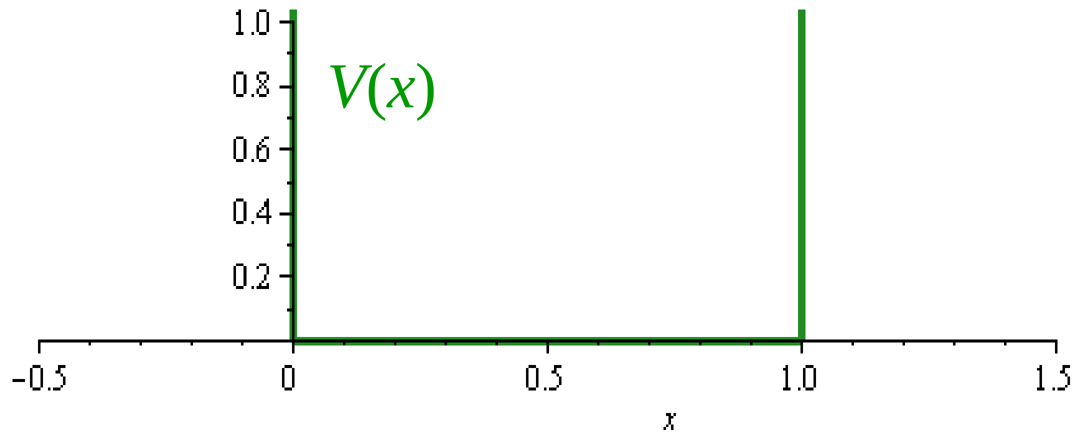
Physics PY4118
Physics of Semiconductor Devices

Coupled States

1D infinite square well (1)

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

$$V(x) = \begin{cases} 0 & \text{if } 0 < x < L \\ \infty & \text{otherwise} \end{cases}$$



$$\psi(x) = 0 \quad \text{if } x < 0 \text{ or } x > L$$

Outside of the well, the wave function must vanish

In remaining region, we need to solve:

$$E\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} \quad \rightarrow \psi = \left\{ \begin{array}{c} \cancel{\cos(kx)} \\ \sin(kx) \\ e^{\pm ikx} \end{array} \right\}$$

1D infinite square well (2)

Choose the real solution: $\psi = \sin(kx)$

Boundary Conditions:

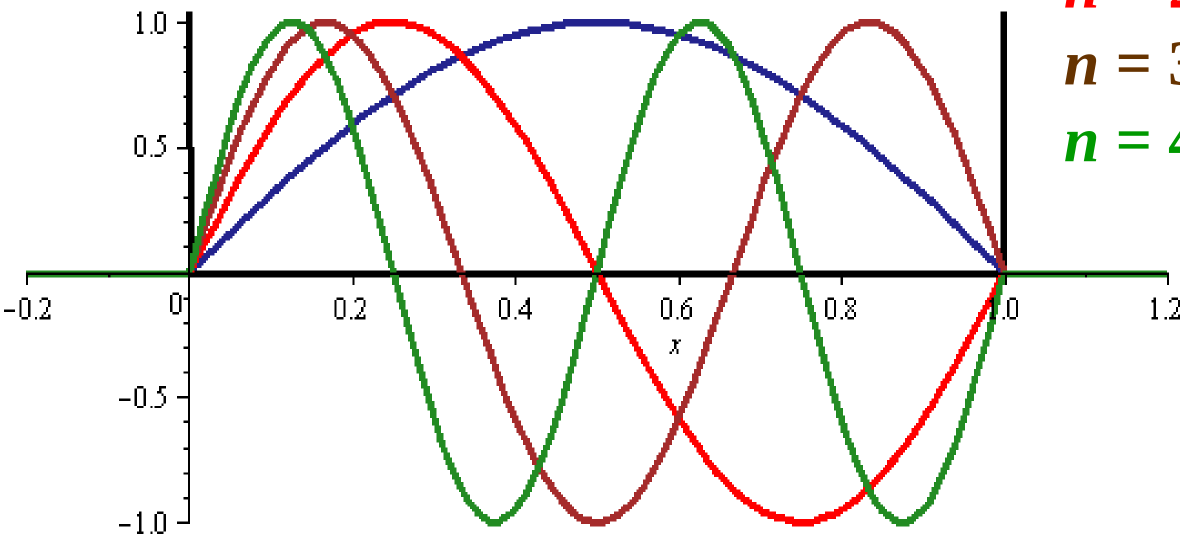
Must vanish at x = 0, and at x = L

$$0 = \psi(L) = \sin(kL) \qquad kL = n\pi \rightarrow k = \frac{n\pi}{L} \qquad \boxed{n = 1, 2, 3, \ldots}$$

$$E\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} \rightarrow E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2\pi^2 n^2}{2mL^2} = E_n$$

