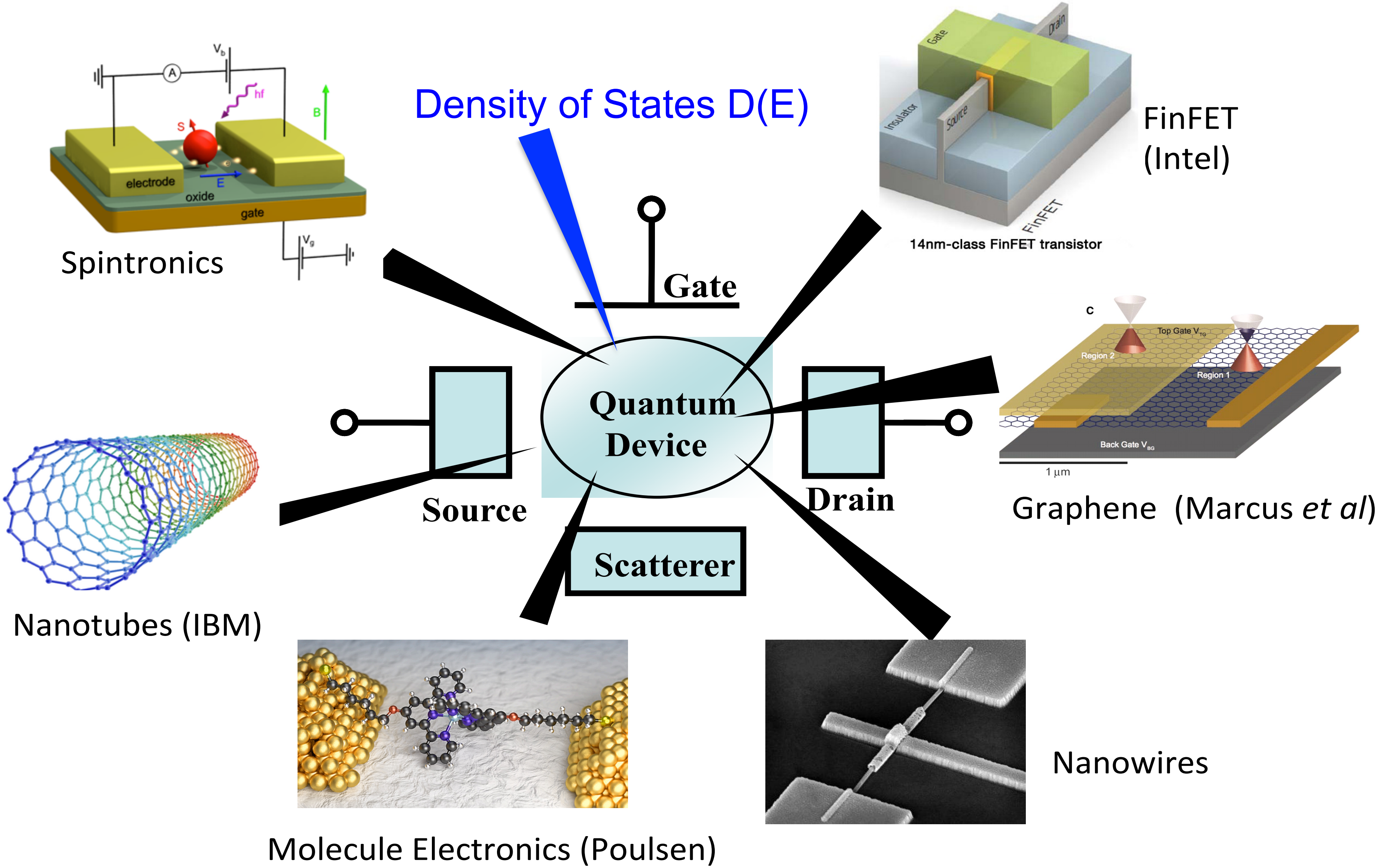
Fundamentals of NanoElectronics

Lecture – VI

UNIFIED FORMALISM



Schrödinger Eq. in 1-D (Free Electron)

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + U(\vec{r}) \right) \Psi$$

(Schrödinger Equation)

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial^2 x}$$

(constant potential U=0 & 1-D)

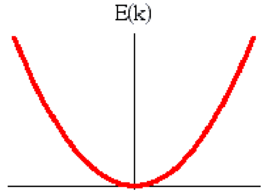
$$\Psi = A e^{-iEt/\hbar} e^{ikx}$$

(solution of PDE for constant coefficients in space and/or time)

$$i\hbar \cdot \frac{-iE}{\hbar} \cdot \Psi = -\frac{\hbar^2}{2m} (ik_x)^2 \cdot \Psi$$

