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Name of student

Roshni Sahoo

Institution

St. Xavier's College (Autonomous), Mumbai

E-mail

roshni.tulip@gmail.com

Phone Number

(+91) 9082172580

Permanent Address

B-202, Suvarnarekha, RBI Officer's Quarters, Dr. B.A. Road, Hindmata, Dadar(East), Mumbai - 400014

Name of Mentor

Prof. Vijay A. Singh

Affiliation

Centre for Excellence in Basic Sciences (UM-DAE CEBS), Mumbai

Name of the HBCSE Co-mentor

Dr. Praveen Pathak

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Date

Roshni Sahoo

Signature of NIUS Student

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Overview

Section 1 is an extension of the paper[1] titled 'Theory of photoluminescence spectra of porous silicon'by George C. John and Vijay A. Singh in which a theoretical formalism based on the quantum confinement model for explaining the photoluminescence spectra of porous silicon is described. The expressions for the photoluminescence spectra originating from the distribution of the dot and column sizes in the porous silicon is derived. Further, due to the presence of local inhomogeneities arising from regions having an excess concentration of either dots or columns, the edges of the photoluminescence spectrum is modelled using a methodology similar to the Lifshitz argument[2].

According to the quantum confinement model, the energy upshift of the electrons due to confinement is proportional to 1/d^2 where d is the diameter of the confinement. However, in this report, the confinement energy is proportional to 1/d$^\alpha$ where $1 < \alpha < 2$. This is justified in Section 2. The nature of the photoluminescence curve due to the distribution of dot sizes and how the maximum intensity of the photoluminescence scales with α is studied. There is a downshift in the confinement energy (as a result of the size distribution of dots) at the location of the PL peak from the mean confinement energy (as it had also been obtained for columns). This downshift in the confinement energy permits a smaller and physically realizable exciton binding energy. Further, we observe how this downshift varies with α. An approximate expression for the full width at half maximum for the photoluminescence spectrum is also derived and its variation with determined.

Section 2 focuses on the mass of charge carriers in different semiconducting materials and how that governs the electronic properties of quantum dots. When an electron from the valence band jumps into the conduction band an electron-hole pair is formed. This electron-hole pair experiences confinement due to the nanometre dimensions of the quantum dot. The dielectric coating of the quantum dot provides a large spherical potential barrier to the confined particle. This confined particle is then modelled using the particle in box model, where the energy of the particle is inversely proportional to d^2. This model, however, assumes two things – 1) the mass of the carrier is same inside and outside the dot and 2) the potential barrier is infinitely large. Both of these assumptions are not entirely correct as the charge carrier experiences a different mass inside and outside the quantum dot on account of different semiconducting materials.

Moreover, the barrier is finitely large.

Thus, in the paper[3] ‘Revisiting Quantum Mechanics with BenDaniel-Duke boundary condition, the varying mass of charge carriers and finite potential barrier is considered. As a result, the energy of the confined particle is not inversely proportional to d^2, rather it is inversely proportional to d^α where $1 < \alpha < 2$. This result agrees better with experiments than the simple QC model. Additionally, the charge density turns out to be non-zero at the boundary of the quantum dot which can exhibit surface-related effects. In case we consider an infinite barrier potential like in the simple QC model, this charge density would be zero thus downplaying said surface-related effects.

In section 3, the tunnelling of charged carriers through a graded semiconductor heterostructure is investigated. To begin with, the tunnelling of an alpha particle through a coulombic barrier potential is studied where the final expression for the tunnelling probability is determined using Gamow’s theory. This exercise then helps us derive the expression for the tunnelling probability of a charged carrier through a graded heterostructure where the mass of the charge carrier as well as the potential barrier varies linearly with distance. This probability is also calculated using numerical methods on a computer to check the validity of the expression obtained analytically.

1 Quantum Dots - Photoluminescence Spectra

Porous silicon is a disordered system consisting of an intricate network of crystallites of varying shapes and sizes. Porous silicon (PS) exhibits photoluminescence (PL) which can be explained by employing the quantum confinement model. According to this model, the confinement of electrons in the column- like and dot- like structures that are present in the porous silicon make it luminescent.

1.1 PL Spectra Derivation

The growth of dot-like structures in porous silicon (PS) is a stochastic process and hence we can assume that the diameter of these dots has a Gaussian distribution about some mean diameter d_o.

$$P_d = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(d-d_o)^2}{2\sigma^2}\right] \tag{1}$$

Thus, the number of electrons participating in the photoluminescence process is proportional to d^3 and hence,

$$N_e = N_e(d) = ad^3 \tag{2}$$

where a is a constant.

So we can say that the probability distribution of the electrons participating in the photoluminescence process in a given sample of porous silicon is given by the product of Equation (1) and Equation (2).

$$P_{ed} = \frac{1}{\sqrt{2\pi}\sigma} bd^3 \exp\left[-\frac{(d-d_o)^2}{2\sigma^2}\right] \tag{3}$$

where b is a suitable normalization constant.

Now, the energy upshift due to the confinement of the electrons is generalized and said to be proportional to $1/d^\alpha$.

The energy of the photoluminescence $\hbar\omega$ is,

$$\hbar\omega = E_g - E_b + \frac{c}{d^\alpha} \tag{4}$$

where E_g is the bulk silicon band gap and E_b is the exciton binding energy.

The energy upshift due to the confinement is then defined as,

$$\Delta E = \hbar\omega - (E_g - E_b) \tag{5}$$

At this point, we also introduce a mean upshift energy corresponding to the mean diameter of the dots,

$$\Delta E_o = \frac{c}{d_o^\alpha} \tag{6}$$

Now, we want to get the expression for the PL curve as a function of the energy upshift ΔE. To do so, we must first understand how to change the variable of a probability distribution function.

So, let X be a continuous random variable with probability distribution function f(x) and Y = s(X) is continuous decreasing function with inverse X = t(Y).
The cumulative probability distribution function is given by,

$$F_Y(y) = P(Y \leq y)$$

$$P(Y \leq y) = P(s(X) \leq y) = P(X \geq t(y))$$

Using Rule of Complementary events,

$$P(X \geq t(y)) = 1 - P(X \leq t(y))$$

Using the definition of Probability,

$$F_Y(y) = 1 - \int_c^{t(y)} f(x)\,dx$$

The derivative of the cumulative distribution function gives the probability distribution function $f_Y(y)$

$$f_Y(y) = F_Y'(y)$$

$$f_Y(y) = f(t(y)) \times |t'(y)| \tag{7}$$

Equation (7) allows us to change the variable of P_{ed} in Equation (3) from d to ΔE.

ΔE is a strictly decreasing function (since d is always positive).

From this we get,

$$d = \left(\frac{c}{\Delta E}\right)^{1/\alpha} = t(\Delta E) \tag{8}$$

$$t'(\Delta E) = -\frac{1}{\alpha}\frac{1}{\Delta E}\left(\frac{c}{\Delta E}\right)^{1/\alpha} \tag{9}$$

$$P_{ed}(t(\Delta E)) = \frac{b}{\sqrt{2\pi}\sigma}\left(\frac{c}{\Delta E}\right)^{3/\alpha} exp\left[-\frac{d_o^2}{2\sigma^2}\left[\left(\frac{\Delta E_o}{\Delta E}\right)^{1/\alpha} - 1\right]^2\right] \tag{10}$$

From Equation (7) we get,

$$P(\Delta E) = P_{ed}(t(\Delta E)) \times |t'(\Delta E)| \tag{11}$$

Substituting Equation (9) and Equation (10) in Equation (11) we get,

$$\boxed{P(\Delta E) = \frac{1}{\sqrt{2\pi}\sigma}\frac{b}{\alpha\Delta E}\left(\frac{c}{\Delta E}\right)^{4/\alpha} exp\left[-\frac{d_o^2}{2\sigma^2}\left[\left(\frac{\Delta E_o}{\Delta E}\right)^{1/\alpha} - 1\right]^2\right]} \tag{12}$$

This is the required expression for the PL curve of dots along the energy axis.

