University of Michigan – Shanghai Jiao Tong University Joint Institute
Center of Optics and Optoelectronics

VE 320 – Summer 2012
Introduction to Semiconductor Device

Instructor: Professor Hua Bao

Previous Lecture

- In order to understand the transport property of semiconductor, we need to understand the chemical composition and atomic arrangements.
- Crystalline structure can be built by repeating basic building blocks… Bravais lattice, basis
- Diamond and zinc-blende structure
- To identify crystal planes…Miller Indices, vector indices

Looking ahead …

Number of atoms/volume from crystal structure

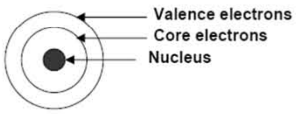
Number of electrons available for conduction

Number of electrons/atoms

$$n \neq \rho \times N$$

II	III	IV	V	VI
4 Be	5 B	6 C	7 N	8 O
12 Mg	13 Al	14 Si	15 P	16 S
30 Zn	31 Ga	32 Ge	33 As	34 Se
48 Cd	49 In	50 Sn	51 Sb	52 Te
80 Hg	81 Tl	82 Pb	83 Bi	84 Po

Classical Model (Drude Model)

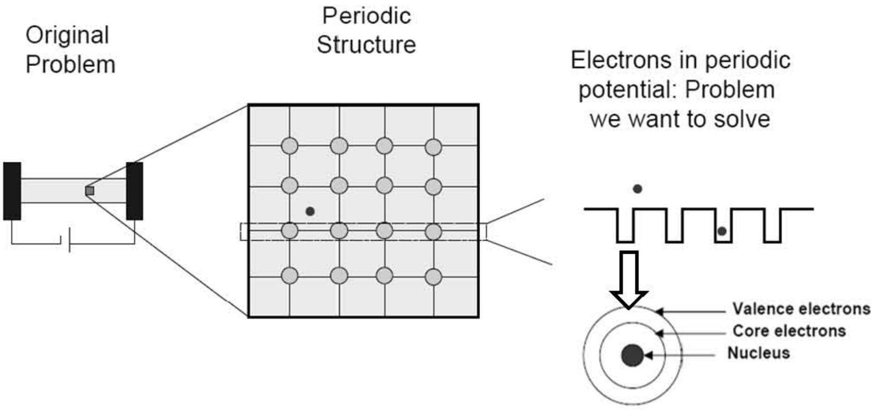


"Free" valence electrons contribute to conductivity

? ⇨ **Quantum Mechanics!**

Don't be afraid. We will keep things simple.

Do I really need quantum mechanics?



If it were large objects, Newton's mechanics would work fine, but in amicro-world…

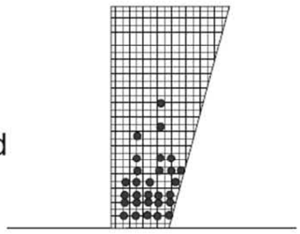
Carrier Density

Carrier number = Number of states x filling factor

Quantum Mechanics

Statistical Mechanics

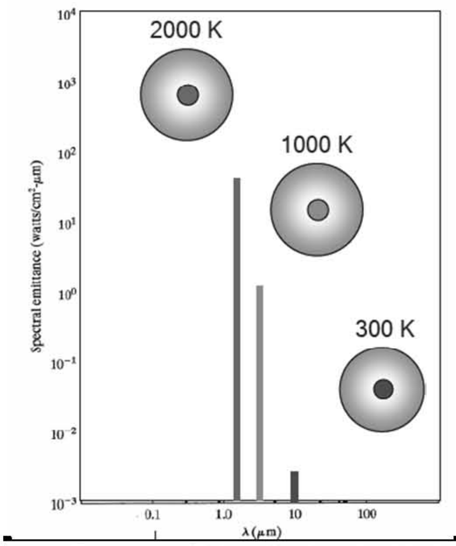
Total number of occupants
= Number of apartments
X The fraction occupied



