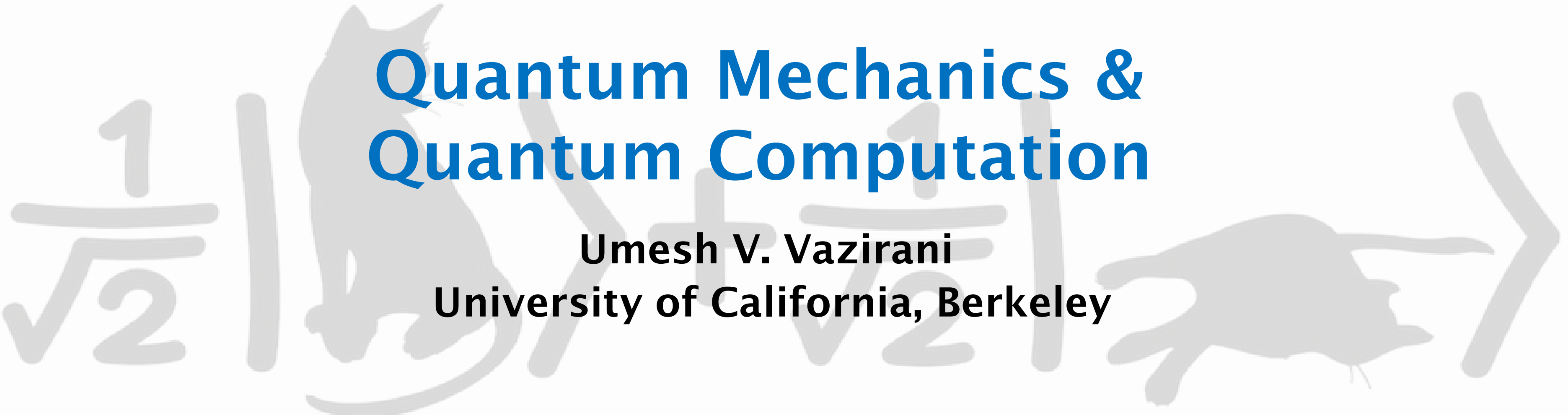


Quantum Mechanics & Quantum Computation

Umesh V. Vazirani

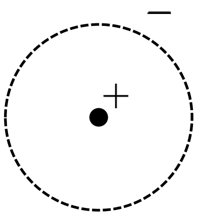
University of California, Berkeley

Lecture 13: Particle in a Box & implementing qubits

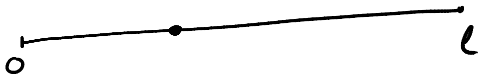
Continuous quantum states

Particle in a box

- Toy model for a hydrogen atom.

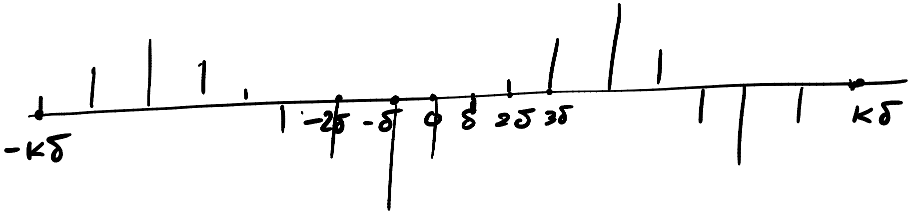


1 Dim.



1) How to describe the state
2) What is the Hamiltonian.
3) Energy eigenstates.
4) Implement qubits.

$$P[j\delta] = |\alpha_{j\delta}|^2$$



$$|\psi\rangle = \sum_{j=-k}^{k} \alpha_{j\delta} |j\delta\rangle$$

$$\| |\psi\rangle \|^2 = \sum_{-k}^{k} |\alpha_{j\delta}|^2 = 1.$$

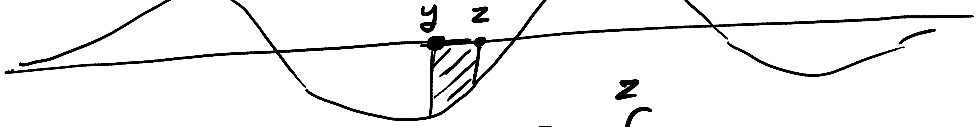
$$\psi(x) \sim \alpha_{\underline{\underline{j}}\delta}$$