For small σ the PL line shape is approximately Gaussian. However, for significant value of σ, the $(1/\Delta E)^{1/\alpha}$ factor in the exponential outweighs the polynomial dependence in the pre-factor resulting in an asymmetrical curve with a shoulder on the high-energy side. Furthermore, this term in the exponential is also responsible for the decrease in the maximum value of the PL as α increases. This is clearly seen in the plots for $P(\Delta E)$ given in Section 1.4.

Now, just to check if our generalized expression for the PL spectra for any value of α agrees with the one given in the paper for $\alpha = 2$. Substitute $\alpha = 2$ in Equation (12)

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

This is the same as expression (2.10) given in the paper *"Theory of the photoluminescence spectra of porous silicon"*.

Now, we move on to derive an expression for the energy upshift due to confinement at the peak of the PL curve, i.e. ΔE_p. This is where we observe the downshift that we mentioned in Section .

1.2 Confinement energy at PL spectra peak

The energy upshift due to confinement ΔE at the peak of the PL spectra is termed as ΔE_p. Before we begin the derivation for ΔE_p, let us restate the expression for the PL spectra due to dots.

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

To find the peak ΔE_p, we must differentiate the above equation and equate it to 0.

For simplicity, re-write the above equation as,

$$P(\Delta E) = k\Delta E^{-(4+\alpha)/\alpha}\exp\left[-aF(\Delta E)\right]$$

where,

$$k = \frac{bc^{4/\alpha}}{\sqrt{2\pi}\sigma\alpha}, a = \frac{1}{2}\left[\frac{d_o}{\sigma}\right]^2, F(\Delta E) = \left[\left(\frac{\Delta E_o}{\Delta E}\right)^{1/\alpha} - 1\right]^2$$

$$P'(\Delta E) = 0$$

$$P'(\Delta E) = -(4+\alpha)(\Delta E)^{-(4+2\alpha)/\alpha} + 2a(\Delta E_o)^{2/\alpha}(\Delta E)^{-(2\alpha+6)/\alpha} - 2a(\Delta E_o)^{1/\alpha}(\Delta E)^{-(2\alpha+5)/\alpha} = 0$$

Taking $\Delta E^{-(2\alpha+6)/\alpha}$ common and dividing both sides by the same (Since $\Delta E \neq 0$), we get,

$$-(4+\alpha)(\Delta E)^{2/\alpha} + 2a(\Delta E_o)^{2/\alpha} - 2a(\Delta E_o\Delta E)^{1/\alpha} = 0$$

$$\Rightarrow -(4+\alpha)(\Delta E_p)^{2/\alpha} + (\Delta E_o)^{2/\alpha}\left(\frac{d_o}{\sigma}\right)^2 - \left(\frac{d_o}{\sigma}\right)^2(\Delta E_o\Delta E_p)^{1/\alpha} = 0$$

Dividing both sides by $(\Delta E_o)^{2/\alpha}$

$$-(4+\alpha)\left(\frac{\Delta E_p}{\Delta E_o}\right)^{2/\alpha}+\left(\frac{d_o}{\sigma}\right)^2-\left(\frac{d_o}{\sigma}\right)^2\left(\frac{\Delta E_p}{\Delta E_o}\right)^{1/\alpha}=0$$

let $t=\left(\frac{\Delta E_p}{\Delta E_o}\right)^{1/\alpha}$

$$(4+\alpha)t^2+\left(\frac{d_o}{\sigma}\right)^2 t-\left(\frac{d_o}{\sigma}\right)^2=0$$

Solving for t using the quadratic formula we get,

$$t=\left(\frac{\Delta E_p}{\Delta E_o}\right)^{1/\alpha}=\frac{1}{2(4+\alpha)}\left[-\left(\frac{d_o}{\sigma}\right)^2\pm\sqrt{\left(\frac{d_o}{\sigma}\right)^4+4(4+\alpha)\left(\frac{d_o}{\sigma}\right)^2}\right]$$

Since t cannot be negative,

$$\left(\frac{\Delta E_p}{\Delta E_o}\right)^{1/\alpha}=\left\{\frac{1}{2(4+\alpha)}\left(\frac{d_o}{\sigma}\right)\left[-\frac{d_o}{\sigma}+\left[\left(\frac{d_o}{\sigma}\right)^2+4(4+\alpha)\right]^{\frac{1}{2}}\right\}$$

Therefore,

$$\boxed{\Delta E_p=\Delta E_o\left\{\frac{1}{2(4+\alpha)}\left(\frac{d_o}{\sigma}\right)\left[-\frac{d_o}{\sigma}+\left[\left(\frac{d_o}{\sigma}\right)^2+4(4+\alpha)\right]^{\frac{1}{2}}\right\}^{\alpha}} \tag{13}$$

This is the value of ΔE_p where $P(\Delta E)$ is maximum.

For $\alpha=2$

$$\Delta E_p=\Delta E_o\left\{\frac{1}{2(4+2)}\left(\frac{d_o}{\sigma}\right)\left[-\frac{d_o}{\sigma}+\left[\left(\frac{d_o}{\sigma}\right)^2+4(4+2)\right]^{\frac{1}{2}}\right\}^{2}$$

$$\boxed{\Delta E_p=\Delta E_o\left\{\frac{1}{12}\left(\frac{d_o}{\sigma}\right)\left[-\frac{d_o}{\sigma}+\left[\left(\frac{d_o}{\sigma}\right)^2+24\right]^{\frac{1}{2}}\right\}^{2}}$$

Now, we make some approximations to get an expression for ΔE_p when the mean diameter of dots d_o is appreciably greater than the variance of the distribution of the diameters σ. Mathematically, this means:

$$\frac{\sigma}{d_o} \longrightarrow 0$$

To begin deriving our approximate expression for ΔE_p, consider these terms from the expression given in Equation (13)

$$\left[\left(\frac{d_o}{\sigma}\right)^2 + 4(4+\alpha)\right]^{1/2}$$
$$\Rightarrow \left(\frac{d_o}{\sigma}\right)\left[1 + 4(4+\alpha)\left(\frac{\sigma}{d_o}\right)^2\right]^{1/2}$$

Using Binomial approximation for $\frac{\sigma}{d_o} \to 0$, the above expression is approximately

$$\approx \left(\frac{d_o}{\sigma}\right)\left[1 + 2(4+\alpha)\left(\frac{\sigma}{d_o}\right)^2\right]$$

Substituting this expression back to Equation (13) for ΔE_p, we get,

$$\boxed{\Delta E_p = \Delta E_o}$$

So, when $\frac{\sigma}{d_o}$ is very small, the confinement energy at the peak is almost equal to confinement energy corresponding to the mean diameter.

However, this may not always be true and we must derive an expression for when $\frac{\sigma}{d_o}$ is considerable (but still small).

Consider again these terms from Equation (13) and expand it using Taylor series,

$$\left[\left(\frac{d_o}{\sigma}\right)^2 + 4(4+\alpha)\right]^{1/2}$$

to get

$$\approx \left(\frac{d_o}{\sigma}\right)\left[1 + 2(4+\alpha)\left(\frac{\sigma}{d_o}\right)^2 - \frac{1}{2}\frac{1}{2}\frac{1}{2!}[4(4+\alpha)]^2\left(\frac{\sigma}{d_o}\right)^4\right]$$

$$\approx \left(\frac{d_o}{\sigma}\right)\left[1 + 2(4+\alpha)\left(\frac{\sigma}{d_o}\right)^2 - 2(4+\alpha)^2\left(\frac{\sigma}{d_o}\right)^4\right]$$

Substituting the above expression back into Equation for ΔE_p, we get,

$$\Delta E_p = \Delta E_o\left[\frac{1}{2(4+\alpha)}\left(\frac{d_o}{\sigma}\right)\left\{2(4+\alpha)\frac{\sigma}{d_o} - 2(4+\alpha)^2\left(\frac{\sigma}{d_o}\right)^3\right]^\alpha$$

$$= \Delta E_o\left[1 - (4+\alpha)\left(\frac{\sigma}{d_o}\right)^2\right]^\alpha$$

$$\boxed{\Delta E_p = \Delta E_o\left[1 - \alpha(4+\alpha)\left(\frac{\sigma}{d_o}\right)^2\right]} \tag{14}$$

Now this is the expression for ΔE_p when $\frac{\sigma}{d_o}$ is appreciable and we can clearly see that it is less than ΔE_o. This is known as the downshift wherein the confinement energy at the PL peak is smaller than the confinement energy at mean diameter d_o.