Quantum Concepts …

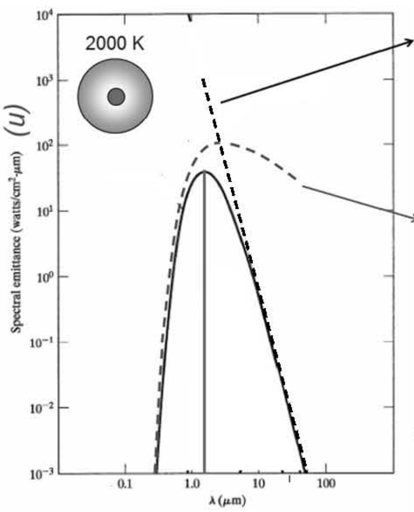
- Blackbody Radiation
- Photoelectric Effect
- Bohr Effect
- Wave Particle Duality

Blackbody Radiation



- Emitting wavelength of blackbody is temperature-dependent.
- Higher temperature, lower emission wavelength
- Becomes visible ~ 3000 K

Planck's Formula



Rayleigh-Jeans Formula

$$u(\lambda, T) \propto k_B T / \lambda^4$$

$$\log(u) = -4\log(\lambda) + \log(T)$$

Wein's Formula

$$u \propto \frac{e^{-\beta/\lambda T}}{\lambda^5}$$

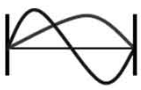
Plank's fitting formula

$$u(\lambda, T) \propto \frac{1}{\lambda^5}\left[\frac{1}{e^{\beta/\lambda T} - 1}\right]$$

Interpretation of Planck's Formula

$$u(f,T) = u(\lambda,T)\frac{d\lambda}{df} \sim \frac{1}{\lambda^5}\left[\frac{1}{e^{\beta/\lambda T}-1}\right]\frac{d\lambda}{df} \qquad \lambda = \frac{c}{f}$$

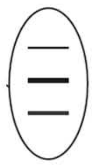
$$\sim f^2 \times hf \times \left(\frac{1}{e^{hf/kT}-1}\right)$$



nos. of modes

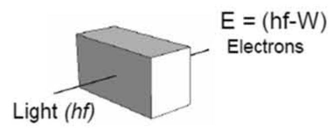
Energy of the mode

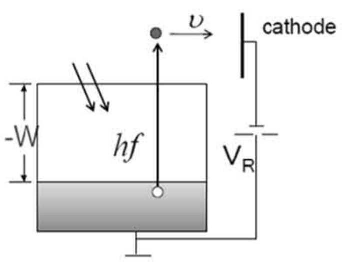
Occupation number



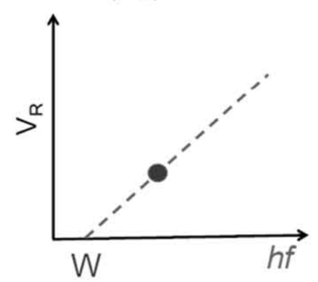
EM emission in discrete quanta of $E = hf$

Photoelectric Effect

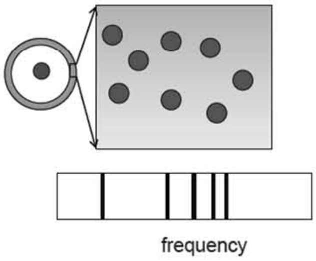




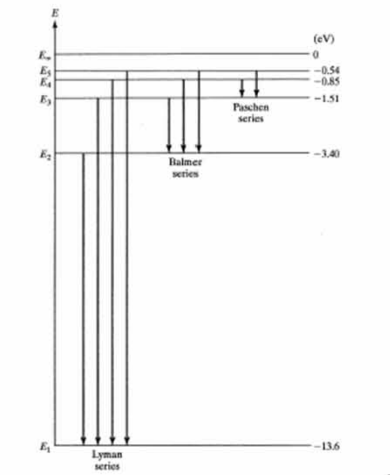
$$qV_R \approx \left(\tfrac{1}{2}\right)m_0\upsilon^2 = hf - W$$