$\delta \to 0$ $\quad\quad k \to \infty$

$$\| |\psi(x)\rangle \|^2 = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

$$= \int_{-\infty}^{\infty} \psi(x)^* \psi(x)\, dx$$

$\psi(x)$



$$\int_y^z |\psi(x)|^2 dx = P[\text{electron between } y \,\&\, z] = \int_y^z \psi(x)^* \psi(x)\, dx$$

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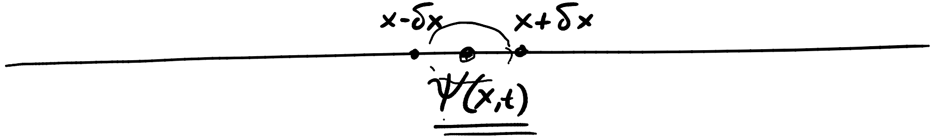
Schrodinger Eqn for 1-D free particle

$\psi(x,t)$

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}}_{H}\psi(x,t)$$

$$\frac{\partial \psi(x,t)}{\partial t} \propto \frac{\partial^2 \psi(x,t)}{\partial x^2}$$



$$\text{change} \propto \frac{\psi(x+\delta x) + \psi(x-\delta x)}{2} - \psi(x)$$

$$= \frac{[\psi(x+\delta x) - \psi(x)] - [\psi(x) - \psi(x-\delta x)]}{2}$$

$$\propto \frac{\psi'(x) - \psi'(x-\delta x)}{2} \propto \psi''(x)$$

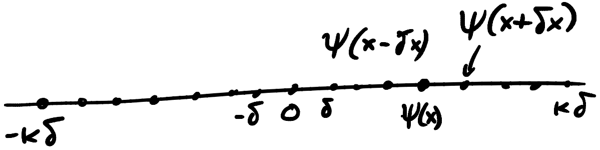
$$\frac{\partial^2 \psi(x)}{\partial x^2}.$$

$$H = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}.$$

$$E = \frac{1}{2}mv^2 = \frac{P^2}{2m}$$

$$\left.\begin{aligned}\hat{P} &= -i\hbar\frac{\partial}{\partial x}\end{aligned}\right\}$$

$$H = \frac{\hat{P}^2}{2m} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$



$$\frac{\partial\psi}{\partial x} \propto \psi(x+\delta x) - \psi(x-\delta x)$$

$$i\frac{\partial}{\partial x} = \begin{bmatrix} 0 & i & & 0 \\ -i & \ddots & \ddots & \\ & \ddots & \ddots & i \\ 0 & & -i & 0 \end{bmatrix} \begin{bmatrix} \psi(-k\delta) \\ \vdots \\ \psi(x) \\ \vdots \\ \psi(k\delta) \end{bmatrix} = \begin{bmatrix} \\ \psi(x+\delta x) - \psi(x-\delta x) \\ \\ \end{bmatrix}$$

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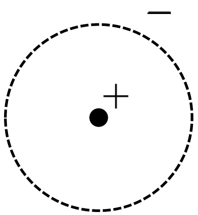
Lecture 13: Particle in a Box & implementing qubits

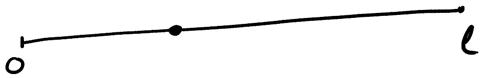
Particle in a box

Particle in a box

- Toy model for a hydrogen atom.



1 Dim.



1) How to describe the state
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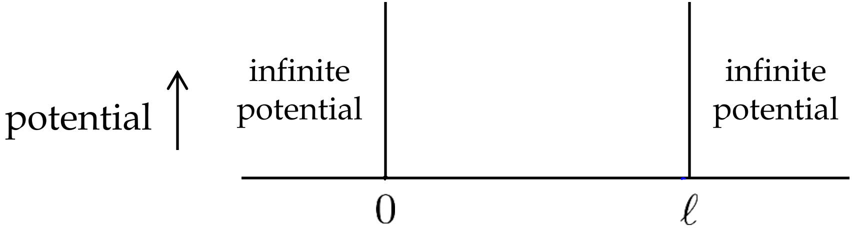


