SEMICONDUCTOR NANOSTRUCTURES

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Motivation

- How quantum effects govern properties of semiconductor nanostructures – specifically quantum dots
- Importance of effective mass of carriers in semiconductor quantum dots
- Lays base for further work on graded semiconductor heterostructures

Quantum Dots

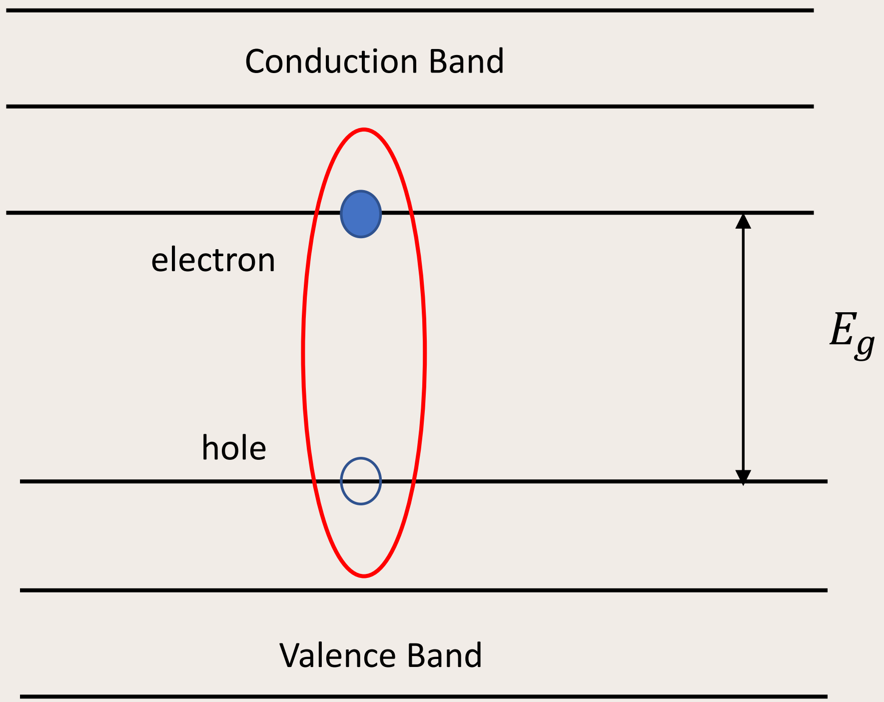
What are they?

- Spherically symmetric semiconductor particles of nanometre size
- Their small size necessitates the use of quantum mechanics to study their properties
- Exhibit luminescence – useful for opto-electronic devices

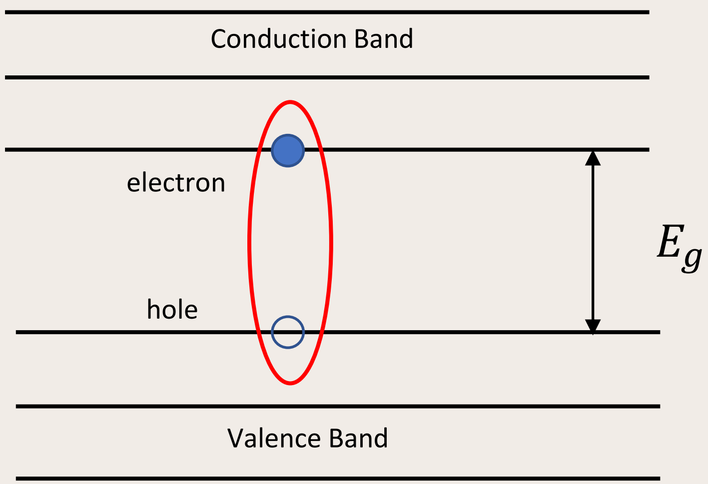
Quantum Dots

Quantum Confinement

- ➢Semiconductors have energy gap in their band structure
- ➢Electron in valence band can gain energy and jump to conduction band
- ➢Electron-hole pair is created



