EEE6212 “Semiconductor Materials” -Quantum Mechanics

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Outline

- Purpose
- Time independent Schroedinger equation
- Infinite Well – derivations
- Application – approximating a semiconductor QW
- In-plane dispersion
- Summary

Purpose

- Quantum structures are at the heart of many (most?) semiconductor electronic or photonic devices
- Will discuss how the time independent Schroedinger equation is employed to solve the modes of an infinite quantum well
- Look at the application of this approximation to a semiconductor quantum well – see xls!
- Discuss the kinetic energy of carriers in-plane

Time Independent Schroedinger

- Wave mechanics analog to Hamilton's formulation in classical mechanics ….Time-independent potentials – self explanatory…
- KE and PE sum to total energy – eigenvalues of linear operators

$$\mathcal{T}\psi + \mathcal{V}\psi = E\psi$$

- Eigenfunction Ψ describes state of the system
- Operators-
  - T- kinetic energy
  - V- potential energy
  - E- total energy
  - p - linear momentum

$$\mathcal{T} = \frac{\mathcal{P}^2}{2m}$$

$$\mathcal{P} = -i\hbar\nabla = -i\hbar\left(\frac{\partial}{\partial x}\mathbf{i} + \frac{\partial}{\partial y}\mathbf{j} + \frac{\partial}{\partial z}\mathbf{k}\right)$$

TISE (2)

- Inserting more explicit form of T

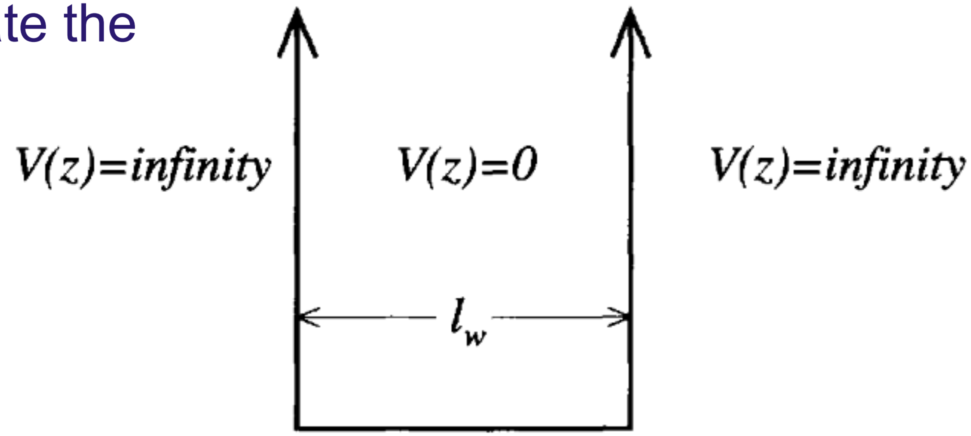
$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi+V(x,y,z)\psi=E\psi$$

- V(x,y,z) – potential energy of the system in spatial coordinates
- Restrict ourselves to 1D – 1D TISE for a particle of mass m is;-

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\psi(z)+V(z)\psi(z)=E\psi(z)$$

Infinite Well TISE

- Outside the well, V(z) =∞ , So Ψ (z)= 0 – wavefunction does not penetrate the barriers



- Inside the well, set datum level V(z) =0

- TISE simplifies to….

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\psi(z) = E\psi(z)$$

Infinite Well TISE (2)

- Need to remember maths for differential equations….
- This 2nd order DE implies that the solution for Ψ is a linear combination of functions f(z), which when differentiated twice, give –f(z)
- Let's try…. $\psi(z) = A\sin kz + B\cos kz$

➔ $$\frac{\hbar^2 k^2}{2m}\left(A\sin kz + B\cos kz\right) = E\left(A\sin kz + B\cos kz\right)$$

➔ $$\therefore \frac{\hbar^2 k^2}{2m} = E$$

Infinite Well TISE (3)