This downshift increases with increasing α and this can be demonstrated as follows,

Let $d_o = 30\,\text{Å}$,

$\sigma = 4\,\text{Å}$

for $\alpha = 1$,

$$\Delta E_p = \Delta E_o\left\{\frac{1}{10}\left(\frac{30}{4}\right)\left[-\frac{30}{4} + \left[\left(\frac{30}{4}\right)^2 + 20\right]^{1/2}\right\}^1$$

$$\Delta E_p = 0.498\,eV$$

for $\alpha = 2$,

$$\Delta E_p = \Delta E_o\left\{\frac{1}{12}\left(\frac{30}{4}\right)\left[-\frac{30}{4} + \left[\left(\frac{30}{4}\right)^2 + 24\right]^{1/2}\right\}^2$$

$$\Delta E_p = 0.448\,eV$$

for $\alpha = 3$,

$$\Delta E_p = \Delta E_o \left\{ \frac{1}{14} \left(\frac{30}{4} \right) \left[-\frac{30}{4} + \left[\left(\frac{30}{4} \right)^2 + 28 \right]^{1/2} \right\}^3$$

$$\Delta E_p = 0.393\, eV$$

Thus, E_p is becoming smaller and smaller as α is increasing which means it's moving farther away from E_o indicating an increase in the downshift.

1.3 Full width at half maximum of PL curve

The full width at half maximum or FWHM can be approximated by ignoring the pre-factor in the expression for the PL curve. In doing so we get,

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

As it is a decreasing exponential function, the maximum value is the constant term c

$$P(\Delta E)_{max} = c$$

The FWHM is the width of the curve at half its maximum value.

$$\frac{P(\Delta E)_{max}}{2} = P(\Delta E)$$

$$\frac{c}{2} = c \exp \left\{ -\frac{1}{2} \left(\frac{d_o}{\sigma} \right)^2 \left[\left(\frac{\Delta E_o}{\Delta E} \right)^{1/\alpha} - 1 \right]^2 \right\}$$

$$\exp(-\ln 2) = \exp \left\{ -\frac{1}{2} \left(\frac{d_o}{\sigma} \right)^2 \left[\left(\frac{\Delta E_o}{\Delta E} \right)^{1/\alpha} - 1 \right]^2 \right\}$$

$$2\ln 2 = \left(\frac{d_o}{\sigma}\right)^2 \left[\left(\frac{\Delta E_o}{\Delta E}\right)^{1/\alpha} - 1\right]^2$$

$$\left(\frac{\Delta E_o}{\Delta E}\right)^{1/\alpha} = 1 \pm \frac{\sigma}{d_o}\sqrt{2\ln 2}$$

$$\frac{\Delta E}{\Delta E_o} = \left(1 \pm \frac{\sigma}{d_o}\right)^{-\alpha}$$

$$\boxed{\Delta E_{FWHM} = \Delta E_o \left[\left(1 - \frac{\sigma}{d_o}\right)^{-\alpha} - \left(1 + \frac{\sigma}{d_o}\right)^{-\alpha}\right]}$$

This is the expression for the FWHM of the PL spectra due to dots.

Now, consider small $\frac{\sigma}{d_o}$

$$\Delta E_{FWHM} = \Delta E_o \left\{ \frac{\left(1 + \frac{\sigma}{d_o}\right)^{\alpha} - \left(1 - \frac{\sigma}{d_o}\right)^{\alpha}}{\left[\left(1 + \frac{\sigma}{d_o}\right)\left(1 - \frac{\sigma}{d_o}\right)\right]^{\alpha}} \right\}$$

$$\Delta E_{FWHM} \approx \Delta E_o \left\{ \frac{1 + \alpha\frac{\sigma}{d_o} - 1 + \alpha\frac{\sigma}{d_o}}{\left[1 - \left(\frac{\sigma}{d_o}\right)^2\right]^{\alpha}} \right\}$$

$$\Delta E_{FWHM} \approx \Delta E_o \left\{ \frac{2\alpha\frac{\sigma}{d_o}}{\left[1 - \alpha\left(\frac{\sigma}{d_o}\right)^2\right]} \right\}$$

$$\Delta E_{FWHM} \approx \frac{2\alpha\Delta E_o(d_o/\sigma)}{\left[\left(\frac{d_o}{\sigma}\right)^2 - \alpha\right]} \approx \frac{2\alpha\Delta E_o\sigma}{d_o} \tag{15}$$

FWHM can also be obtained using a different method,

$$\Delta E_{FWHM} = 2|\delta(\Delta E)|_{d=d_o}$$

$$\Delta E_{FWHM} = \frac{2\alpha c\delta d}{(d_o)^{\alpha+1}}$$

$$\Delta E_{FWHM} \approx \frac{2\alpha\Delta E_o\sigma}{d_o}$$

In the above equation, the denominator decreases as α increases and the numerator increases as α increases, thus overall ΔE_{FWHM} increases as α increases and results in a broader shape. This is demonstrated with some calculations as well as in the plots for $P(\Delta E)$ in Section 1.4.

**Note that, the formula for FWHM which is obtained by ignoring the pre-factor is the same as that for columns.*

The variation for FWHM with α is demonstrated as follows,

$d_o = 30$ Å

$\sigma = 4$ Å

For $\alpha = 1$,

$$\Delta E_{FWHM} \approx \frac{2 \times 0.539 \times (7.5)}{\left[(7.5)^2 - 1\right]}$$

$$\Delta E_{FWHM} \approx 146\ meV$$

For $\alpha = 2$,

$$\Delta E_{FWHM} \approx \frac{4 \times 0.539 \times (7.5)}{\left[(7.5)^2 - 2\right]}$$

$$\Delta E_{FWHM} \approx 298\ meV$$

For $\alpha = 3$,

$$\Delta E_{FWHM} \approx \frac{6 \times 0.539 \times (7.5)}{\left[(7.5)^2 - 3\right]}$$

$$\Delta E_{FWHM} \approx 455 \; meV$$

As expected, the FWHM of the PL curve increases with increasing α.

1.4 Plots of the PL spectra

Now, we plot the PL spectra due to dots for $\alpha = 1, 2, 3$.

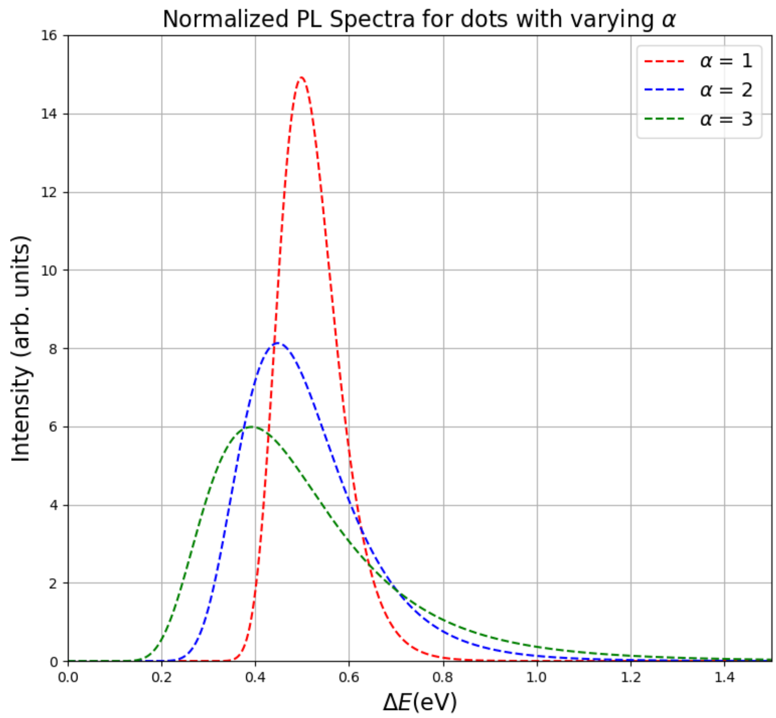


Figure 1: Theoretical PL spectra (normalized) due to dots using different quantum confinement models. Red dashed line is for $\alpha = 1$ (peak at 0.498 eV). Blue dashed line is for $\alpha = 2$ (peak at 0.448 eV). Green dashed line is for $\alpha = 3$ (peak at 0.393 eV)

In Fig. 1 we can clearly observe what we have been claiming about the trends of the confinement energy at the peak ΔE_p and the FWHM ΔE_{FWHM} in Section 1.2 and Section 1.3. We can see that with increasing α, the ΔE_p of the the PL curve shifts further away from the mean upshift ΔE_o. Similarly, the width of the peak also increases with increasing α.