Small size of dots → confinement of e-h pair

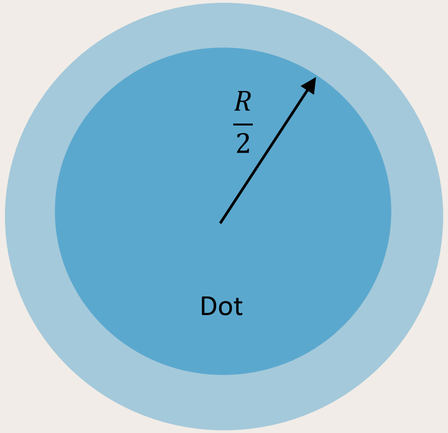


- Electron confined in spherically symmetric potential barrier
- Energy of confined electron is calculated using the particle in a box model.

$$E \propto \frac{1}{R^2}$$

Where R is diameter of the quantum dot

- Confinement causes enhancement of band gap



A Quantum Dot Model

- Simple Quantum Confinement model assumes –
  - Mass of carrier inside and outside the quantum dot are same
  - Potential barrier is infinite

In the paper,

Revisiting Quantum Mechanics with the BenDaniel-Duke boundary condition, the mass of carriers and finite barrier potential is considered.

Singh, V. A., & Kumar, L. (2006). Revisiting elementary quantum mechanics with the BenDaniel-Duke boundary condition. *American journal of physics*, *74*(5), 412-418.

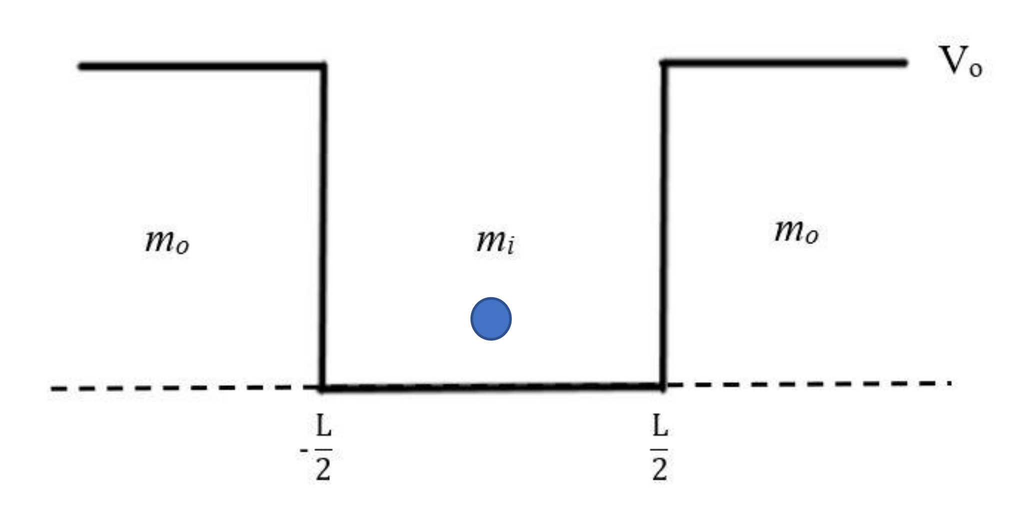
Mass Discontinuity

- Electron experiences a different mass in semiconductors

Mass inside the quantum dot = m_i

Mass outside the quantum dot = m_o

$$\beta = \frac{m_i}{m_o}$$



The Hamiltonian for position-dependent mass:

$$H = -\frac{\hbar^2}{2}\frac{d}{dx}\left(\frac{1}{m^*(x)}\frac{d}{dx}\right) + V(x)$$

Time Independent Schrodinger's Equation:

$$H\psi(x) = E\psi(x)$$

Example:
GaAs
$\beta = 0.067$

InAs
$\beta = 0.02$

Wavefunction:

For $|x| \leq \frac{L}{2}$

For even states,

$$\psi_n(x) = A_I \cos\left(k_{n,in}\, x\right)$$

For odd states,

$$\psi_n(x) = A_I \sin\left(k_{n,in}\, x\right)$$

For $|x| > \frac{L}{2}$

$$\psi_n(x) = B_I\, e^{-k_{n,out}\, x}$$

Wave vectors are,

$$k_{n,in} = \sqrt{\frac{2m_i E_n}{\hbar^2}}$$

$$k_{n,out} = \sqrt{\frac{2m_o(V_o - E_n)}{\hbar^2}}$$

Boundary Conditions

1. Wavefunctions must be continuous across boundary

2. Continuity of derivative of wavefunctions – BenDaniel-Duke boundary condition

$$\left.\frac{1}{m_i}\frac{d\psi(x)}{dx}\right|_{x\to\frac{L}{2}^-} = \left.\frac{1}{m_o}\frac{d\psi(x)}{dx}\right|_{x\to\frac{L}{2}^+}$$

On applying BC & some other manipulations,

$$-\beta k_{n,out} = k_{n,in}\cot\left(\frac{k_{n,in}L}{2}\right)$$

$$\beta k_{n,out} = k_{n,in}\tan\left(\frac{k_{n,in}L}{2}\right)$$

$$k_{n,in} = \sqrt{\frac{2m_i E_n}{\hbar^2}}$$

$$k_{n,out} = \sqrt{\frac{2m_o(V_o - E_n)}{\hbar^2}}$$

Asymptotic Analysis

Carried out to obtain an expression for E_n

For infinite barrier,

$$V_o \to \infty$$

$$\frac{k_{n,in}\,L}{2} = \frac{\pi}{2}$$

For a large but finite barrier,

$$\frac{k_{n,in}\,L}{2} = \frac{\pi}{2} - \epsilon$$

Small positive number

$$\boxed{E_n = \frac{C_1}{L^2} - \frac{C_2}{L^3} = \frac{C}{L^\alpha}\ (1 < \alpha < 2)}$$

- Confinement energy dependence is *weaker* than inverse quadratic behaviour
- Agrees with experimental results better than quantum confinement model where

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

Charge Density at Boundary

$$\text{charge density } \rho(x) = |\psi(x)|^2$$

$$\boxed{\rho\left(\frac{L}{2}\right) \propto \frac{1}{\beta^2}}$$

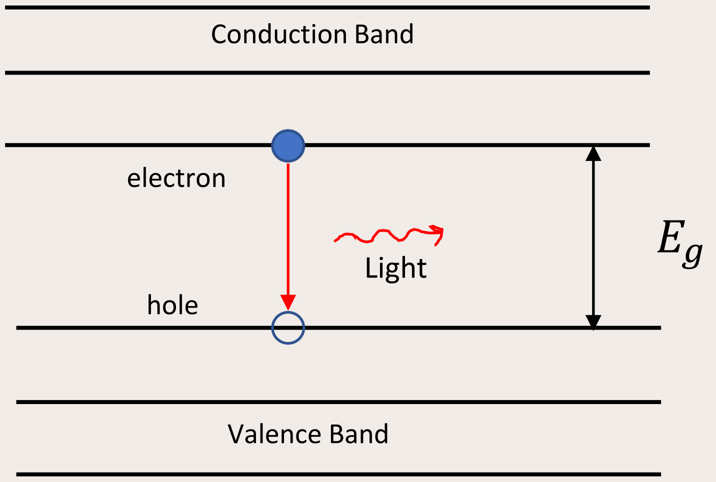
$$\beta = \frac{m_i}{m_o}$$

For $\beta < 1$ the charge density at boundary is non-zero

- Charge carriers at the boundary can exhibit surface-related effects
- In case of infinite barrier potential, $\rho\left(\frac{L}{2}\right)$ is 0
  - significance of surface effects is downplayed

Photoluminescence

- Porous Silicon exhibits photoluminescence
    - Due to nanostructures – quantum dots and wires
- Electrons in valence band get excited to conduction band
- Subsequently de-excite and emit light



$$\boxed{\hbar\omega = E_g + E_{confinement} - E_b}$$

E_b = exciton binding energy, E_g = band gap of semiconductor

Theory

$$\mathrm{E}_{\text{confinement}} = \Delta E = \frac{c}{d^2}$$

- Dot sizes have a Gaussian distribution about mean d_o

$$\Delta E_o = \frac{c}{d_o^2}$$

$$P(\Delta E) = \frac{1}{\sqrt{2\pi}\sigma}\frac{b}{2\Delta E}\left(\frac{\mathrm{c}}{\Delta E}\right)^2 \exp\left[-\frac{d_o^2}{2\sigma^2}\left[\left(\frac{\Delta E_o}{\Delta E}\right)^{\frac{1}{2}} - 2\right]^2\right]$$

PL Curve

- The peak of the PL curve is at a value of ΔE smaller than ΔE_o
    - Happens due to statistical distribution of dot sizes

John, G. C., Singh, V. A. (1994). Theory of the photoluminescence spectra of porous silicon. Physical Review B, 50(8), 5329.