- Need to consider boundary conditions to determine the constant k

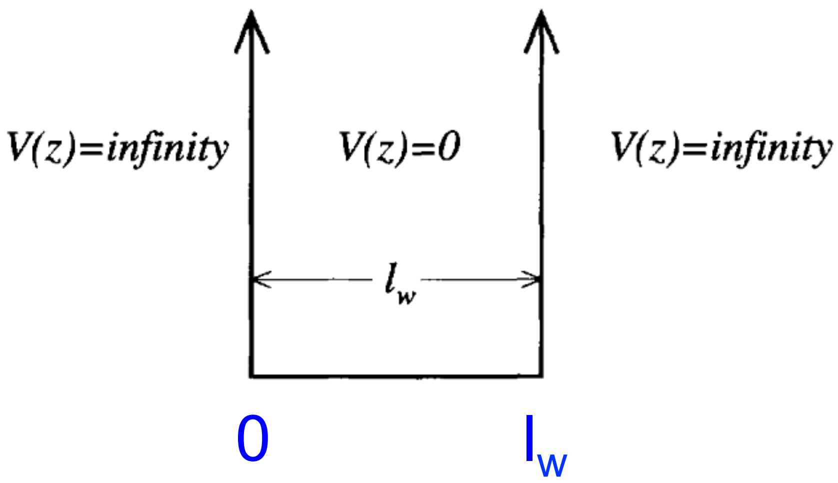
$$\mathcal{T} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\psi(z) \quad \rightarrow \quad \mathcal{T} = -\frac{\hbar^2}{2m}\frac{\partial}{\partial z}\left(\frac{\partial}{\partial z}\psi(z)\right)$$

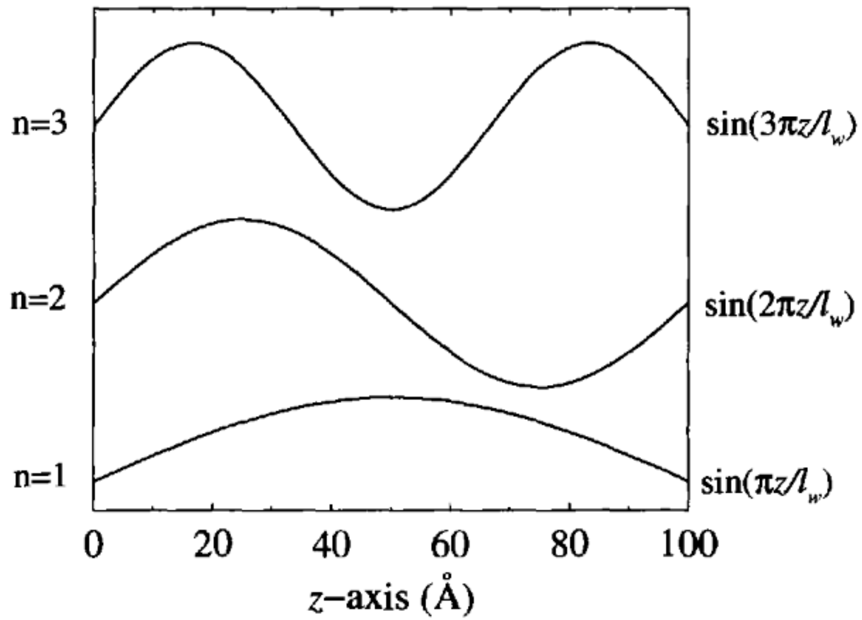
- Ψ(z) is continuous if we have finite values for KE (if not continuous dΨ/dz contains poles)

- Ψ(z) is continuous, and is zero in the barrier, so is zero at the edges of the well

Infinite Well TISE (4)

- Set origin as left hand edge of the well





$$\psi(z) = A\sin kz + \cancel{B\cos kz}$$

Infinite Well TISE (5)

- And $\Psi(0) = \Psi(l_w) = 0$, so $$k = \frac{\pi n}{l_w}$$
- Where n is an integer representing a series of solutions
- Substituting into $$\frac{\hbar^2 k^2}{2m} = E$$

$$\boxed{E_n = \frac{\hbar^2 \pi^2 n^2}{2m l_w^2}}$$

Infinite Well TISE (5)

- Last step is to determine A coefficient in $\psi(z) = A\sin kz.$

- Particle is confined to the well so $\int_0^{l_w} \psi^*(z)\psi(z)\ \mathrm{d}z = 1$