2 Quantum Mechanics with BenDaniel- Duke boundary condition

Generalizing the Asymptotic Analysis from the paper titled 'Revisiting Elementary quantum mechanics with the BenDaniel-Duke boundary condition' by Vijay A. Singh and Luv Kumar.

2.1 The Square Well Potential

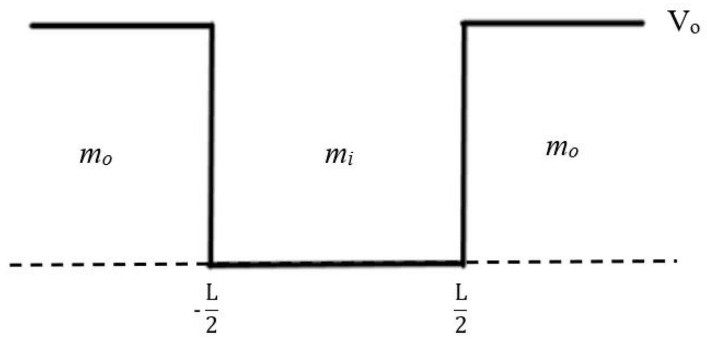


Figure 2: Square Well

The potential function is written as,

$$V = \begin{cases} V_o & \text{if } |x| > \frac{L}{2}, \\ 0 & \text{if } |x| \leq \frac{L}{2}, \end{cases}$$

In this paper, the effective mass of the electron inside the well is m_i and the mass outside the well is m_o.

The Time Independent Schrodinger Equation in such a case is given by,

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

Solving for the above differential equation, we get two types of solutions - odd and even.

Even Solutions.

$$\Psi_n(x) = \begin{cases} A_I \cos(k_{n,in}x) & \text{if } |x| \leq \frac{L}{2}, \\ B_I e^{-k_{n,out}|x|} & \text{if } |x| > \frac{L}{2}, \end{cases}$$

Odd Solutions.

$$\Psi_n(x) = \begin{cases} A_I \sin(k_{n,in}x) & \text{if } |x| \leq \frac{L}{2}, \\ B_I e^{-k_{n,out}|x|} & \text{if } |x| > \frac{L}{2}, \end{cases}$$

The wave vectors are:

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

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

There are 2 boundary conditions for the wavefunctions of a particle in a square well potential:

1. The wavefunctions are continuous across the boundaries of the well at $\pm\frac{L}{2}$
2. The continuity of the derivative of the wavefunctions is given by the BenDaniel- Duke boundary condition.

Applying these two boundary conditions to the odd and even solutions, we get 4 sets of equations as follows:

$$A_I \sin\left(\frac{k_{n,in}L}{2}\right) = B_I e^{-\frac{k_{n,out}L}{2}} \tag{16}$$

$$\frac{A_I k_{n,in}}{m_i} \cos\left(\frac{k_{n,in}L}{2}\right) = \frac{-B_I k_{n,out}}{m_o} e^{-\frac{k_{n,out}L}{2}} \tag{17}$$

$$A_I \cos\left(\frac{k_{n,in}L}{2}\right) = B_I e^{-\frac{k_{n,out}L}{2}} \tag{18}$$

$$\frac{A_I k_{n,in}}{m_i} \sin\left(\frac{k_{n,in}L}{2}\right) = \frac{B_I k_{n,out}}{m_o} e^{-\frac{k_{n,out}L}{2}} \tag{19}$$

From Equation (2) and Equation (4), we get the following,

$$-\beta k_{n,out} = k_{n,in} \cot\left(\frac{k_{n,in}L}{2}\right) \tag{20}$$

$$\beta k_{n,out} = k_{n,in} \tan\left(\frac{k_{n,in}L}{2}\right) \tag{21}$$

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

2.2 Generalizing the Asymptotic Analysis

Rewriting Equation (6) which holds for $n = 1, 3, 5...$

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

For very large values of V_o,

$$k_{n,in} \tan\left(\frac{k_{n,in}L}{2}\right) \longrightarrow \infty$$

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

However, we don't want an infinite barrier, rather, a large *but* **finite** barrier. In which case,

For the ground state,

$$\frac{k_{1,in}L}{2} = \frac{\pi}{2} - \epsilon$$

For the second excited state,

$$\frac{k_{3,in}L}{2} = \frac{3\pi}{2} - \epsilon$$

For the fourth excited state,

$$\frac{k_{5,in}L}{2} = \frac{5\pi}{2} - \epsilon$$

Thus, in general

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

where, ϵ is a very small positive real number.

Now, Equation (5) holds for $n = 2, 4, 6, ...$

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

For very large values of V_o,

$$k_{n,in} \cot\left(\frac{k_{n,in}L}{2}\right) \longrightarrow \infty$$

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

For the first excited state,

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

For the third excited state,

$$\frac{k_{4,in}L}{2} = 2\pi - \epsilon$$

Thus, in general we can say that

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

Thus, we see that for all values of n where $n = 1, 2, 3, 4, 5, ...$

$$\frac{k_{n,in}L}{2} = \frac{n\pi}{2} - \epsilon \tag{22}$$

where ϵ is a small positive real number.

Now, substituting Equation (7) in Equation (6),

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

$$\frac{\tan(n\pi/2) - \tan\epsilon}{1 + \tan(n\pi/2)\tan\epsilon} = \frac{\beta k_{n,out}L}{n\pi - 2\epsilon}$$

The expression on the left can be re-written as,

$$\frac{1-\dfrac{\tan\epsilon}{\tan(n\pi/2)}}{\dfrac{1}{\tan(n\pi/2)}+\tan\epsilon}=\frac{\beta k_{n,out}L}{n\pi-2\epsilon}$$

$$\frac{1}{\tan\epsilon}=\frac{\beta k_{n,out}L}{n\pi-2\epsilon}$$

Since ϵ is a very small positive number, $\tan\epsilon \approx \epsilon$

$$\frac{1}{\epsilon}=\frac{\beta k_{n,out}L}{n\pi-2\epsilon}$$

Re-arranging the terms we get,

$$\epsilon=\frac{n\pi}{\beta k_{n,out}L+2}, \qquad \text{for } n=1,3,5,7,... \tag{23}$$

Now, if we substitute Equation (7) in Equation (5) for the **odd** states we get the same expression for ϵ, i.e.,

$$\epsilon=\frac{n\pi}{\beta k_{n,out}L+2}, \qquad \text{for } n=2,4,6,8... \tag{24}$$

Now, we define the parameter σ as,

$$\sigma=\beta^2\frac{2m_oV_o}{\hbar^2}L^2$$

Since we are dealing with very large values of V_o, it is safe to say that

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

It is important to state here that we strictly consider the cases where $V_o > E_n$. Hence, n cannot be so large that E_n exceeds V_o.