We will solve Schrödinger's equation:

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

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

$$H = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

Eigenstate $\psi(x) = e^{ikx}$

$$H\,\psi(x) = \frac{-\hbar^2}{2m}\frac{\partial^2 e^{ikx}}{\partial x^2} = \frac{-\hbar^2}{2m}(ik)^2 e^{ikx}$$

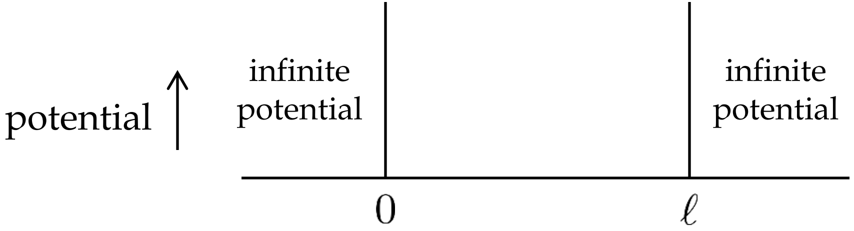
$$= \frac{\hbar^2 k^2}{2m} e^{ikx} = E_k e^{ikx}$$

$$\left.E_k = \frac{\hbar^2 k^2}{2m}.\right\} \quad e^{ikx} \quad \& \quad e^{-ikx}$$

$$\psi_E(x) = A e^{ikx} + B e^{-ikx} \qquad E_k$$

$$= C \sin kx + D \cos kx$$

Boundary conditions.



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

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

$\psi_E(0) = 0 \qquad 0 = D\cdot 1 \Rightarrow D = 0$

$\psi_E(\ell) = 0 \qquad C \sin k\ell = 0 \qquad k\ell = n\pi \qquad n$ is an integer.

$$k_n = \frac{n\pi}{\ell}$$

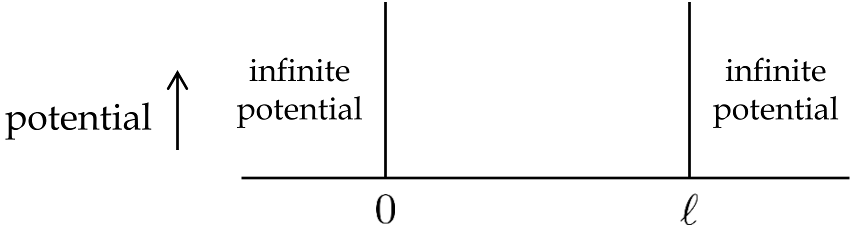
$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2m\ell^2}$$

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

$$\int_0^\ell |\psi_n(x)|^2 dx = 1 = \int_0^\ell C^2 \sin^2\frac{n\pi}{\ell}x\, dx \iff 2 = \int_0^\ell C^2 [\underbrace{\sin^2 + \cos^2}_{=1}]\, dx$$

$$2 = C^2\ell \Rightarrow C = \sqrt{\frac{2}{\ell}}.$$

$$\psi_n(x) = \sqrt{\frac{2}{\ell}}\sin\left(\frac{n\pi}{\ell}x\right), \quad E_n = \frac{\hbar^2 n^2\pi^2}{2m\ell^2}.$$



We will solve Schrödinger's equation:

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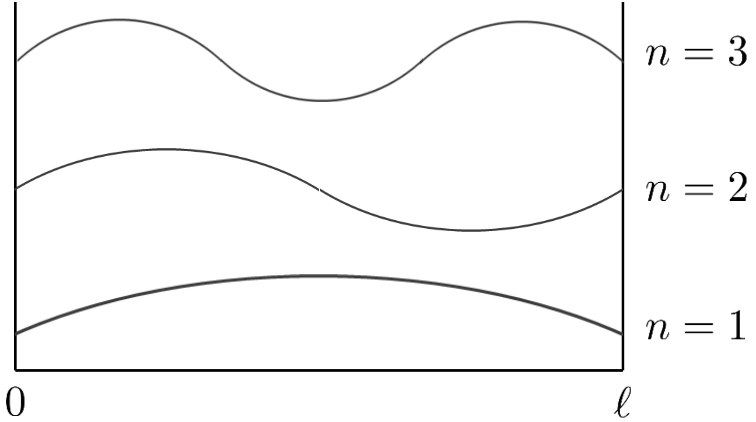
Boundary conditions: $\psi(0) = \psi(\ell) = 0$

