Note Title 1/15/2008

$$\hat{H}\psi_n(r) = E_n \psi_n(r)$$

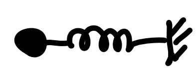
Remember: This is the space part. The time dependent part is $e^{-i\omega_n t}$, where $E_n = \hbar\omega_n$:

$$\boxed{\psi_n(r,t) = \psi_n(r)\, e^{-i\omega_n t}}$$

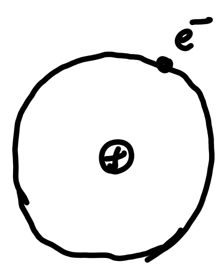
Example: what is the $\hat{H}$ for these potentials:

1D Simple Harmonic Oscillator (SHO),

$$\hat{H} = \underbrace{\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}}_{T} + \underbrace{\frac{1}{2}m\omega^2 x^2}_{V}$$



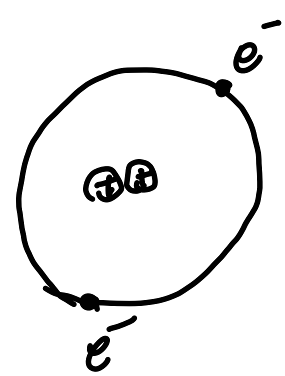
Hydrogen atom,



$$\hat{H} = \underbrace{-\frac{\hbar^2}{2m}\nabla^2}_{T_e} \underbrace{-\frac{\hbar^2}{2M}\nabla^2}_{T_p} \underbrace{-\frac{e^2}{4\pi\epsilon_0 r}}_{V_{ep}}$$

electron proton

Hellium atom,



$$\hat{H} = T_{e_1} + T_{e_2} + T_{p_1} + T_{p_2} +$$

$$V_{e_1e_2} + V_{e_1p_1} + V_{e_1p_2} + V_{e_2p_1} + V_{e_2p_2} + V_{p_{12}}$$

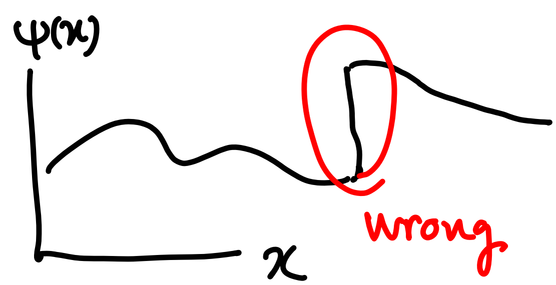
Using the Schrödinger wave equation

$$\hat{H}\psi_n(r) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\psi_n(r) = E_n\psi_n(r)$$

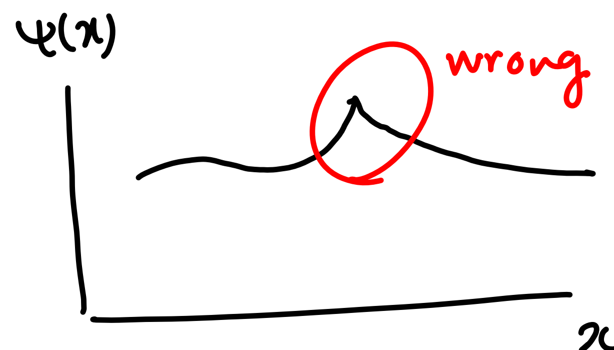
$$\psi_n(r,t) = \underbrace{\psi_n(r)}_{\text{Stationary state (time independent)}} e^{-i\omega_n t} \qquad E_n = \hbar\omega_n$$

Boundary conditions:

① ψ is continous



② $\frac{d\psi}{dx}$ is continous if V is finite.



③ $\psi(x \to \pm\infty) = 0$

wave function normalization

$$\int_{-\infty}^{\infty} |\psi(r)|^2 d^3r = 1$$

Wavefunctions are orthonormal

$$\hat{H}\psi_n = E_n\psi_n \implies \psi_1, \psi_2, \ldots$$

$$\int_{-\infty}^{\infty} \psi_n^*(r)\,\psi_m(r)\,d^3r = \underbrace{\delta_{nm}}_{\text{Kronecker delta}} \begin{cases} 1 & n=m \\ 0 & n\neq 0 \end{cases}$$

Completeness

ψ_n's make a complete space.

So any $\psi(r)$ can be expanded by ψ_n's:

$$\psi(r) = \sum_n a_n \psi_n(r)$$

Inversion Symmetry in V(r)

$$\underbrace{\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)}_{\hat{H}_n}\psi_n = E_n\psi_n$$

If $V(r)$ is symmetric: $V(r) = V(-r)$,

eigenfunctions have either odd or even

parity:

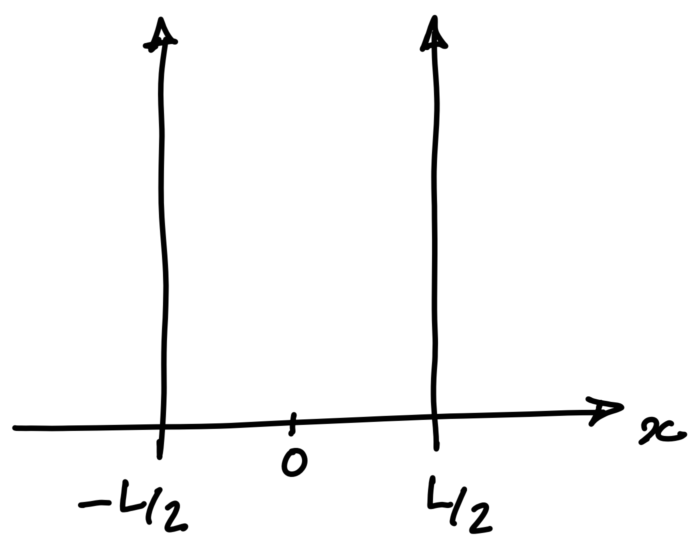
Even parity: $\psi_n(r) = \psi_n(-r)$

odd parity: $\psi_n(r) = -\psi_n(-r)$

Example 1D rectangular potential well
with infinite barrier energy

$V = 0 \quad -\frac{L}{2} < x < \frac{L}{2}$

$V = \infty \quad$ elsewhere



$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\psi'' = -\underbrace{\frac{2mE}{\hbar^2}}_{k^2}\psi$$

$$\Rightarrow \quad \psi = A e^{ikx} + B e^{-ikx}$$

B.C.

$$\psi(-\tfrac{L}{2}) = \psi(\tfrac{L}{2}) = 0 \quad \Rightarrow$$

$$\begin{cases} \psi(-\frac{L}{2}) = A e^{-ikL/2} + B e^{ikL/2} = 0 \\ \psi(\frac{L}{2}) = A e^{ikL/2} + B e^{-ikL/2} = 0 \end{cases}$$

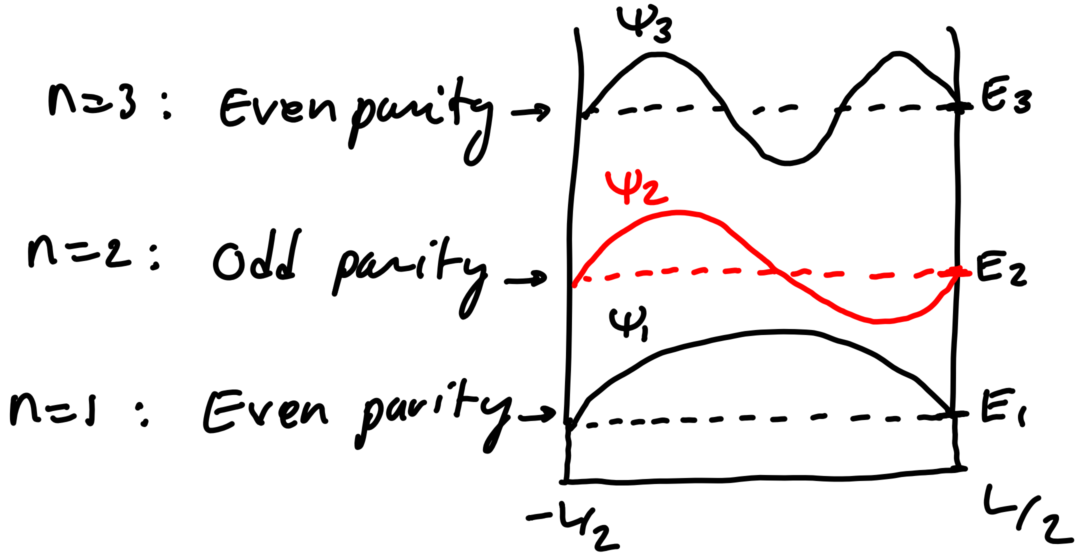
$$\begin{vmatrix} e^{-ikL/2} & e^{ikL/2} \\ e^{ikL/2} & e^{-ikL/2} \end{vmatrix} = \underbrace{e^{-ikL} - e^{ikL}}_{\downarrow} = 0$$

$$\cancel{\cos kL} - i\sin kL - (\cancel{\cos kL} + i\sin kL)$$

$$\Rightarrow \quad \sin kL = 0 \quad \Rightarrow \quad k_n L = n\pi \qquad n = 1, 2, \dots$$

$$\Rightarrow \boxed{\begin{aligned} & k_n = \frac{n\pi}{L} \\ & E = \frac{\hbar^2 k^2}{2m} \Rightarrow E_n = \frac{\hbar^2}{2m} \frac{n^2\pi^2}{L^2} \end{aligned}}$$

$$\left.\begin{aligned} k_n = \frac{n\pi}{L} \\ k = \frac{2\pi}{\lambda} \end{aligned}\right\} \quad \frac{2\pi}{\lambda_n} = \frac{n\pi}{L} \Rightarrow \boxed{L = n\frac{\lambda_n}{2}} \qquad n = 1, 2, \dots$$



n=3 : Even parity
n=2 : Odd parity
n=1 : Even parity
ψ3
ψ2
ψ1
E3
E2
E1
-L/2
L/2