In that case, we can write σ as,

$$\sigma \approx \beta^2 k_{n,out}^2 L^2$$

$$\sqrt{\sigma} = \beta k_{n,out} L$$

Now, we can substitute $\sqrt{\sigma}$ back in the expression for ϵ given in Equation (9) to get,

$$\epsilon = \frac{n\pi}{\sqrt{\sigma}+2}, \qquad \text{for all n = 1,2,3,4,5,...} \tag{25}$$

Now that we have the expression for ϵ, we need to substitute it back in Equation (7) so that we can get an expression for the energy of the electron.

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

$$\frac{k_{n,in}L}{2} = \frac{n\pi}{2} - \frac{n\pi}{\sqrt{\sigma}+2}$$

$$\frac{k_{n,in}L}{2} = \frac{n\pi}{2}\left[1 - \frac{2}{\sqrt{\sigma}+2}\right]$$

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

$$\implies \frac{2m_iE_nL^2}{\hbar^2} = n^2\pi^2\left[1 - \frac{2}{\sqrt{\sigma}+2}\right]^2$$

$$\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2m_iL^2}\left[1 - \frac{4}{\sqrt{\sigma}+2}\right]} \tag{26}$$

Thus, we can see that energy of a particle in a square well potential with mass discontinuity increases by n^2 and decreases by L^α.

$$E_n \propto \frac{n^2}{L^\alpha} \qquad 1 < \alpha < 2$$

The energy of a particle in an infinite potential well is,

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

The energy of the confined particle is no longer proportional to $1/L^2$ but rather to $1/L^\alpha$. This particular result is interesting because it agrees much better with experimental results.

2.2.1 Normalization of wavefunction

Consider the wavefunctions for a particle in the state $n = 1, 3, 5...$,

$$\Psi_n(x) = \begin{cases} A_I \cos(k_{n,in}x) & \text{if } |x| \le \frac{L}{2}, \\ B_I e^{-k_{n,out}|x|} & \text{if } |x| > \frac{L}{2}, \end{cases}$$

To find the normalization constant A_I we must do the following,

$$\int_{-\infty}^{\infty} \Psi^*(x)\Psi(x)\,dx = 1$$

$$2B_I^2 \int_{L/2}^{\infty} \exp\left(-2k_{n,out}x\right) dx + 2A_I^2 \int_0^{L/2} \cos^2(k_{n,in}x)\,dx = 1$$

$$2B_I^2 \left[\frac{\exp\left(-2k_{n,out}x\right)}{-2k_{n,out}}\right]_{L/2}^{\infty} + A_I^2 \left[\frac{\sin(2k_{n,in}x)}{2k_{n,in}} + x\right]_0^{L/2} = 1$$

$$B_I^2 \left[\frac{\exp\left(-k_{n,out}L\right)}{k_{n,out}}\right] + A_I^2 \left[\frac{\sin(k_{n,in}L)}{2k_{n,in}} + \frac{L}{2}\right] = 1$$

From Equation (3) we get,

$$A_I^2 \cos^2\left(\frac{k_{n,in}L}{2}\right) = B_I^2 \exp\left(-k_{n,out}L\right)$$

This gives us,

$$A_I^2\left[\frac{\cos^2(k_{n,in}L/2)}{k_{n,out}}\right]+A_I^2\left[\frac{\sin(k_{n,in}L)}{2k_{n,in}}+\frac{L}{2}\right]=1$$

The term on the left can be further simplified to,

$$A_I^2\left[\frac{\cos(k_{n,in}L)+1}{2k_{n,out}}\right]+A_I^2\left[\frac{\sin(k_{n,in}L)}{2k_{n,in}}+\frac{L}{2}\right]=1$$

Thus, A_I can be written as,

$$\boxed{A_I=\left[\frac{L}{2}\left(1+\frac{sin(k_{n,in}L)}{k_{n,in}L}\right)+\left(\frac{1+\cos(k_{n,in}L)}{2k_{n,out}}\right)\right]^{-1/2}} \tag{27}$$

This is the normalization constant for the particle in states $n = 1, 3, 5, ...$

The wavefunctions for the particle in states $n = 1, 3, 5...$ is given by,

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

Substituting Equation (7) in the above equation, we get

$$\Psi_n(x)=A_I\cos\left(\frac{(n\pi-2\epsilon)x}{L}\right)$$

$$\Psi_n(x)=A_I\cos(\frac{n\pi x}{L})\cos(\frac{2\epsilon x}{L})+\sin(\frac{n\pi x}{L})\sin(\frac{2\epsilon x}{L})$$

ϵ is a very small positive quantity, thus

$$\frac{\epsilon}{L}<<1$$

$$\cos(\frac{2\epsilon x}{L})\approx 1$$

$$\sin(\frac{2\epsilon x}{L})\approx\frac{2\epsilon x}{L}$$

The wavefunction then becomes,

$$\boxed{\Psi_n(x) \approx A_I \left[\cos(\frac{n\pi x}{L}) + \frac{2\epsilon x}{L}\sin(\frac{n\pi x}{L})\right]} \tag{28}$$

2.3 Charge Density at Boundary

The charge density inside the well is given by,

$$\rho(x) = |\Psi(x)|^2$$

for $n = 1, 3, 5, ...$

$$\Psi(x) = A_I \cos(k_{n,in}x)$$

At the boundary, $x = \pm L/2$

$$\rho(L/2) = A_I^2 \cos^2(k_{n,in}L/2)$$

Using Equation (7),

$$\rho(L/2) = A_I^2 \cos^2(\frac{n\pi}{2} - \epsilon)$$

$$\rho(L/2) = A_I^2 \sin^2 \epsilon$$

$$\rho(L/2) = A_I^2 \epsilon^2$$

Substituting ϵ from equation (10), we get

$$\rho(L/2) = \frac{A_I^2 n^2 \pi^2}{\sigma}$$

$$\sigma \propto \beta^2$$

$$\rho(L/2) \propto \frac{1}{\beta^2}$$

Therefore, as the value of β decreases significantly, the charge density at the boundary of the well increases. Thus, the charge density at the boundary is inversely proportional to β^2

Now, if you were to consider the eigenfunctions of the particle in states $n = 2, 4, 6...$, you would get the exact same relationship between charge density at boundary and β. This is demonstrated as follows,

Consider $n = 2, 4, 6, ...$

$$\Psi_n(x) = A_I \sin(k_{n,in} x)$$

At the boundary, $x = \pm L/2$

$$\rho(L/2) = A_I^2 \sin(k_{n,in} L/2)$$

Using Equation (7),

$$\rho(L/2) = A_I^2 \sin\left(\frac{n\pi}{2} - \epsilon\right)$$

$$\rho(L/2) = A_I^2 \left[\sin(\frac{n\pi}{2}) \cos\epsilon - \cos(\frac{n\pi}{2}) \sin\epsilon\right]$$

$$\rho(L/2) = A_I^2 \sin^2 \epsilon$$

ϵ is a very small positive number,

$$\rho(L/2) = A_I^2 \epsilon^2$$

Substituting ϵ from equation (10), we get

$$\rho(L/2) = \frac{A_I^2 n^2 \pi^2}{\sigma}$$

$$\sigma \propto \beta^2$$

$$\rho(L/2) \propto \frac{1}{\beta^2}$$

Thus, the charge density at the boundary for the particle in any excited state increases as β decreases.

In case we had considered an infinite potential barrier like in the simple quantum confinement model rather than a finite (but large) potential barrier, the charge density in the boundary would have turned out to be 0. Which means that, various surface-related phenomena arising from quantum dots due to the presence of surface charges would not predicted by the simple quantum confinement model.

3 Graded Heterostructures - Quantum Tunneling

3.1 Gamow's Theory of Alpha Decay

α decay is a type of radioactive transmutation in which a heavy unstable nucleus emits an alpha-particle (He atom with +2 charge) and transforms into a different atomic nucleus with atomic number that is reduced by 2 and mass number reduced by 4.

Inside the nucleus of a heavy atom, the α particle is trapped by the attractive nuclear forces. In order to escape from the nucleus it has to overcome the Coulomb potential barrier. When it does so, it is said to “tunnel" through the barrier and hence the phenomena is known as quantum tunneling.