Dispersion Relation

$$E = \frac{\hbar^2 k_x^2}{2m}$$



Free Electron Theory

Schrödinger Eq. in 2-D (Free Electron)

$$i\hbar\frac{\partial\Psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right)\Psi$$

(Schrödinger Equation)

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial^2 x} - \frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial^2 y}$$

(constant potential U=0 & 2-D)

$$\Psi = Ae^{-iEt/\hbar}e^{ikx}e^{iky}$$

(constant coefficients space and/or time)

$$E\Psi = \frac{\hbar^2 k_x^2}{2m}\Psi + \frac{\hbar^2 k_y^2}{2m}\Psi$$

Dispersion Relation

$$E = \frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

Time Independent Schrödinger Equation

(Time Dependent Schrödinger Equation)

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + U(\vec{r}) \right) \Psi$$

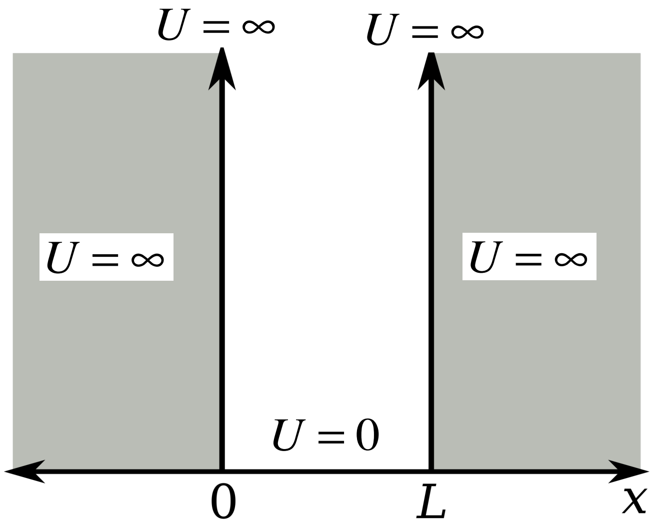
No Time Variance

$$\Psi(r,t) = \Phi(r) e^{-iEt/\hbar}$$

(Time Independent Schrödinger Equation)

$$E\Phi(r) = -\frac{\hbar^2}{2m} \nabla^2 \Phi(r) + U(r)\Phi(r)$$

Particle in a Box



$$i\hbar\frac{\partial\Psi}{\partial t}=\left(-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r})\right)\Psi$$

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

Time Independent Problem

$$\Psi(x=0)=0$$

$$\Psi=Ae^{ikx}+Be^{-ikx}$$

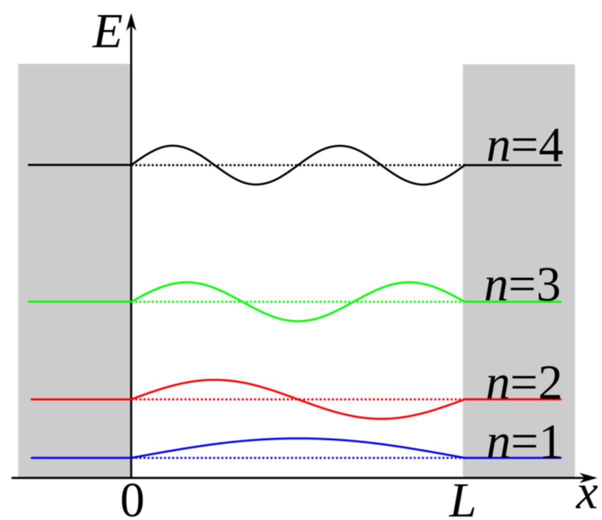
$$\Psi=A\sin kx \qquad A=-B$$

$$\Psi(x=L)=0$$

$$\sin kL=0$$

$$E=\frac{\hbar^2k^2}{2m}=\frac{\hbar^2}{2m}\frac{\pi^2}{L^2}n^2$$

(Discrete Energy Levels)



$$E_4=16E_1$$

$$E_3=9E_1$$

$$E_2=4E_1$$

$$E_1=\hbar^2\pi^2/2mL^2$$

Time-Independent Schrödinger Equation

(Time Dependent Schrödinger Equation)

$$i\hbar\frac{\partial\Psi}{\partial t}=\left(-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r})\right)\Psi$$

(Amplitude is not constant)