- Which gives

$$A = \sqrt{(2/l_w)}$$

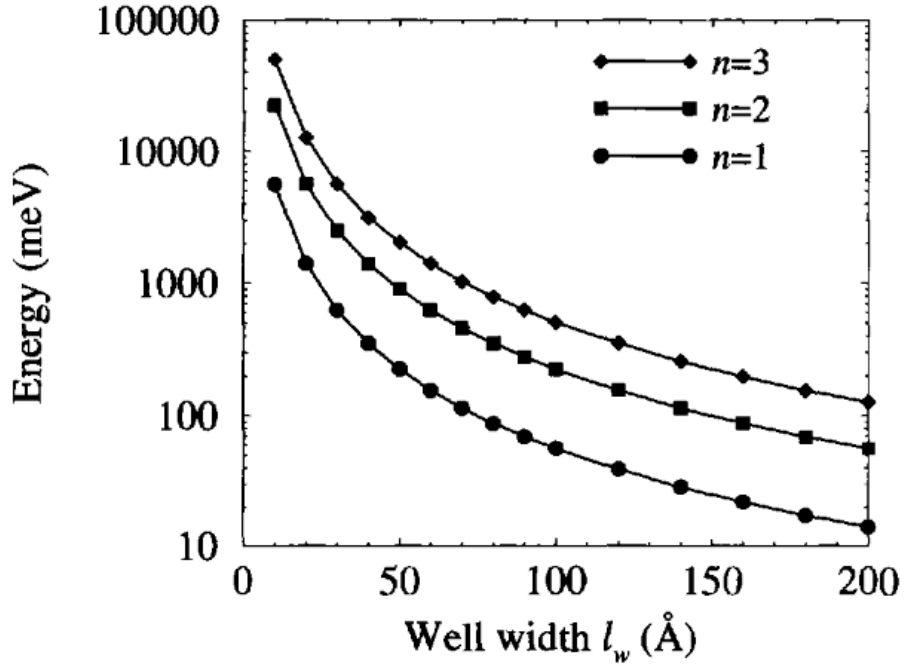
$$\boxed{\psi_n(z) = \sqrt{\frac{2}{l_w}}\sin\left(\frac{\pi n z}{l_w}\right)}$$

Effect of Various Parameters

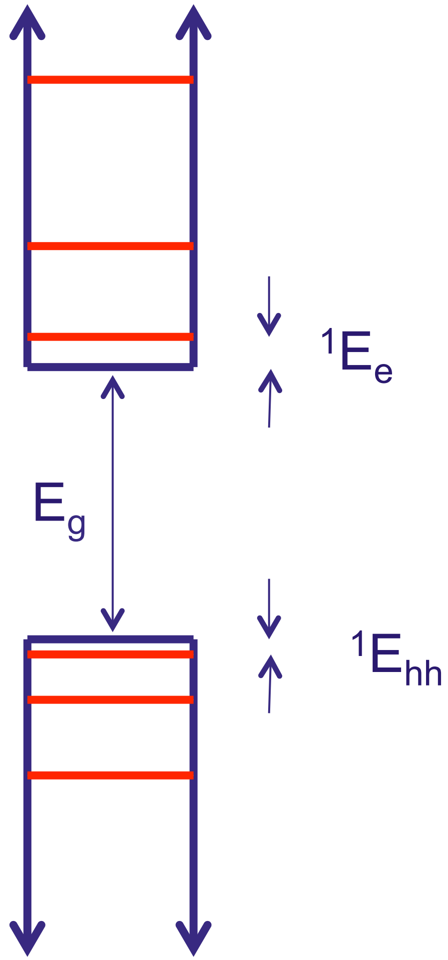
- Confinement energy $$E_n = \frac{\hbar^2 \pi^2 n^2}{2 m l_w^2}$$

- $m \uparrow \quad E_n \downarrow$
- $l_w \uparrow \quad E_n \downarrow\downarrow$
- $n \uparrow \quad E_n \uparrow\uparrow$

Example for electrons in infinite GaAs QW



Infinite QW - Approximation



- Consider a GaAs quantum well in an infinite barrier

- What is emission/ absorption energy of e1hh1 transition?

- E_g =1.42 eV
- m_e = 0.06 m*
- m_{hh} = 0.51 m*

In-plane Dispersion

- We have considered an infinite potential in z, how about the motion of the particle in x, y ? Need to consider all terms of KE operator-

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi + V(z)\psi = E\psi$$

- V(z) van be written as the sum of independent functions
V = V(x) + V(y) + V (z), so eigenfunction of the system can be written as product

$$\psi(x,y,z) = \psi_x(x)\psi_y(y)\psi_z(z)$$

- So -

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi_x}{\partial x^2}\psi_y\psi_z+\frac{\partial^2\psi_y}{\partial y^2}\psi_x\psi_z+\frac{\partial^2\psi_z}{\partial z^2}\psi_x\psi_y\right) + V(z)\psi_x\psi_y\psi_z = E\psi_x\psi_y\psi_z$$