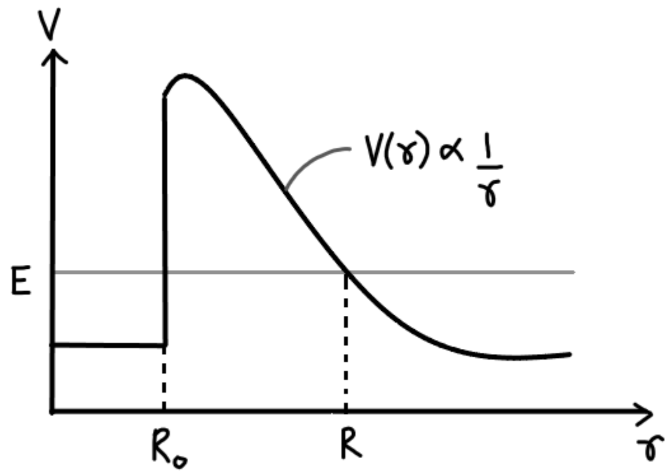


Figure 3: Coulomb barrier potential

We need to find the transmission probability of the α particle that escapes the barrier. In order to find this, recall the rectangular barrier transmission probability,

$$T = \left\{ 1 + \frac{sin^2h(kL)}{\frac{4E}{V_o}\left(1 - \frac{E}{V_o}\right)} \right\}^{-1} \tag{29}$$

where $V_o =$ barrier height, $L =$ barrier width

$E =$ energy of particle in well

$$k = \frac{\sqrt{2m(V_o - E)}}{\hbar}$$

This is the transmission probability of a particle tunnelling through a rectangular barrier of height V_o with an energy $E < V_o$

For wide barrier, i.e.,

$$kL >> 1$$

$$L >> \frac{1}{k}$$

$$T \approx \frac{16E}{V_o}\left(1 - \frac{E}{V_o}\right)e^{-2kL} \tag{30}$$

Ignoring the pre-factor as it is order unity, we get

$$T \approx e^{-2kL} \tag{31}$$

Now, we need to use the transmission probability of a particle tunneling through a rectangular barrier to find the transmission probability of an α particle tunneling through the Coulomb barrier.

To do so, we divide the Coulomb barrier potential into N rectangular wells of width Δr as shown in Figure 2.

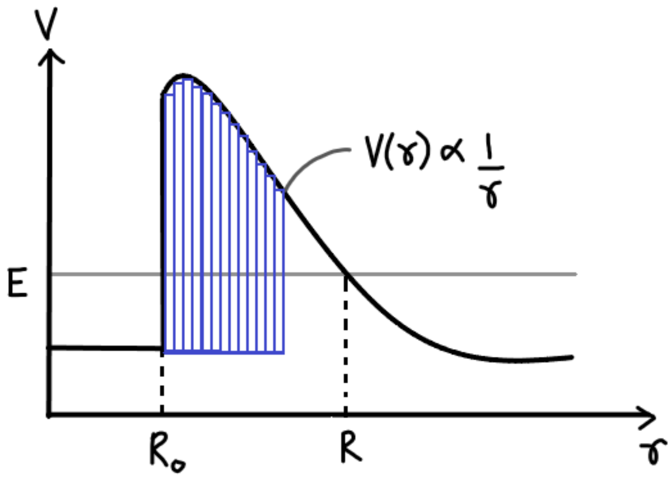


Figure 4: Coulomb barrier potential divided into N rectangular potential wells each of width Δr

It is important to note that in order for the wide barrier approximation to hold true,

$$\Delta r >> \frac{1}{k}$$

The transmission coefficient for a given rectangular barrier of width Δr is,

$$T_i = \exp\left\{\frac{-2}{\hbar}\Delta r\sqrt{2m_\alpha(V_i - E)}\right\} \tag{32}$$

$$V_i = V(r_i) = \frac{2kZe^2}{r_i}$$

The total transmission coefficient then becomes.

$$T = \exp\left[\frac{-2}{\hbar}\sum_{i=1}^{N}\sqrt{2m_\alpha(V_i - E)}\Delta r\right] \tag{33}$$

To compute the expression for T in Equation 33, we have to revisit trapezoidal rule of integration.

3.1.1 Trapezoidal Rule

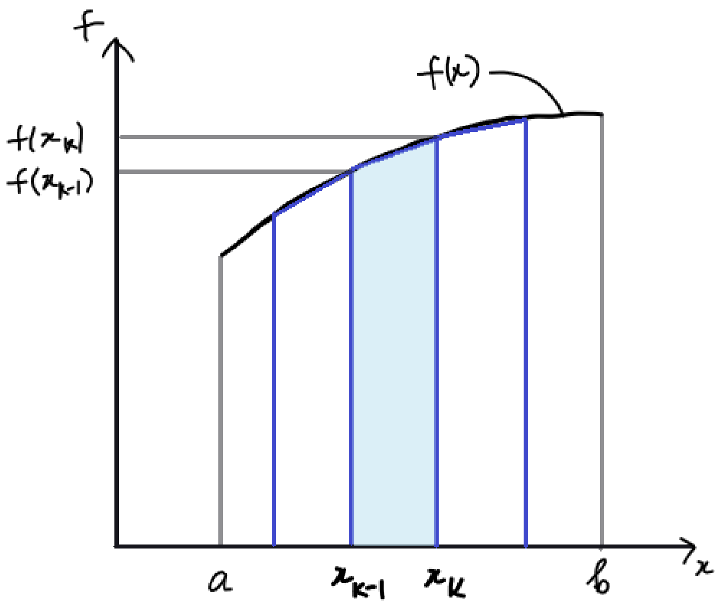


Figure 5: Area under the curve f(x) divided into N trapezoids

Divide a function f(x) from a to b into N regions such that,

$$a = x_o < x_1 < x_2 < ... < x_N = b$$

The length of each division is,

$$\Delta x_k = x_k - x_{k-1}$$

Integration of f(x) from a to b can be approximated by

$$\int_a^b f(x)\,dx = \sum_{k=1}^{N} \left[\frac{f(x_{k-1}) + f(x_k)}{2} \Delta x \right] \tag{34}$$

where

$$\Delta x_k = \Delta x \qquad \text{i.e., all the trapezoids have same height}$$

Integrating f(x) in a small interval from x_{k-1} to x_k, we get

$$\int_{x_{k-1}}^{x_k} = \frac{\Delta x}{2} \bigg(f(x_{k-1}) + f(x_k) \bigg)$$

Suppose that $\Delta f(x_k)$ is so small that,

$$f(x_{k-1}) \approx f(x_k)$$

i.e.,

$$\Delta f(x_k) << f(x_k)$$

then,

$$\int_{x_{k-1}}^{x_k} = f(x_k)\Delta x$$

For the interval [a,b] then,

$$\int_a^b f(x)\,dx = \Delta x \sum_{k=1}^{N} f(x_k) \tag{35}$$

3.1.2 Gamow Tunneling Formula

Rewrite Equation 33 using Equation 35

$$T \approx \exp\left[\frac{-2\sqrt{2m_\alpha}}{\hbar}\int_{R_o}^{R}\sqrt{V(r)-E}\,dr\right] \tag{36}$$

where $V(r) = \frac{2kZe^2}{r}$

Equation 36 holds true when these two conditions are satisfied:

The first condition is that,

$$|\Delta\sqrt{V(r)-E}| << \sqrt{V(r)-E}$$

$$\frac{1}{2\sqrt{V(r)-E}}\frac{dV}{dr}\Delta r << \sqrt{V(r)-E}$$

$$\boxed{\frac{dV}{dr} << \frac{2[V(r)-E]}{\Delta r}}$$

The second condition is that,

$$\boxed{\Delta r >> \frac{\hbar}{\sqrt{2m_\alpha(V_i-E)}}}$$

This is essential for the tunneling expression of a wide rectangular barrier (Equation 30) to hold true.

The integral in Equation 36 has to be computed.