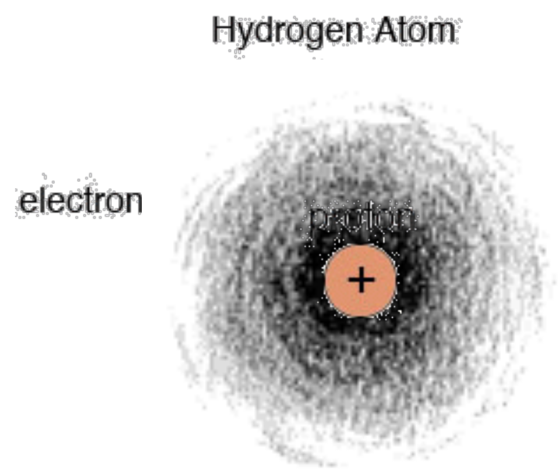
$$\Psi(r,t)=\Phi(r)e^{-iEt/\hbar}$$

(Time Independent Schrödinger Equation)

$$E\Phi(r)=-\frac{\hbar^2}{2m}\nabla^2\Phi(r)+U(r)\Phi(r)$$

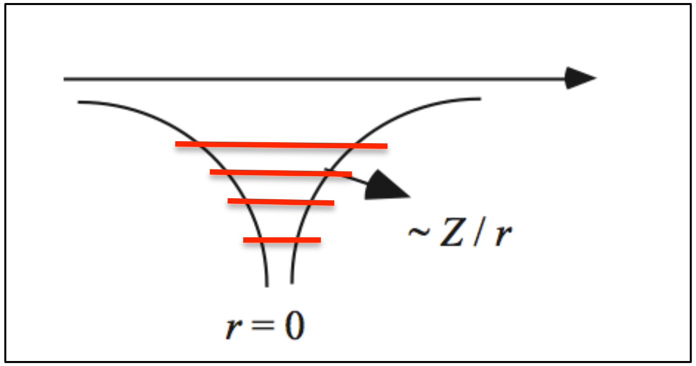
$$U(r)=-\frac{Zq^2}{4\pi\varepsilon_o r}$$

$$E=-\frac{E_0}{n^2}$$

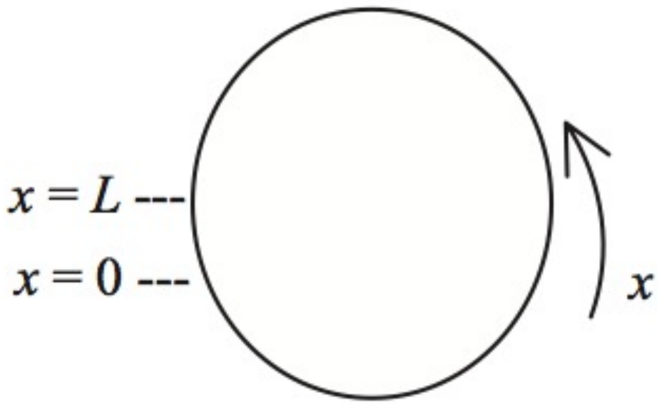


Probability Density:

$$P(r,t)=\Psi(r,t)^*\Psi(r,t)=\Phi(r)^*\Phi(r)=\left|\Phi^2(r)\right|$$



Periodic Boundary



$$i\hbar\frac{\partial\Psi}{\partial t}=\left(-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r})\right)\Psi$$