Origin of Quantization



Analyze spectra of hydrogen



Empirical equation:

$$E_{m,n} = const \times \left(\frac{1}{m^2} - \frac{1}{n^2} \right)$$

Bohr Atom

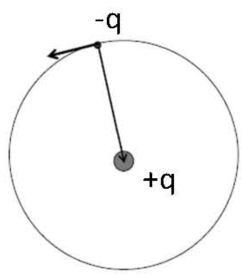
Assuming the angular momentum are quantized:

$$\boxed{L_n = mvr_n = n\hbar} \qquad n = 1,2,3, \ldots\ldots$$

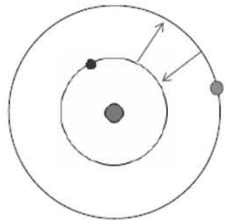
$$v = \frac{n\hbar}{mr_n}$$

$$F = \frac{mv^2}{r_n} = \frac{q^2}{4\pi\varepsilon_0 {r_n}^2}$$

$$r_n = \frac{4\pi\varepsilon_0 \, (n\hbar)^2}{mq^2}$$



Bohr Atom Cont'd



$$r_n = \frac{4\pi\varepsilon_0 (n\hbar)^2}{mq^2}$$

$$KE = \frac{1}{2}mv^2 = \frac{1}{2}\frac{q^2}{4\pi\varepsilon_0 r_n}$$

$$PE = -\frac{q^2}{4\pi\varepsilon_0 r_n}$$

$$E_{m,n} = const \times \left(\frac{1}{m^2} - \frac{1}{n^2}\right)$$

$$E_n = KE + PE = -\frac{1}{2}\frac{q^2}{4\pi\varepsilon_0 r_n} = -\frac{13.6}{n^2} \quad \text{eV}$$

Wave-Particle Duality

Photons act both as wave and particle, what about electrons ?

Remember
$E = mc^2$?

$$E = \sqrt{m_0^2 c^4 + p^2 c^2}$$

$$hf = pc$$

m_0=0 (photon rest mass)

$$\begin{aligned} p &= hf / c \\ &= h / \lambda \quad \text{(because } c = \lambda f\text{)} \\ &= \hbar k \quad \text{(because } k = 2\pi / \lambda\text{)} \end{aligned}$$

Wave vector and momentum are connected!

Schrodinger Equation for Electrons

$$E = \sqrt{{m_0}^2c^4 + p^2c^2} \approx m_0c^2\left[1 + p^2c^2/2{m_0}^2c^4 + \ldots\right]$$

$$E - m_0c^2 \;=\; V \;+\; (p^2/2m_0)$$

$$hf = \hbar\omega \;=\; V \;+\; (\hbar^2k^2/2m_0)$$

Schrodinger Equation (cont'd)

$$\hbar\omega \;=\; (\hbar^2k^2/2m_0) + V$$

Assume, $\Psi(x,t) = A\exp(-i(\omega t - kx))$

$$d\Psi/dt = -i\omega\Psi \quad \text{and} \quad d^2\Psi/dx^2 = -k^2\Psi$$

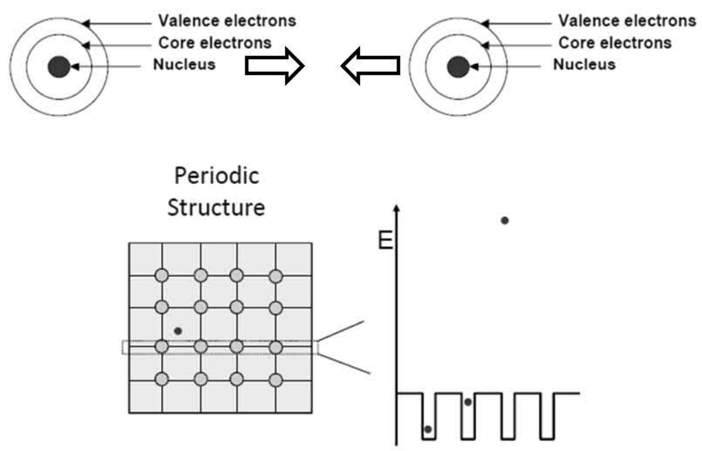
$$i\hbar\frac{d\Psi}{dt} = \left(-\frac{\hbar^2}{2m_0}\frac{d^2\Psi}{dx^2}\right) + V\Psi$$

This is the Schrodinger Equation electrons for one-dimensional problems.

What have we learned so far?