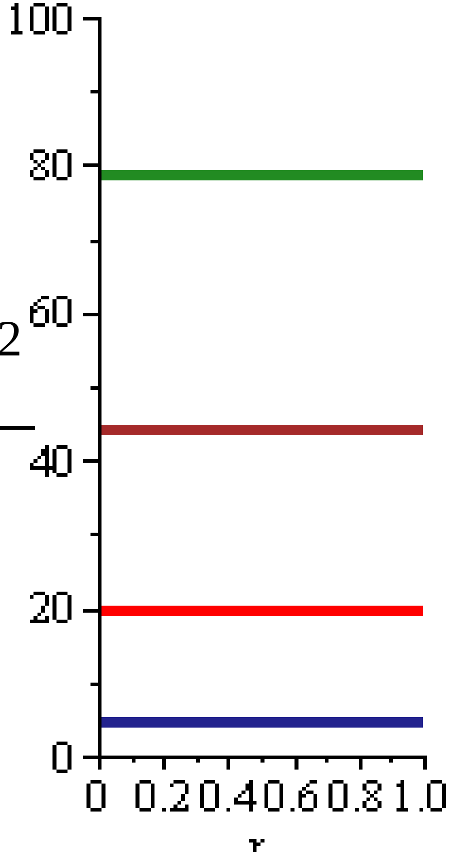
1D infinite square well (3)

$$\psi(x) = \sin\left(\frac{\pi n x}{L}\right)$$



$n = 1$
$n = 2$
$n = 3$
$n = 4$

$$\frac{E_n m L^2}{\hbar^2}$$

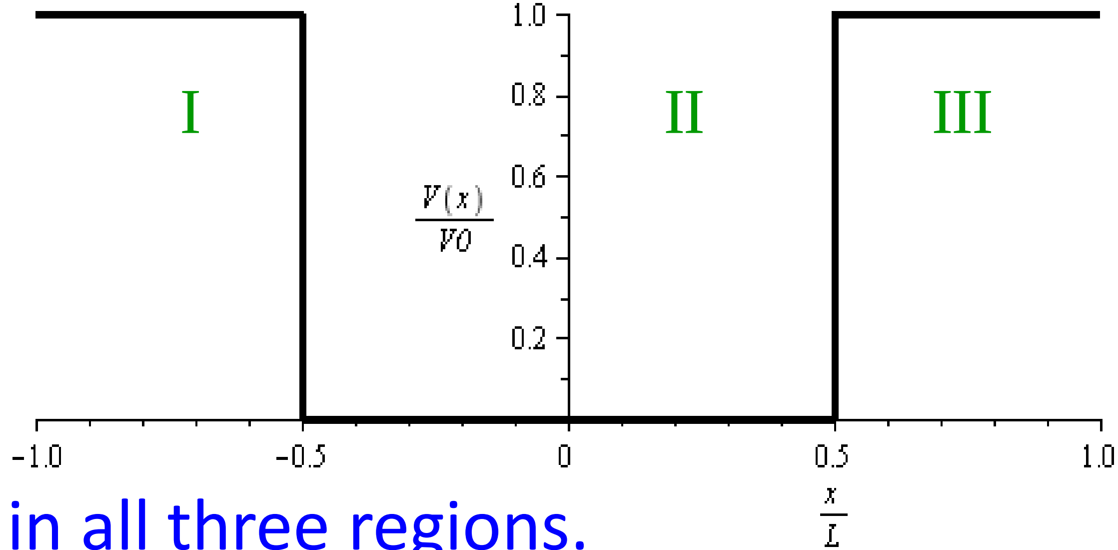


Energy Diagram

The Finite Square Well (1)

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

$$V(x) = \begin{cases} 0 & \text{if } |x| < \frac{1}{2}L \\ V_0 & \text{otherwise} \end{cases}$$



We need to solve equation in all three regions.

In region II, we get solutions like before: $\psi(x) = \cos(kx)$

$$\psi(x) = \sin(kx)$$

The solution no longer vanishes at the boundaries

In regions I and III, we solve a different equation

The Finite Square Well (2)

In the well: $k^2 = \dfrac{2mE}{\hbar^2}$

In the barrier:

$$E\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi \quad \Rightarrow \quad \frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (V_0 - E)\psi$$