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial^2 x}$$

Time Independent Problem

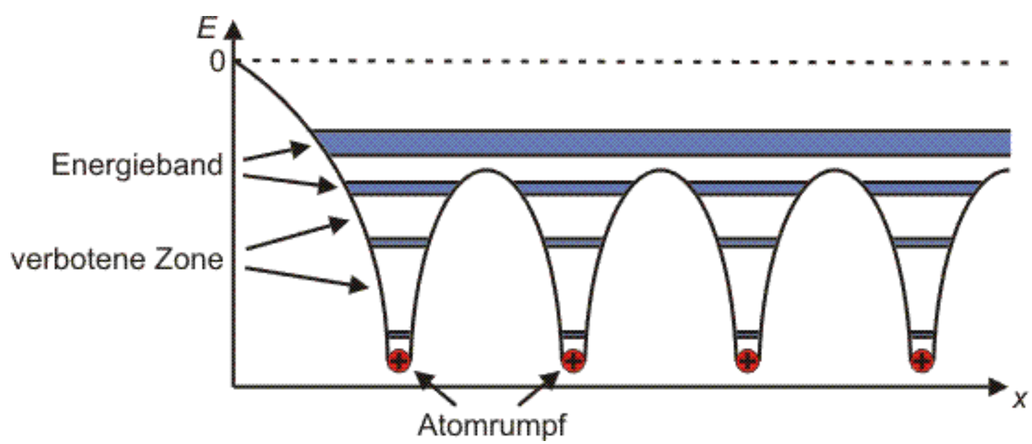
$$\Psi=Ae^{-iEt/\hbar}e^{ikx}$$

$$\Psi(0)=\Psi(L)\quad\Rightarrow\quad e^{ikx}=e^{ik(x+L)}$$

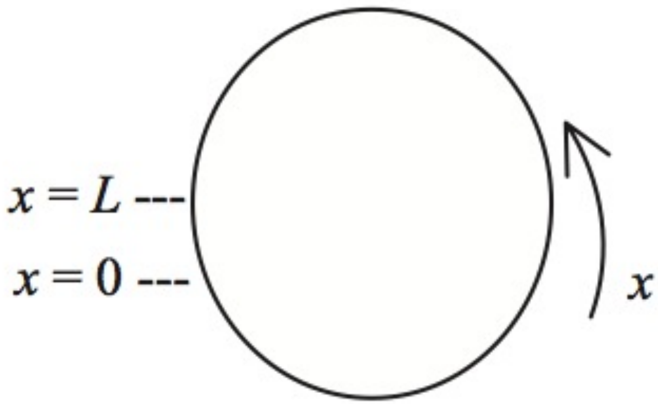
$$e^{ikL}=1\quad\Rightarrow\quad k_n=\frac{n2\pi}{L}$$

(Periodic Boundary Condition)

$$n=\ldots-2\quad -1\quad 0\quad 1\quad 2\quad \ldots$$



Periodic Boundary



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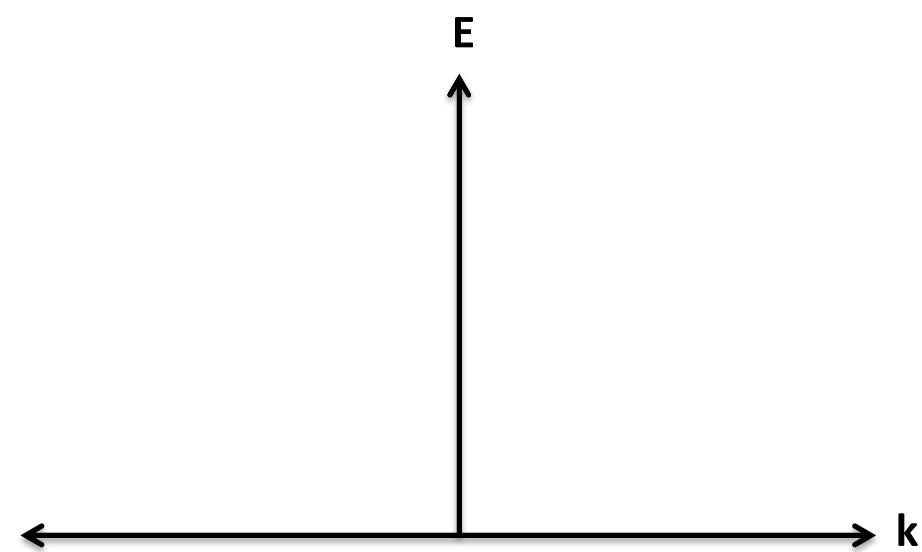
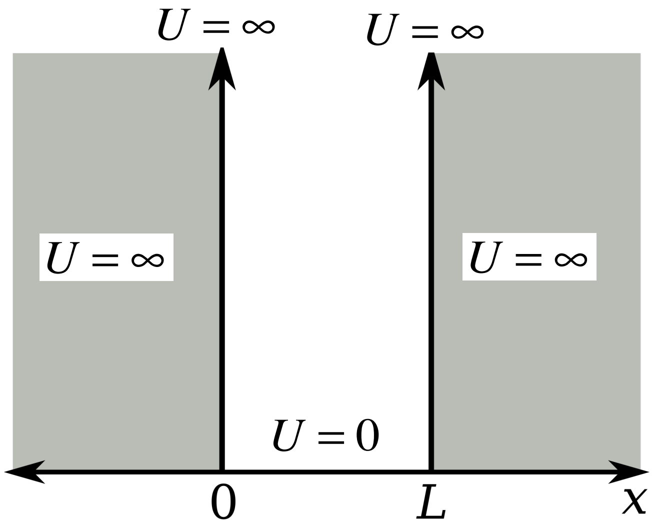


Particle in a Box



$$i\hbar\frac{\partial\Psi}{\partial t}=\left(-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r})\right)\Psi$$