- Classical theory is not consistent with experimental observation. That's the origin of quantum mechanics
- We saw how Schrodinger equation can arise as a consequence of quantization and relativity, *but this is not a derivation.*

Solution of Schrodinger's Equation



Time-independent Shrodinger's Equation

Assume

$$-\frac{\hbar^2}{2m_0}\frac{d^2\Psi}{dx^2}+U(x)\Psi=i\hbar\frac{d\Psi}{dt} \qquad \Psi(x,t)=\psi(x)\,e^{-iEt/\hbar}$$

$$-e^{-\frac{iEt}{\hbar}}\frac{\hbar^2}{2m_0}\frac{d^2\psi(x)}{dx^2}+e^{-\frac{iEt}{\hbar}}U(x)\psi(x)=i\hbar\frac{-iE}{\hbar}\psi(x)e^{-\frac{iEt}{\hbar}}$$

$$-\frac{\hbar^2}{2m_0}\frac{d^2\psi}{dx^2}+U(x)\psi=E\psi$$

$$\frac{d^2\psi}{dx^2}+\frac{2m_0}{\hbar^2}(E-U)\psi=0$$

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Time-independent Schrodinger's Equation

$$\frac{d^2\psi}{dx^2}+\frac{2m_0}{\hbar^2}(E-U)\psi=0$$

If E >U, then ....

$$k\equiv\frac{\sqrt{2m_0[E-U]}}{\hbar} \qquad \frac{d^2\psi}{dx^2}+k^2\psi=0 \qquad \psi(x)=A\sin(kx)+B\cos(kx)$$
$$\equiv A_+e^{ikx}+A_-e^{-ikx}$$

If U>E, then ....

$$\alpha\equiv\frac{\sqrt{2m_0[U-E]}}{\hbar} \qquad \frac{d^2\psi}{dx^2}-\alpha^2\psi=0 \qquad \psi(x)=De^{-\alpha x}+Ee^{+\alpha x}$$

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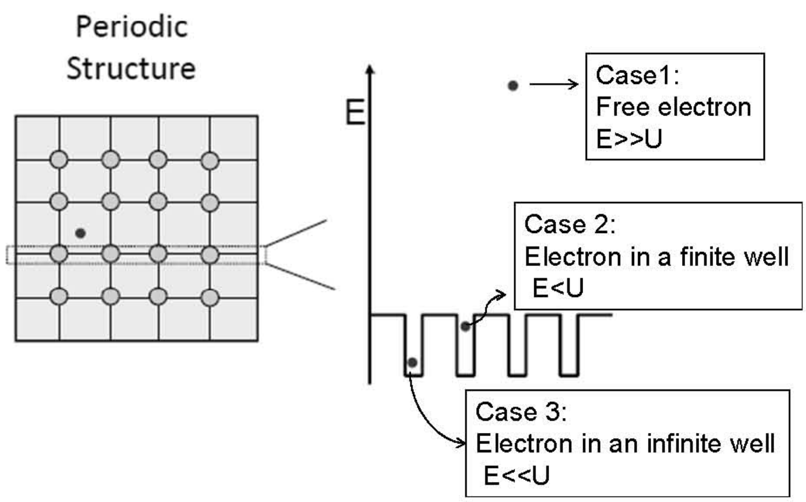
Basic Steps to Solve the Equation

$$-\frac{\hbar^2}{2m_0}\frac{d^2\psi}{dx^2}+U(x)\psi=E\psi$$

- Obtain U(x) and the boundary conditions for a given problem.
- Solve the 2[nd] order equation – pretty basic
- Interpret $|\psi|^2=\psi^*\psi$ as the probability of finding an electron at x
- Compute anything else you need, e.g.,

$$p=\int_0^\infty \Psi^*\left[\frac{\hbar}{i}\frac{d}{dx}\right]\Psi\,dx \qquad E=\int_0^\infty \Psi^*\left[-\frac{\hbar}{i}\frac{d}{dt}\right]\Psi\,dx$$