E is the energy of the α particle, therefore,

$$E = \frac{2kZe^2}{R}$$

and

$$V(r) = \frac{2kZe^2}{r}$$

$$V(r) - E \ = 2kZe^2\left[\frac{1}{r} - \frac{1}{R}\right]$$

Equation 36 can be re-written as,

$$T \approx \exp\left\{ \frac{-2\sqrt{2m_\alpha}}{\hbar} \int_{R_o}^{R} \sqrt{2kZe^2}\left[\frac{1}{r} - \frac{1}{R}\right]^{1/2} dr \right\}$$

let

$$C = \frac{-2\sqrt{2m_\alpha}}{\hbar}\sqrt{2kZe^2}$$

$$T \approx \exp\left\{ \frac{C}{\sqrt{R}} \int_{R_o}^{R} \left[\frac{R}{r} - 1\right]^{1/2} dr \right\}$$

let

$$I = \int_{R_o}^{R} \left[\frac{R}{r} - 1\right]^{1/2} dr$$

let

$$\frac{R}{r} = \frac{1}{x}$$

then

$$I = R\int_{R_o/R}^{1} \frac{\sqrt{1-x}}{\sqrt{x}}\, dx$$

let

$$\sqrt{x} = t$$

then

$$I = 2R\int_{\sqrt{R_o/R}}^{1} \sqrt{1-t^2}\, dt$$

let

$$t = \sin\theta$$

then

$$I = 2R\int_{\sin^{-1}\sqrt{R_o/R}}^{\pi/2} \sqrt{1-\sin^2\theta}\cos\theta\, d\theta$$

$$= R\Big[\sin\theta\cos\theta + \theta\Big]_{\sin^{-1}\sqrt{R_o/R}}^{\pi/2}$$

$$= R\left[\frac{\pi}{2} - \sqrt{\frac{R_o}{R}}\cos\theta - \sin^{-1}\sqrt{\frac{R_o}{R}}\right]$$

Assume that $\frac{R_o}{R}$ is a small number.

This can be demonstrated using Uranium - 238 which undergoes α decay.

Number of nucleons = 238

The nuclear radius R_o,

$$R_o = a_o A^{1/3}$$

$$= 1.3\,\text{fm} \times (238)^{1/3} \approx 8\,\text{fm}$$

To find an estimate of R, let the α particle have $E = 5\,\text{Mev}$.

$$E = \frac{2kZE^2}{R}$$

$$R = \frac{2kZe^2}{E} = \frac{2 \times 9 \times 10^9 \times 92 \times (1.6 \times 10^{-19})^2}{5MeV} \approx 53\,\text{fm}$$

Now,

$$\frac{R_o}{R} = \frac{8}{53} \approx 0.15 \text{ which is a small number}$$

$$\theta = \sin^{-1}\sqrt{\frac{R_o}{R}} \longrightarrow \sin\theta = \sqrt{\frac{R_o}{R}}$$

This implies that $\sin\theta$ is a small number such that $\sin\theta \approx \theta$ in which case,

$$\cos\theta \approx 1$$

Finally,

$$I = R\left[\frac{\pi}{2} - 2\sqrt{\frac{R_o}{R}}\right]$$

Therefore

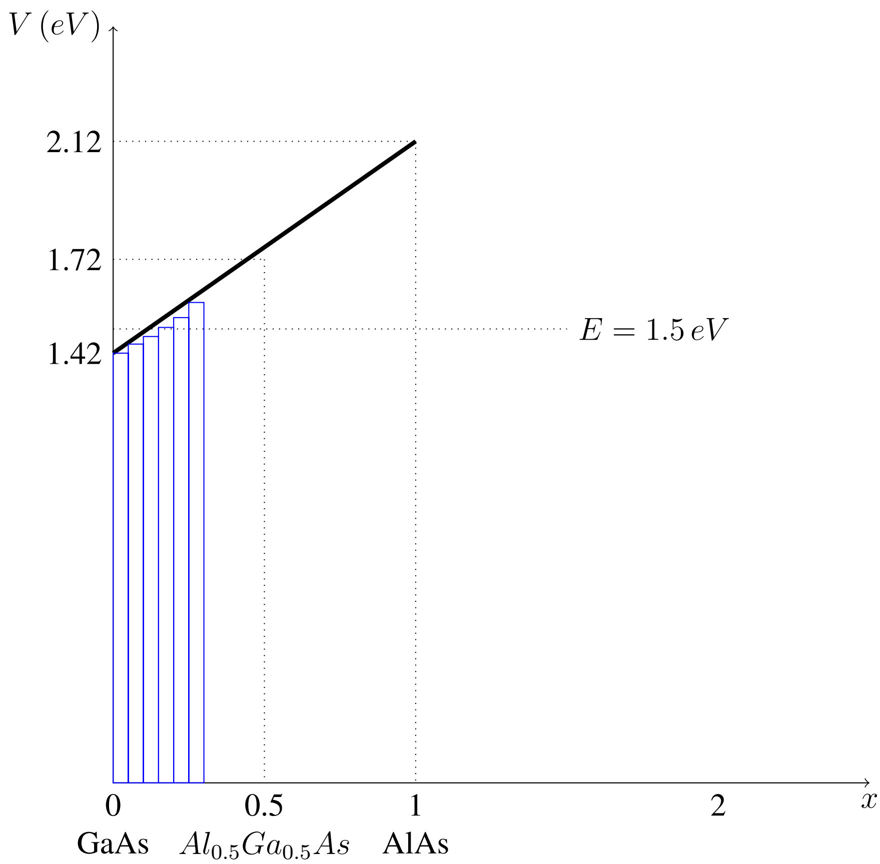
$$T = \exp\left\{C\sqrt{R}\left[\frac{\pi}{2} - 2\sqrt{\frac{R_o}{R}}\right]\right\}$$

Substituting the value of C and R (in terms of E) we get,

$$\boxed{T = \exp\left\{-4\pi\left(\frac{2m_\alpha k^2 Z^2 e^4}{4\hbar^2 E}\right)^{1/2} + 8\sqrt{ZR_o}\left(\frac{m_\alpha k e^2}{\hbar^2}\right)^{1/2}\right\}} \tag{37}$$

This is the transmission probability for an α particle trapped in a nucleus.

3.2 $Al_xGa_{1-x}As$ Graded Heterostructure



In a linearly graded heterojunction, the effective mass of the charge carriers is also going to vary linearly with the concentration (c). For example, in $Al_xGa_{1-x}As$, the effective mass of electrons is $0.063m_o$ in GaAs and $0.15m_o$ in AlAs, where m_o is the free electron mass. So, we can write the variation in the effective mass of the electron as,

$$m_e = m_o(0.063 + \delta_m c) \tag{38}$$

where δ_m is the change in the mass.

The band gap for GaAs $= 1.42$ eV.

The band gap for AlAs $= 2.12$ eV.

If the potential is varying linearly with concentration then, it can be written as:

$$V = (1.42 + \delta_v c)\,eV \tag{39}$$

This linear variation of the potential is demonstrated in the figure above.

However, the concentration 'c' is varying linearly with distance 'x', therefore, the effective mass and potential is also varying linearly with x.

$$c \propto x$$

$$m_e = m_o(0.063 + \delta_m x)$$

$$V = (1.42 + \delta_v x)\,[eV]$$

Suppose we want to find the transmission probability of charged carriers through a graded heterojunction such as $Al_xGa_{1-x}As$, we will follow a method similar to the one we used for finding the probability of transmission of an $\alpha-$ particle from the nucleus.

Divide the potential barrier into N rectangular barriers of width Δr.