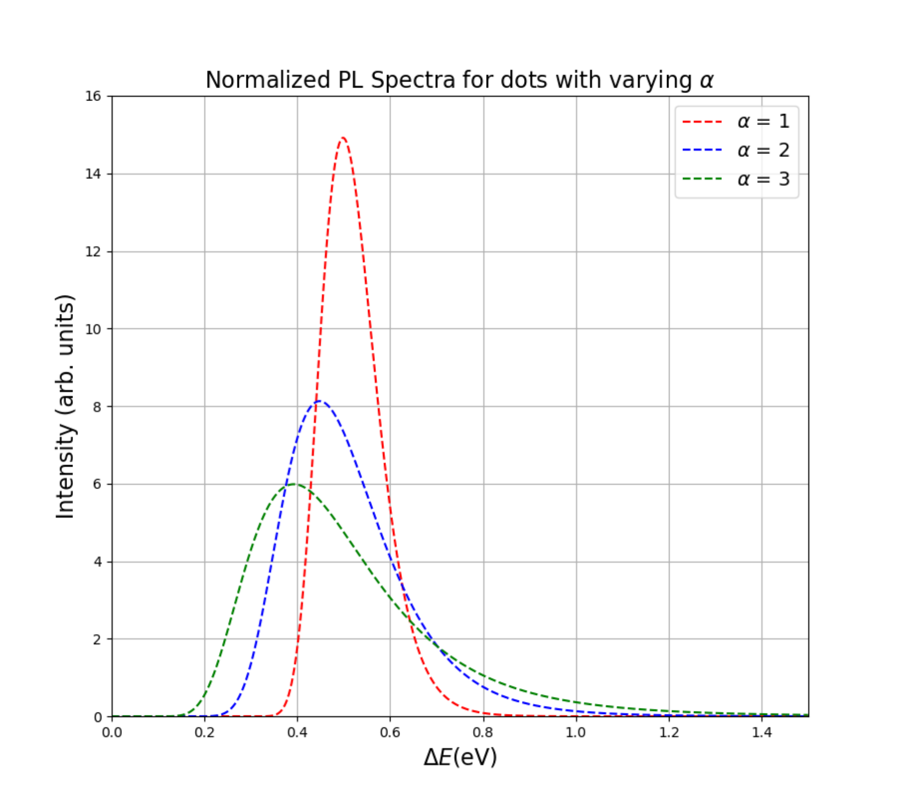
➢ Infra-quadratic energy upshift

$$\Delta E = \frac{c}{d^{\alpha}} \ (1 < \alpha < 2)$$

$$P(\Delta E) = \frac{1}{\sqrt{2\pi}\sigma} \frac{b}{\alpha \Delta E} \left(\frac{\mathrm{c}}{\Delta E}\right)^{\frac{4}{\alpha}} \exp\left[-\frac{d_o^2}{2\sigma^2} \left[\left(\frac{\Delta E_o}{\Delta E}\right)^{\frac{1}{\alpha}} - 2 \right]^2 \right]$$

For $\alpha < 2$

- ➢ At PL peak, ΔE is larger than that for $\alpha = 2$
- ➢ Width of the curve is smaller



Acknowledgement

This research project is supported by the National Initiative on Undergraduate Science (NIUS) undertaken by the Homi Bhabha Centre for Science Education (HBCSE-TIFR), Mumbai, India.

I am grateful to my project mentor Prof. Vijay A. Singh (UM-DAE CEBS, Mumbai) for his continued guidance and support.

THANK YOU

References

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