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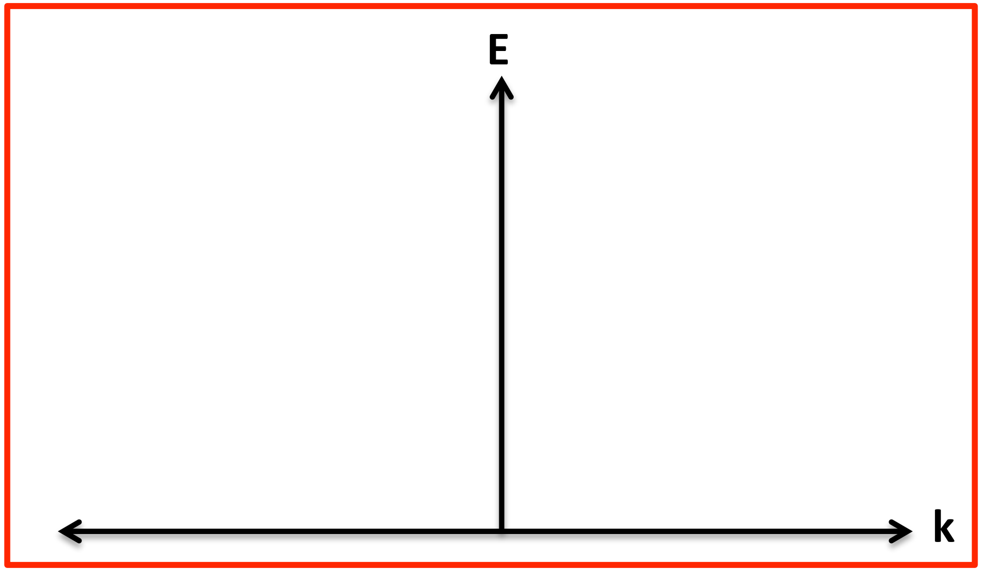
(Discrete Energy Levels)



How to Solve Schrödinger Equation

Schrödinger Equation

$$E\Phi(r) = -\frac{\hbar^2}{2m}\nabla^2\Phi(r) + U(r)\Phi(r)$$

(Time Independent Schrödinger Equation)

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Howto solve this relation?

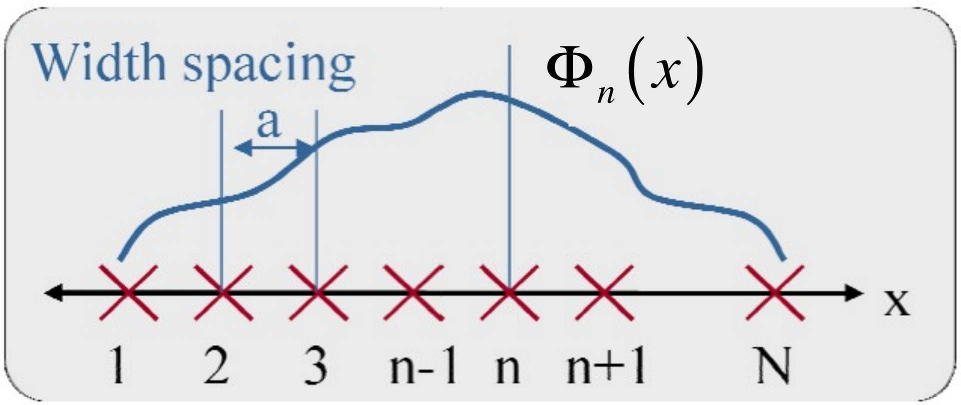
$$E\Phi(x) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)\right]\Phi(x)$$

1-D Schrödinger Equation

Numerical solution → algebraic relations

Method of Finite Differences

Lattice of discrete points



Wavefunction as a vector

$$\Phi(x) \rightarrow \begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_N \end{bmatrix}$$

Schrodinger Equation

$$E\Phi(x) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x) \right]\Phi(x) \Rightarrow$$

Matrix Relation

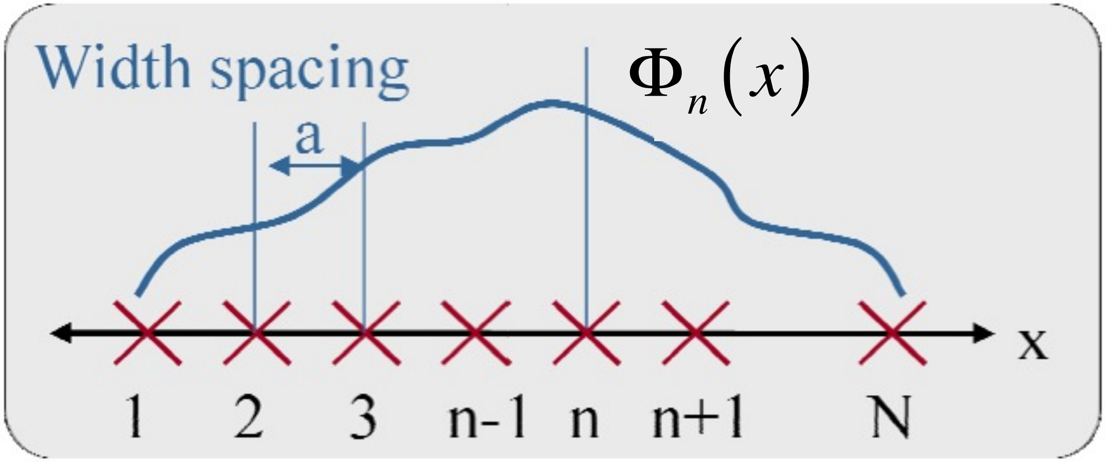
$$\mathrm{E}\begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_N \end{bmatrix} = \overbrace{\begin{bmatrix} \\ & H & \\ \\ \end{bmatrix}}^{N \times N} \begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_N \end{bmatrix}$$