The tunnelling probability of a rectangular barrier is well established and is equal to,

$$T = \left\{ 1 + \frac{sin^2h(kL)}{\frac{4E}{V_o}\left(1 - \frac{E}{V_o}\right)} \right\}$$

Using the wide barrier approximation, i.e.,

$$kL >> 1$$

$$L >> \frac{1}{k}$$

$$T = \frac{16E}{V_o}\left(1 - \frac{E}{V_o}\right)e^{-2kL} \tag{40}$$

where L is the length of the barrier and E is the energy of the charged carrier.

$$k = \sqrt{\frac{2m_e(V_o - E)}{\hbar^2}}$$

Suppose we take the energy of the charge carrier (electron) to be about 1.5 eV, the maximum value that the pre-exponential factor can take is 3.3, so we can approximate T as,

$$\boxed{T \approx e^{-2kL}}$$

Now, since we divided the potential barrier into N rectangular barriers of length Δr, we must ensure that for the wide barrier approximation to hold,

$$\boxed{\Delta r >> \frac{1}{k}}$$

The tunnelling probability of the i^{th} barrier is,

$$T_i = exp\left\{ -\frac{2}{\hbar}\sqrt{2m_i(V_i - E)}\Delta r \right\}$$

where,

$$V_i = 1.42 + \delta_v x_i$$

$$m_i = 0.063 + \delta_m x_i$$

$$\delta_v = 0.7$$

$$\delta_m = 0.087$$

The total transmission probability is then,

$$T = exp\left\{ \frac{-2}{\hbar} \sum_{i=1}^{N} \sqrt{2m_i(V_i - E)}\Delta r \right\}$$

From trapezoidal rule of integration, we have found that

$$\int_a^b f(x)dx = \Delta x \sum_{k=1}^{N} f(x_k)$$

Here,

$$f(x_k) = \sqrt{2m_i(V_i - E)}$$

$$\Delta r = \Delta x$$

$$\rightarrow f(x) = \sqrt{2m(x)[V(x) - E]}$$

Therefore,

$$T = exp\left\{\frac{-2}{\hbar}\int_a^b \sqrt{2m(x)(V(x) - E)}\,dx\right\} \tag{41}$$

where,

$$m(x) = 0.063 + \delta_m x$$

$$V(x) = 1.42 + \delta_v x$$

The upper limit is 1 but the lower limit has to be calculated based on the energy of the charge carrier.

Here, $E = 1.5$ eV.

$$1.5 = 1.42 + \delta_v x_o$$

$$x_o = \frac{0.08}{\delta_v}$$

Equation 4 can then be written as,

$$T = exp\left\{\frac{-2}{\hbar}\int_{0.08/\delta_v}^1 \sqrt{2m(x)[V(x) - E]}\,dx\right\} \tag{42}$$

We must solve the integral in Equation 5 now in order to find the expression for the transmission probability.

So, let

$$I = \int_{0.08/\delta_v}^1 \sqrt{2m(x)[V(x) - E]}\,dx$$

$$I = \sqrt{2}\int_{0.08/\delta_v}^1 \sqrt{m_o(0.063 + \delta_m x)(1.42 + \delta_v x - E)}\,dx$$

$$I = \sqrt{2m_o}\int_{0.08/\delta_v}^1 \sqrt{\delta_m\delta_v x^2 + x[0.06\delta_v + \delta_m(1.42 - E)] + 0.06(1.42 - E)}\,dx$$

We see that the integral is of the form

$$I = \int_{0.08/\delta_v}^1 \sqrt{cx^2 + bx + a}\,dx$$

$$I = \sqrt{c}\int_{0.08/\delta_v}^1 \sqrt{x^2 + \frac{b}{c}x + \frac{a}{c}}\,dx$$

$$I=\sqrt{c}\int_{0.08/\delta_v}^{1}\sqrt{\left(x+\frac{b}{2c}\right)^2+\sqrt{\left(\frac{a}{c}-\frac{b^2}{4c^2}\right)}^2}\,dx \tag{43}$$

———————————————————————————-

Any integral of the form:

$$I'=\int\sqrt{x^2+d^2}$$

is equal to,

$$I'=\frac{x}{2}\sqrt{x^2+d^2}+\frac{d^2}{2}log|x+\sqrt{x^2+d^2}|+C \tag{44}$$

———————————————————————————-

In order to make use of the result that we have obtained in Equation 7 , we need to make a change of variables. Let,

$$x+\frac{b}{2c}=y$$

$$\longrightarrow dx=dy$$

If $x:x_o\to 1$, then $y:x_o+\frac{b}{2c}\to 1+\frac{b}{2c}$

The integral in Equation 6 then becomes,

$$I=\sqrt{c}\int_{x_o+b/2c}^{1+b/2c}\sqrt{y^2+\sqrt{\left(\frac{a}{c}-\frac{b^2}{4c^2}\right)}^2}\,dy$$

Now, we can solve the above integral using the result obtained in Equation 7.

$$I=\sqrt{c}\left[\frac{y}{2}\sqrt{y^2+\left(\frac{a}{c}-\frac{b^2}{4c^2}\right)}+\frac{1}{2}\left(\frac{a}{c}-\frac{b^2}{4c^2}\right)log\left|y+\sqrt{y^2+\left(\frac{a}{c}-\frac{b^2}{4c^2}\right)}\right|\right]_{x_o+b/2c}^{1+b/2c}$$

Applying the limits and simplifying the equation by introducing P and Q as,

$$\sqrt{\frac{a}{c}-\frac{b^2}{4c^2}}=P$$

$$\frac{b}{2c}=Q$$

$$I = \sqrt{c}\Bigg\{\frac{(Q+1)}{2}\sqrt{(Q+1)^2+P^2} + \frac{P^2}{2}\,log\big|(Q+1)+\sqrt{(Q+1)^2+P^2}\big|$$
$$-\frac{(Q-x_o)}{2}\sqrt{(Q+x_o)^2+P^2} - \frac{P^2}{2}\,log\big|(Q+x_o)+\sqrt{(Q+x_o)^2+P^2}\big|\Bigg\} \quad (45)$$

$$I = \sqrt{c}\Bigg\{\frac{(Q+1)}{2}\sqrt{(Q+1)^2+P^2} - \frac{(Q+x_o)}{2}\sqrt{(Q+x_o)^2+P^2}$$
$$+\frac{P^2}{2}\,log\left|\frac{(Q+1)+\sqrt{(Q+1)^2+P^2}}{(Q+x_o)+\sqrt{(Q+x_o)^2+P^2}}\right|\Bigg\} \quad (46)$$

In this case,

$$c = \delta_m\delta_v$$

$$a = 0.06(1.42-E)$$

$$b = 0.06\delta_v + (1.42-E)\delta_m$$

Therefore, the transmission of the charge carrier across the graded hetero-structure can be calculated using the following expression,

$$\boxed{T = exp\Bigg\{\frac{-2\sqrt{2m_o}}{\hbar}I\Bigg\}} \quad (47)$$

where,

$$I = \sqrt{\delta_m\delta_v}\Bigg\{\frac{(Q+1)}{2}\sqrt{(Q+1)^2+P^2} - \frac{(Q+x_o)}{2}\sqrt{(Q+x_o)^2+P^2}$$
$$+\frac{P^2}{2}\,log\left|\frac{(Q+1)+\sqrt{(Q+1)^2+P^2}}{(Q+x_o)+\sqrt{(Q+x_o)^2+P^2}}\right|\Bigg\}$$

$$P = \sqrt{\frac{0.063(1.42-E)}{\delta_m\delta_v} - \left(\frac{0.03}{\delta_m} + \frac{(1.42-E)}{2\delta_v}\right)^2}$$

$$Q = \frac{0.03}{\delta_m} + \frac{(1.42-E)}{2\delta_v}$$

$$x_o = \frac{E-1.42}{\delta_v}$$

It was found that on numerically evaluating Equation 42 using Simpson's 1/3 Rule, the transmission probability was 0.636. Whereas, the analytical solution in Equation 47 gives us the transmission probability as 0.639.

The error in the the transmission probability value computed numerically using Simpson's rule is 0.579 $\%$.

References

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

[2]I.M. Lifshitz, Adv. Phy. 13, 483 (1964)

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

[4]Singh, M., Ranjan, V., Singh, V. A. (2000). The role of the carrier mass in semiconductor quantum dots. International Journal of Modern Physics B, 14(17), 1753-1765.