Solution of Schrodinger's Equation



Five Steps to Solve this Problem

1) $\frac{d^2\psi}{dx^2} + k^2\psi = 0$ ⟶ 2N unknowns for N regions

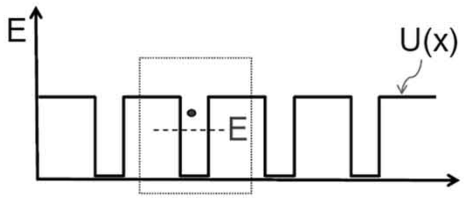
2) $\psi(x = -\infty) = 0$, $\psi(x = +\infty) = 0$ ⟶ Reduces 2 unknowns

3) $\psi\big|_{x=x_B^-} = \psi\big|_{x=x_B^+}$, $\left.\frac{d\psi}{dx}\right|_{x=x_B^-} = \left.\frac{d\psi}{dx}\right|_{x=x_B^+}$ ⟶ Set 2N-2 equations for 2N-2 unknowns (for continuous U)

4) Det (coefficient matrix)=0
And find E by graphical or numerical solution

5) $\int_{-\infty}^{\infty} |\psi(x,E)|^2 \, dx = 1$
for wave function

Case 1: Bounded Levels in a Finite Well

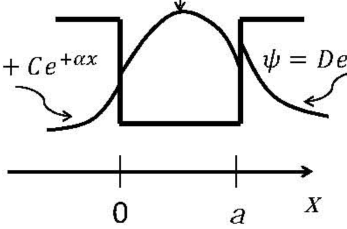


$\psi = A\sin kx + B\cos kx$

Step 1:

$\psi = \cancel{M}e^{-\alpha x} + Ce^{+\alpha x}$

$\psi = De^{-\alpha x} + \cancel{N}e^{+\alpha x}$



Step 2:
Boundary Condition

$\psi(x = -\infty) = 0$

$\psi(x = +\infty) = 0$

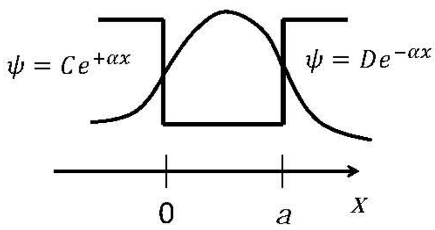
Continuity of Wavefunction

3) $\psi\big|_{x=x_B^-} = \psi\big|_{x=x_B^+}$

$$\left.\frac{d\psi}{dx}\right|_{x=x_B^-} = \left.\frac{d\psi}{dx}\right|_{x=x_B^+} \Rightarrow$$

$$C = B$$
$$\alpha C = -kA$$
$$A\sin(ka) + B\cos(ka) = De^{-\alpha a}$$
$$kA\cos(ka) - kB\sin(ka) = -\alpha De^{-\alpha a}$$

$\psi = A\sin kx + B\cos kx$



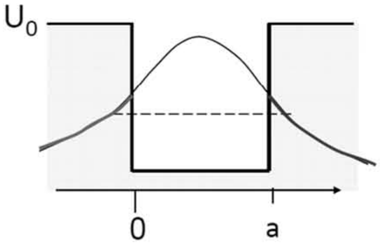
Continuity of Wavefunction

$$C = B$$
$$\alpha C = -kA$$
$$A\sin(ka) + B\cos(ka) = De^{-\alpha a}$$
$$kA\cos(ka) - kB\sin(ka) = -\alpha De^{-\alpha a}$$
$$\Downarrow$$
$$\begin{pmatrix} 0 & 1 & -1 & 0 \\ k & 0 & \alpha & 0 \\ \sin(ka) & \cos(ka) & 0 & -e^{-\alpha a} \\ \cos(ka) & -\sin(ka) & 0 & \alpha e^{-\alpha a}/k \end{pmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Step 4: Bound-level in Finite Well

det (Matrix)=0

$$\tan(\alpha a\sqrt{\xi}) = \frac{2\sqrt{\xi(1-\xi)}}{2\xi - 1} \qquad \xi \equiv \frac{E}{U_0} \quad \alpha \equiv \sqrt{\frac{2mU_0}{\hbar^2}}$$