How to Write Hamiltonian

Schrodinger Equation

$$E\Phi(x)=\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+U(x)\right]\Phi(x) \quad = \quad [H]\Phi(x) \quad = \quad [KE+U]\Phi(x)$$

$$E\Phi(x)=U(x)\Phi(x)$$



Each lattice point

$$E\Phi_n=U_n\Phi_n$$

How to Write Hamiltonian

Schrodinger Equation

$$E\Phi(x) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)\right]\Phi(x) \quad = \quad [H]\Phi(x) \quad = \quad [KE + U]\Phi(x)$$

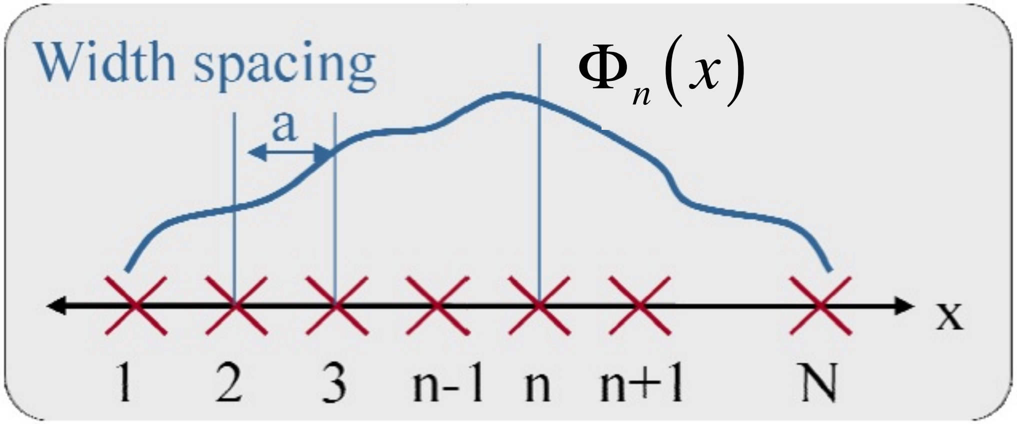
$$E\Phi(x) = U(x)\Phi(x)$$

$$E\begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_N \end{bmatrix} = \underbrace{\begin{bmatrix} U(x=x_1) & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & U(x=x_2) & 0 & & & \vdots \\ \vdots & 0 & \ddots & & & \vdots \\ \vdots & & & \ddots & & \vdots \\ \vdots & & & & \ddots & 0 \\ 0 & \cdots & \cdots & \cdots & 0 & U(x=x_N) \end{bmatrix}}_{U} \begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_N \end{bmatrix}$$

Kronecker Delta Relation

$$U(x) \;\Rightarrow\; U(x=x_n)\delta_{n,m} \quad \text{so} \quad U_{nm} = U(x=x_n)\delta_{n,m}$$

How to Write Hamiltonian



First derivative

$$\left(\frac{d\Phi}{dx}\right)_{n+\frac{1}{2}} \simeq \frac{\Phi_{n+1}-\Phi_n}{a} \quad \text{and} \quad \left(\frac{d\Phi}{dx}\right)_{n-\frac{1}{2}} \simeq \frac{\Phi_n-\Phi_{n-1}}{a}$$

Second derivative

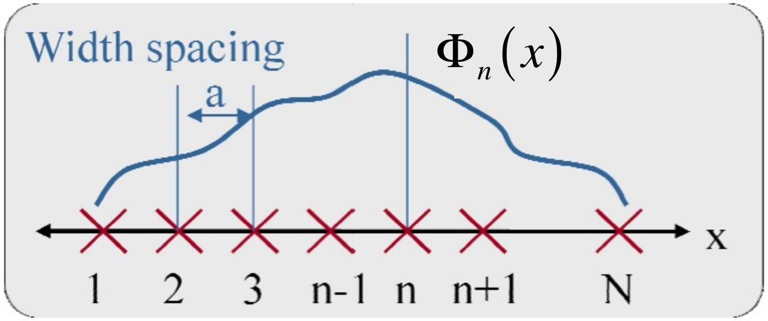
$$\left(\frac{d^2\Phi}{dx^2}\right)_n \simeq \frac{\left(\frac{d\Phi}{dx}\right)_{n+\frac{1}{2}} - \left(\frac{d\Phi}{dx}\right)_{n-\frac{1}{2}}}{a} \quad \Rightarrow \quad \left(\frac{d^2\Phi}{dx^2}\right)_n \simeq \frac{\Phi_{n+1}-2\Phi_n+\Phi_{n-1}}{a^2}$$

