi \quad n \in \mathbb{N}$

$k = \frac{n\pi}{a}$

$\psi(x) = A \sin\left(\frac{n\pi x}{a}\right)$

Normalization

$|\psi|^2 = 1$

↳ $A = \sqrt{\frac{2}{a}}$

$\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$

$k^2 = 2mE/\hbar^2 \rightarrow E = \frac{k^2 \hbar^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$

$E_1 = \frac{\pi^2 \hbar^2}{2ma^2}$

Inf Well-Variational Guess

$$E_1 \leq \langle \Psi | H | \Psi \rangle \equiv \langle H \rangle$$

$$H = V + K \quad \text{In well: } V = 0$$

$$H = K = \frac{p^2}{2m} \quad \hat{p} = -i\hbar \frac{\partial}{\partial x}$$
$$= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

$$\text{Ansatz choice: } \Psi(x) = Ax^2$$

$$\text{Normalization: } 1 = \int_0^a (Ax^2)^* Ax^2 dx = A^2 \int_0^a x^4 dx$$

$$A^2 = \frac{5}{a^5} \quad A = \sqrt{\frac{5}{a^5}} \quad \Psi(x) = \sqrt{\frac{5}{a^5}} x^2$$
$$= A^2 \left[\frac{1}{5} x^5 \right]_0^a = \frac{A^2 a^5}{5} = 1$$

$$\langle H \rangle = \langle V \rangle + \langle K \rangle$$

$$\hookrightarrow \text{In well: } \langle H \rangle = \langle K \rangle = \frac{p^2}{2m} = +\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

$$\langle H \rangle = \langle \Psi | H | \Psi \rangle = \int_0^a (Ax^2) \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) (Ax^2)$$

$$= \frac{\hbar^2 A^2}{2m} \int_0^a x^2 \frac{\partial}{\partial x} [2x] dx = \frac{\hbar^2 A^2}{m} \int_0^a x^2 dx = \frac{\hbar^2 A^2}{m} \left[\frac{1}{3} x^3 \right]_0^a$$
$$= \frac{\hbar^2 A^2}{m} \cdot \frac{1}{3} a^3 = \frac{\hbar^2 \cdot 5}{m a^5} \cdot \frac{1}{3} a^3 = \frac{5}{3} \cdot \frac{\hbar^2}{m a^2}$$

Harmonic oscillator