# Quantum Mechanics & Quantum Computation

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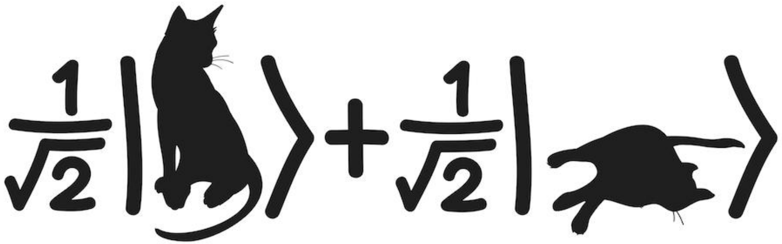
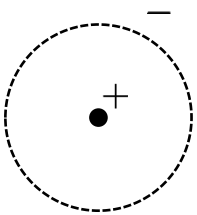


## Lecture 10: Observables, Schrödinger's equation, Particle in a box

Particle in a box

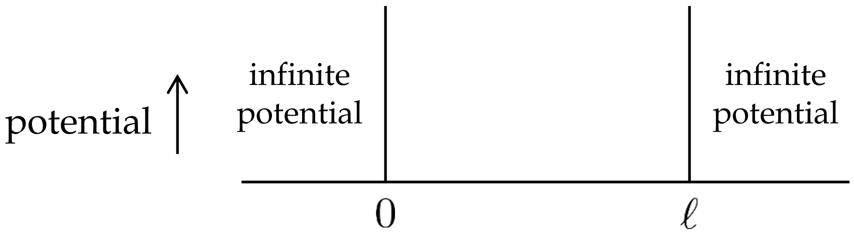
# Particle in a box

- Toy model for a hydrogen atom.




Coulomb attraction confines the electron to within some distance $\ell$

We model this in 1D (radial distance)




We will solve Schrödinger's equation:

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi = \frac{\hat{p}^2}{2m}|\psi\rangle + V(x)|\psi\rangle = \underline{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}}|\psi\rangle$$

Boundary conditions: $\psi(0) = \psi(\ell) = 0$

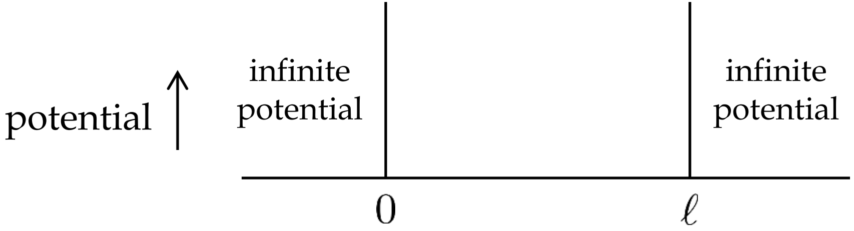
$$H|\phi\rangle = \lambda|\phi\rangle \qquad \psi(0) = |\phi\rangle \Rightarrow \psi(t) = e^{-i\lambda t/\hbar}|\phi\rangle$$

<u>Guess</u> : $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ $\qquad \phi(x) = e^{ikx}$

$$H\phi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}e^{ikx} = \frac{\hbar^2}{2m}k^2 e^{ikx} \qquad E = \frac{\hbar^2 k^2}{2m}.$$

$$\phi_E(x) = Ae^{ikx} + Be^{-ikx} \qquad E_k = \frac{\hbar^2 k^2}{2m}$$

$$= C\sin kx + D\cos kx \qquad e^{ikx} = \cos kx + i\sin kx$$

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$$\phi_E(x) = C\sin kx + D\cos kx \qquad E_k = \frac{\hbar^2 k^2}{2m}$$

$$\phi(0) = 0 = C\times 0 + \cancel{D\times 1} = 0$$

$$\Phi_E(\ell) = 0 = C\sin k\ell$$

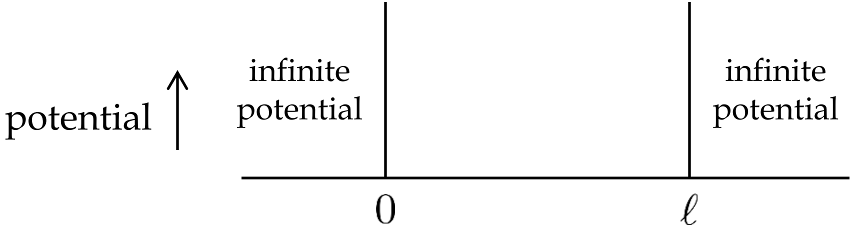
$$k\ell = n\pi \qquad n \text{ integer}$$

$$k_n = \frac{n\pi}{\ell} \qquad E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2\pi^2}{2m l^2}$$

$$\Phi_n(x) = C\sin\frac{n\pi}{\ell}x$$

$$\int_0^\ell C^2\sin^2\frac{n\pi}{\ell}x\,dx = 1 \Rightarrow C^2 = 2/\ell$$

$$C = \sqrt{2/\ell}.$$

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Boundary conditions: $\psi(0) = \psi(\ell) = 0$

Solution: $E_n = \underline{\underline{\frac{\hbar^2 n^2 \pi^2}{2m\ell^2}}}$ $\psi_n(x) = \sqrt{\frac{2}{\ell}}\sin\frac{n\pi x}{\ell}$

Quantization:

$$\psi(x) = \alpha_n \psi_n(x)$$

$$\psi(x,t) = \alpha_n e^{-iE_n t/\hbar} \psi_n(x)$$