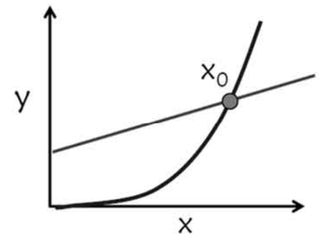
Only unknown is E

(i) Use Matlab function
(ii) Use graphical method

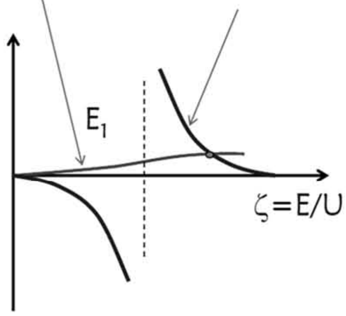
Graphical Method for Bound Levels

$$x^2 = x + 5$$

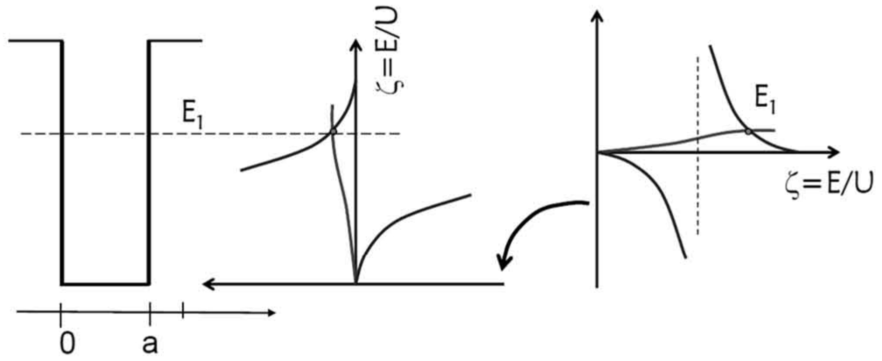
$$y_1 = x^2 \quad y_2 = x + 5$$



$$\tan(\alpha_0 a\sqrt{\xi}) = \frac{2\sqrt{\xi(1-\xi)}}{2\xi - 1}$$

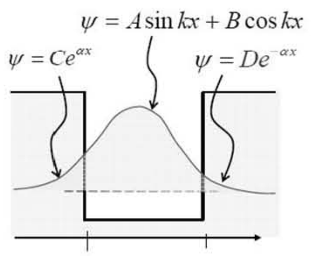


Graphical Method for Bound Levels



Wave Function

Step 5:



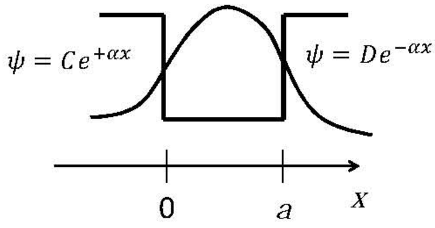
$$\begin{pmatrix} 0 & 1 & -1 & 0 \\ k & 0 & \alpha & 0 \\ \sin(ka) & \cos(ka) & 0 & e^{-\alpha a} \\ \cos(ka) & -\sin(ka) & 0 & -\alpha D e^{-\alpha a}/k \end{pmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{pmatrix} 1 & -1 & 0 \\ 0 & \alpha & 0 \\ \cos(ka) & 0 & e^{-\alpha a} \end{pmatrix} \begin{bmatrix} B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ -kA \\ -A\sin(ka) \end{bmatrix}$$

$$\begin{bmatrix} B \\ C \\ D \end{bmatrix} = \begin{pmatrix} 1 & -1 & 0 \\ 0 & \alpha & 0 \\ \cos(ka) & 0 & e^{-\alpha a} \end{pmatrix}^{-1} \begin{bmatrix} 0 \\ -kA \\ -A\sin(ka) \end{bmatrix}$$

Calculation of Wave Function

$$\psi = A\sin kx + B\cos kx$$



$$\begin{bmatrix} B \\ C \\ D \end{bmatrix} = \begin{pmatrix} 1 & -1 & 0 \\ 0 & \alpha & 0 \\ \cos(ka) & 0 & e^{-\alpha a} \end{pmatrix}^{-1} \begin{bmatrix} 0 \\ -kA \\ -A\sin(ka) \end{bmatrix}$$

$$\boxed{\begin{aligned} &\int_{-\infty}^{\infty} |\psi|^2 dx = 1 \quad \Rightarrow \\ &\int_{-\infty}^{0} C^2 e^{2\alpha x} dx + \int_0^a \left[A\,sin(kx) + B\,sin(kx)\right]^2 dx + \int_a^{\infty} D^2 e^{-2\alpha x} dx \end{aligned}}$$