How to Write Hamiltonian

Schrodinger Equation

$$E\Phi(x)=\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+U(x)\right]\Phi(x) \quad = \quad [H]\Phi(x) \quad = \quad [KE+U]\Phi(x)$$

$$E\Phi(x)=\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right]\Phi(x) \quad = \quad KE\ \Phi(x)$$



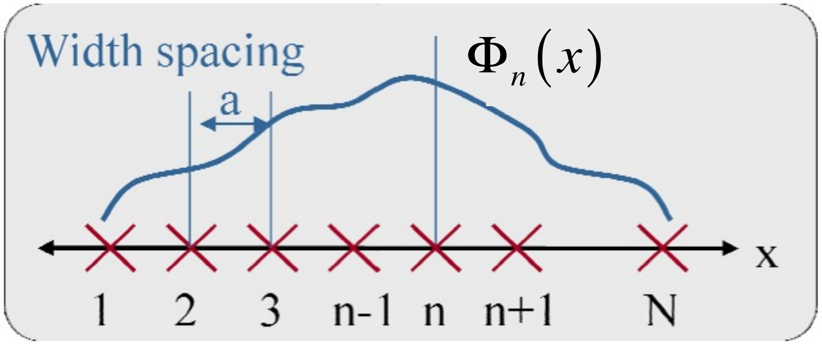
First derivative

$$\left(\frac{d\Phi}{dx}\right)_{n+\frac{1}{2}} \simeq \frac{\Phi_{n+1}-\Phi_n}{a} \quad \text{and} \quad \left(\frac{d\Phi}{dx}\right)_{n-\frac{1}{2}} \simeq \frac{\Phi_n-\Phi_{n-1}}{a}$$

Second derivative

$$\left(\frac{d^2\Phi}{dx^2}\right)_n \simeq \frac{\left(\frac{d\Phi}{dx}\right)_{n+\frac{1}{2}}-\left(\frac{d\Phi}{dx}\right)_{n-\frac{1}{2}}}{a} \quad \Rightarrow \quad \left(\frac{d^2\Phi}{dx^2}\right)_n \simeq \frac{\Phi_{n+1}-2\Phi_n+\Phi_{n-1}}{a^2}$$

How to Write Hamiltonian



$$E\Phi(x) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \right]\Phi(x) = H_1\Phi(x)$$

$$\left(\frac{d^2\Phi}{dx^2}\right)_n \simeq \frac{\Phi_{n+1} - 2\Phi_n + \Phi_{n-1}}{a^2}$$

$$E\Phi_n(x) \simeq \underbrace{\frac{\hbar^2}{2ma^2}}_{t_0}\left[2\Phi_n - \Phi_{n-1} - \Phi_{n+1}\right]$$

There are N equations for n ε {1,2,3,..N}

It is not diagonal !!

$$E\begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_N \end{bmatrix} = \begin{bmatrix} 2t_0 & -t_0 & \cdots & \cdots & \cdots & 0 \\ -t_0 & 2t_0 & -t_0 & & & \vdots \\ \vdots & -t_0 & \ddots & & & \vdots \\ \vdots & & & \ddots & & \vdots \\ \vdots & & & & \ddots & -t_0 \\ 0 & \cdots & \cdots & \cdots & -t_0 & 2t_0 \end{bmatrix}\begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_N \end{bmatrix}$$

How to Write Hamiltonian

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Kronecker Delta Relation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \Rightarrow KE_{nm} = 2t_0\delta_{n,m} - t_0\delta_{n+1,m} - t_0\delta_{n-1,m}$$