In-Plane Dispersion (2)

- Three distnct contributions to Total Energy E in each of the orthogonal axes ; $E = E_x + E_y + E_z$

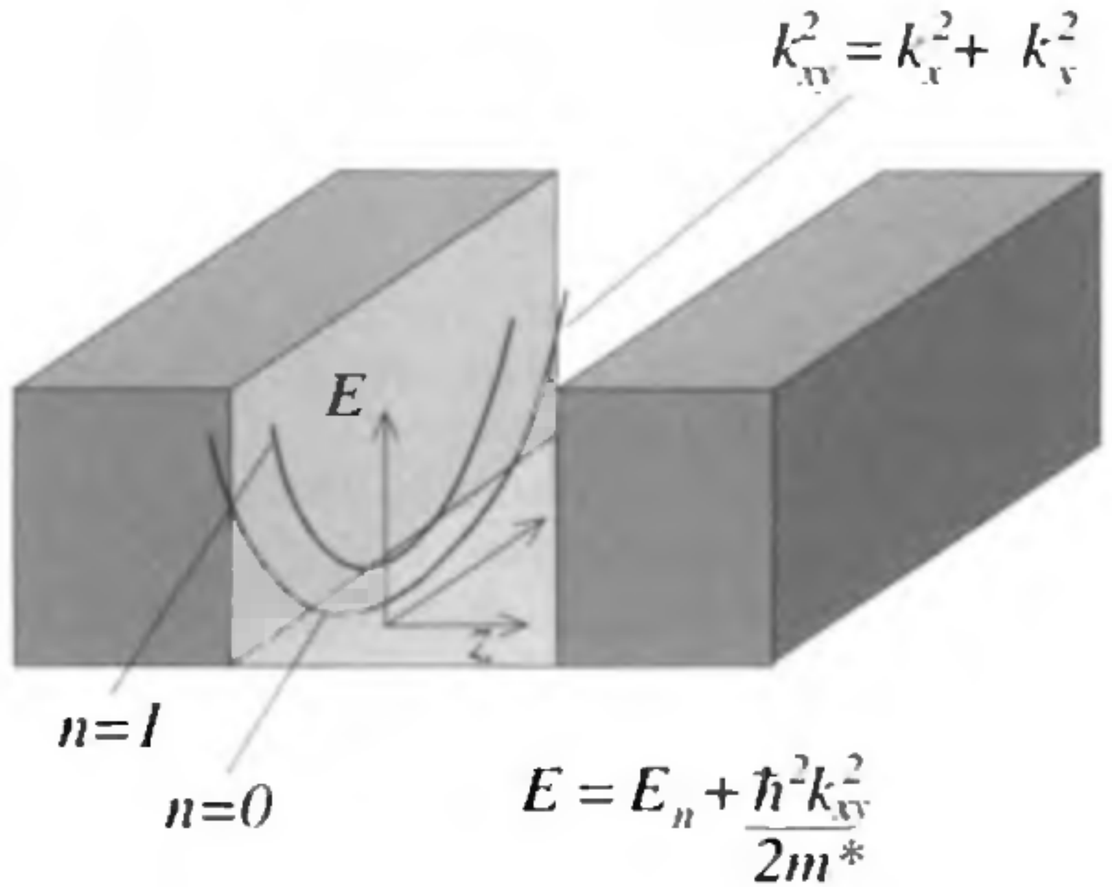
- The motion is decoupled – an equation of motion for each axis

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_x}{\partial x^2}\psi_y\psi_z = E_x\psi_x\psi_y\psi_z$$
$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_y}{\partial y^2}\psi_x\psi_z = E_y\psi_x\psi_y\psi_z$$
$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_z}{\partial z^2}\psi_x\psi_y + V(z)\psi_x\psi_y\psi_z = E_z\psi_x\psi_y\psi_z$$

$$\Rightarrow$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_x}{\partial x^2} = E_x\psi_x$$
$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_y}{\partial y^2} = E_y\psi_y$$
$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_z}{\partial z^2} + V(z)\psi_z = E_z\psi_z$$

In-Plane Dispersion (3)



Summary

- Introduced motivation to understand quantum structures
- Derived confinement energy and form of the wavefunction for particles in an infinite quantum well
- Applied this approximation to a semiconductor quantum well
- Noted how the transition energy/wavelength may be a strong function of well-width
- Seen how the motion (and hence KE) is decoupled in the three orthogonal axes