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

Quantization:

$$\psi(0) = \sum_{n=1}^{\infty} \alpha_n \psi_n(x)$$

$$\psi(t) = \sum_{n=1}^{\infty} \alpha_n e^{-iE_n t/\hbar} \psi_n(x)$$



$E_2 - E_1 = \Delta E$

$\Delta E_H \approx 10$ eV.

$\Delta E_B = \frac{3\hbar^2\pi^2}{2m\ell^2} \simeq 10$ eV

$\ell \approx 3.4$ Å $\approx 3.4 \times 10^{-10}$ m.

Diam of H ≈ 1 Å.

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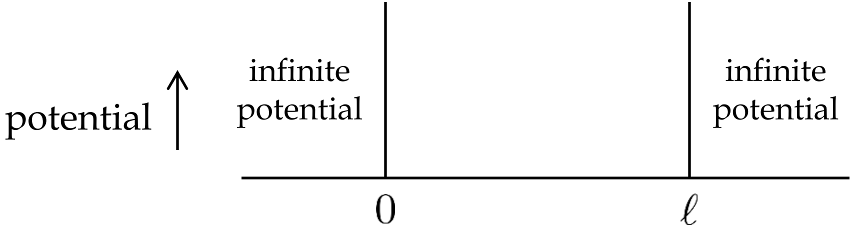
Lecture 13: Particle in a Box & implementing qubits

Implementing qubits



We will solve Schrödinger's equation:

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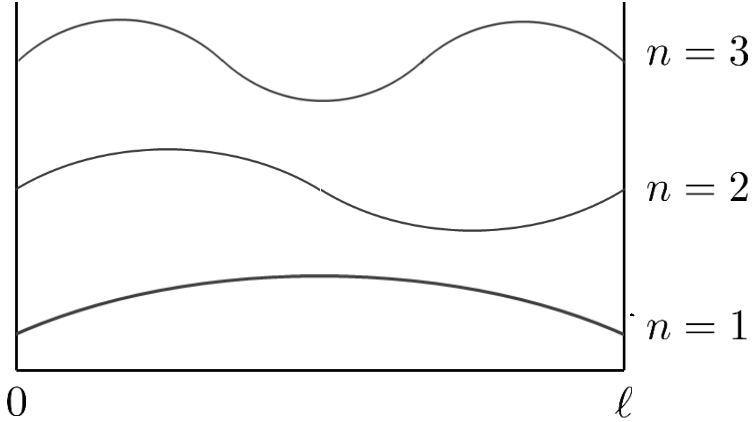
Boundary conditions: $\psi(0) = \psi(\ell) = 0$

$\ell = 3.4$ Angstroms

$E_2 - E_1 = \Delta E_H$

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

Quantization:



$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$

$= \alpha\sqrt{\frac{2}{\ell}}\sin\frac{\pi x}{\ell} + \beta\sqrt{\frac{2}{\ell}}\sin\frac{2\pi x}{\ell}.$

$|\psi(t)\rangle = \alpha|0\rangle e^{-iE_1 t/\hbar} + \beta|1\rangle e^{-iE_2 t/\hbar}$

$= e^{-iE_1 t/\hbar}\left\{\alpha|0\rangle + \beta|1\rangle e^{-i(E_2 - E_1)t/\hbar}\right.$

$= e^{-iE_1 t/\hbar}\left\{\alpha\sqrt{\frac{2}{\ell}}\sin\frac{\pi x}{\ell} + \beta\sqrt{\frac{2}{\ell}}\sin\frac{2\pi x}{\ell}\, e^{-i\Delta E_H t/\hbar}\right.$

$\Delta E_H \simeq 10\,eV$

$\nu = \frac{\Delta E_H}{h} \approx \underline{\underline{2.5\times 10^{15}\,Hz}}$