Total Hamiltonian

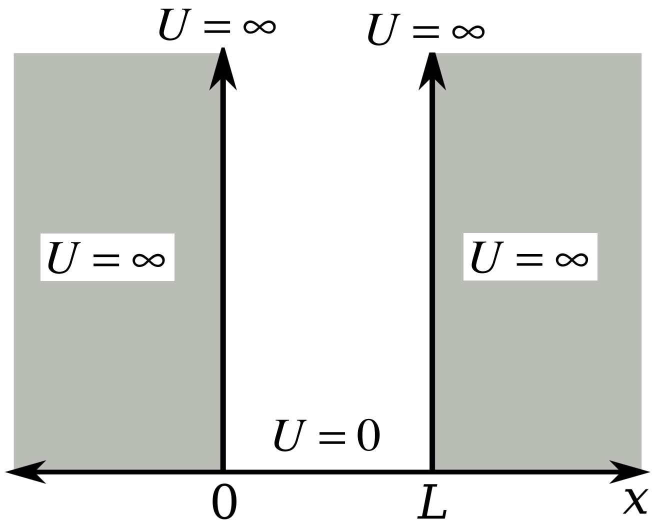
$$E\Phi_n(x) \simeq U(x_n) - t_0\left[\Phi_{n-1} - 2\Phi_n + \Phi_{n+1}\right]$$

$$E\begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_N \end{bmatrix} = \underbrace{\begin{bmatrix} 2t_0 + U(x_1) & -t_0 & \cdots & \cdots & \cdots & 0 \\ -t_0 & 2t_0 + U(x_2) & -t_0 & & & \vdots \\ \vdots & -t_0 & \ddots & & & \vdots \\ \vdots & & & \ddots & & \vdots \\ \vdots & & & & \ddots & -t_0 \\ 0 & \cdots & \cdots & \cdots & -t_0 & 2t_0 + U(x_N) \end{bmatrix}}_{H = KE + U} \begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_N \end{bmatrix}$$

where $t_0 = \dfrac{\hbar^2}{2ma^2}$

Incorporating Boundary Conditions

Particle in a Box



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

Time Independent Problem

$$\Psi(x=0)=0$$

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$$\Psi = A\sin kx \qquad A = -B$$

$$\Psi(x=L)=0$$

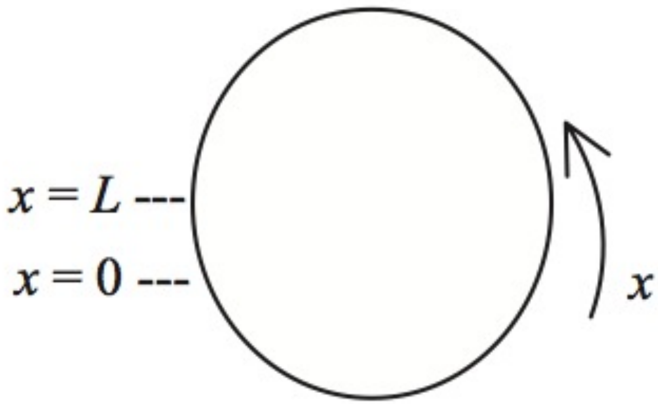
$$\sin kL = 0$$

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\frac{\pi^2}{L^2}n^2$$

(Discrete Energy Levels)

$$E\begin{bmatrix}\Phi_1\\ \Phi_2\\ \vdots\\ \Phi_N\end{bmatrix} = \begin{bmatrix} 2t_0+U(x_1) & -t_0 & \cdots & \cdots & \cdots & 0\\ -t_0 & 2t_0+U(x_2) & -t_0 & & & \vdots\\ \vdots & -t_0 & \ddots & & & \vdots\\ \vdots & & & \ddots & & \vdots\\ \vdots & & & & \ddots & -t_0\\ 0 & \cdots & \cdots & \cdots & -t_0 & 2t_0+U(x_N)\end{bmatrix}\begin{bmatrix}\Phi_1\\ \Phi_2\\ \vdots\\ \Phi_N\end{bmatrix}$$

Periodic Boundary



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Time Independent Problem

$$\Psi = A e^{-iEt/\hbar} e^{ikx}$$

$$\Psi(0) = \Psi(L) \quad \Rightarrow \quad e^{ikx} = e^{ik(x+L)}$$

$$e^{ikL} = 1 \quad \Rightarrow \quad k_n = \frac{n2\pi}{L}$$

(Periodic Boundary Condition)

$$n = \ldots -2 \quad \text{-1} \quad 0 \quad 1 \quad 2 \quad \ldots$$

$$E \begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_N \end{bmatrix} = \begin{bmatrix} 2t_0 + U(x_1) & -t_0 & \cdots & \cdots & \cdots & -t_0 \\ -t_0 & 2t_0 + U(x_2) & -t_0 & & & \vdots \\ \vdots & -t_0 & \ddots & & & \vdots \\ \vdots & & & \ddots & & \vdots \\ \vdots & & & & \ddots & -t_0 \\ -t_0 & \cdots & \cdots & \cdots & -t_0 & 2t_0 + U(x_N) \end{bmatrix} \begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_N \end{bmatrix}$$