Infinite Quantum Well

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad k \equiv \frac{\sqrt{2m_0[E-U]}}{\hbar}$$

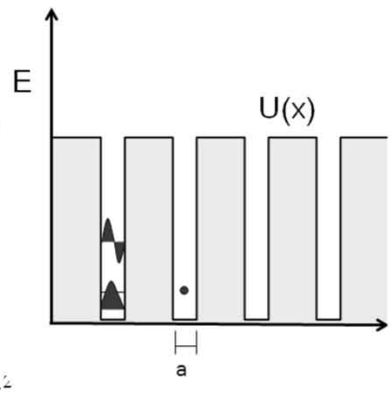
1) Solutions: $\psi = A\sin kx + B\cos(kx)$

2) Boundary conditions

$$\psi(x=0) = 0 = A\,sin\,k(0) + B\,cos\,k(0)$$

$$\psi(x=a) = 0 = A\,sin(ka) = A\,sin(n\pi)$$

$$k_n = \frac{n\pi}{a} = \frac{\sqrt{2m_0 E_n}}{\hbar} \qquad E_n = \frac{\hbar^2 n^2 \pi^2}{2m_0 a^2}$$



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4) Det (coefficient matrix)=0
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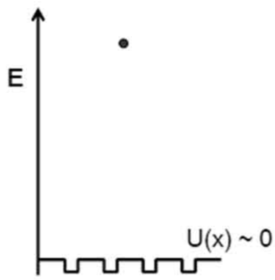
5) $$\int_{-\infty}^{\infty}\left|\psi(x,E)\right|^2 dx=1$$
for wave function

The Case of E >> U

$$\frac{d^2\psi}{dx^2}+k^2\psi=0 \qquad k\equiv\frac{\sqrt{2m_0\left[E-U\right]}}{\hbar}$$



1) Solution $$\psi(x)=A\sin(kx)+B\cos(kx)$$ $$\equiv A_+e^{ikx}+A\_e^{-ikx}$$

2) Boundary condition $\psi(x)=A_+e^{ikx}$ positive going wave

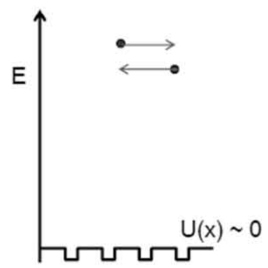
$=A\_e^{-ikx}$ negative going wave

Free Particle

$$\psi(x) = A\sin(kx) + B\cos(kx)$$
$$\equiv A_+ e^{ikx} + A_- e^{-ikx}$$

$\psi(x) = A_+ e^{ikx}$ positive going wave

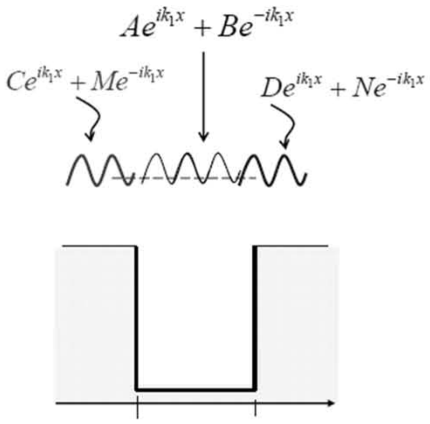
$= A_- e^{-ikx}$ negative going wave



Probability: $|\psi|^2 - \psi\psi^* - |A_+|^2 \; or \; |A_-|^2$

Momentum: $p = \int_0^{\infty} \Psi^* \left[\frac{\hbar}{i}\frac{d}{dx}\right] \Psi \, dx = \hbar k$ or $-\hbar k$

Bounded vs Tunneling State



Boundary conditions
N=0

5 unknowns (C,M,A,B,D)

4 equations from
x=0 and x=a interfaces

No bound levels

Ratios of D/C is of
Interest.