For a bound state: *E<V₀*

$$\Rightarrow \quad \frac{d^2\psi}{dx^2} = \alpha^2\psi$$

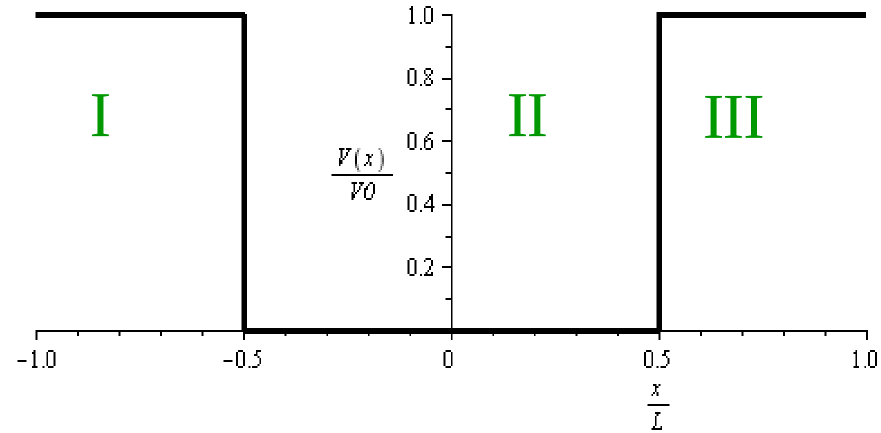
And the solutions are: $\psi(x) = e^{\pm\alpha x} \qquad \alpha^2 = \dfrac{2m(V_0 - E)}{\hbar^2}$

The Finite Square Well (3)

$$\psi_I(x) = Ae^{\alpha x} + Be^{-\alpha x}$$

$$\psi_{II}(x) = C\cos(kx) + D\sin(kx)$$

$$\psi_{III}(x) = Ee^{\alpha x} + Fe^{-\alpha x}$$



Wave function must not blow up at: $x = \pm\infty \quad \rightarrow B = E = 0$

Wave function must be continuous at: $x = \pm\dfrac{L}{2}$

$$\psi_I\left(-\tfrac{1}{2}L\right) = \psi_{II}\left(-\tfrac{1}{2}L\right) \qquad Ae^{-\alpha L/2} = C\cos(kL/2) - D\sin(kL/2)$$

$$\psi_{II}\left(\tfrac{1}{2}L\right) = \psi_{III}\left(\tfrac{1}{2}L\right) \qquad Fe^{-\alpha L/2} = C\cos(kL/2) + D\sin(kL/2)$$

The Finite Square Well (4)

The derivative must be continuous at: $x = \pm \dfrac{L}{2}$

$$\psi_I'\left(-\tfrac{1}{2}L\right) = \psi_{II}'\left(-\tfrac{1}{2}L\right) \qquad A\alpha e^{-\alpha L/2} = Ck\sin\left(kL/2\right) + Dk\cos\left(kL/2\right)$$

$$\psi_{II}'\left(\tfrac{1}{2}L\right) = \psi_{III}'\left(\tfrac{1}{2}L\right) \qquad -F\alpha e^{-\alpha L/2} = -Ck\sin\left(kL/2\right) + Dk\cos\left(kL/2\right)$$

We can find solutions by considering the symmetric and asymmetric solutions separately:

The Finite Square Well (5)

symmetric | antisymmetric

x=-L/2

$$C\cos(kL/2) = Ae^{-\alpha L/2}$$
$$kC\sin(kL/2) = \alpha Ae^{-\alpha L/2}$$

$$-D\sin(kL/2) = Ae^{-\alpha L/2}$$
$$kD\cos(kL/2) = \alpha Ae^{-\alpha L/2}$$

x=-L/2

$$C\cos(kL/2) = Fe^{-\alpha L/2}$$
$$kC\sin(kL/2) = \alpha Fe^{-\alpha L/2}$$

$$D\sin(kL/2) = Fe^{-\alpha L/2}$$
$$-kD\cos(kL/2) = \alpha Fe^{-\alpha L/2}$$

$$A = F \qquad\qquad A = -F$$

$$k\tan(kL/2) = \alpha \qquad\qquad k\cot(kL/2) = -\alpha$$

The Finite Square Well (5)

Need to calculate: k and α

$$k^2 = \frac{2mE}{\hbar^2} \qquad \alpha^2 = \frac{2m(V_0 - E)}{\hbar^2} \qquad \rightarrow k^2 + \alpha^2 = \frac{2m}{\hbar^2} V_0$$

symmetric

$$k \tan(kL/2) = \alpha$$

$$\frac{kL}{2} \tan\left(\frac{kL}{2}\right) = \frac{\alpha L}{2}$$

antisymmetric

$$k \cot(kL/2) = -\alpha$$

$$\frac{kL}{2} \cot\left(\frac{kL}{2}\right) = -\frac{\alpha L}{2}$$

$$\left(\frac{kL}{2}\right)^2 + \left(\frac{\alpha L}{2}\right)^2 = \frac{mL^2}{2\hbar^2} V_0$$

The Finite Square Well (6)

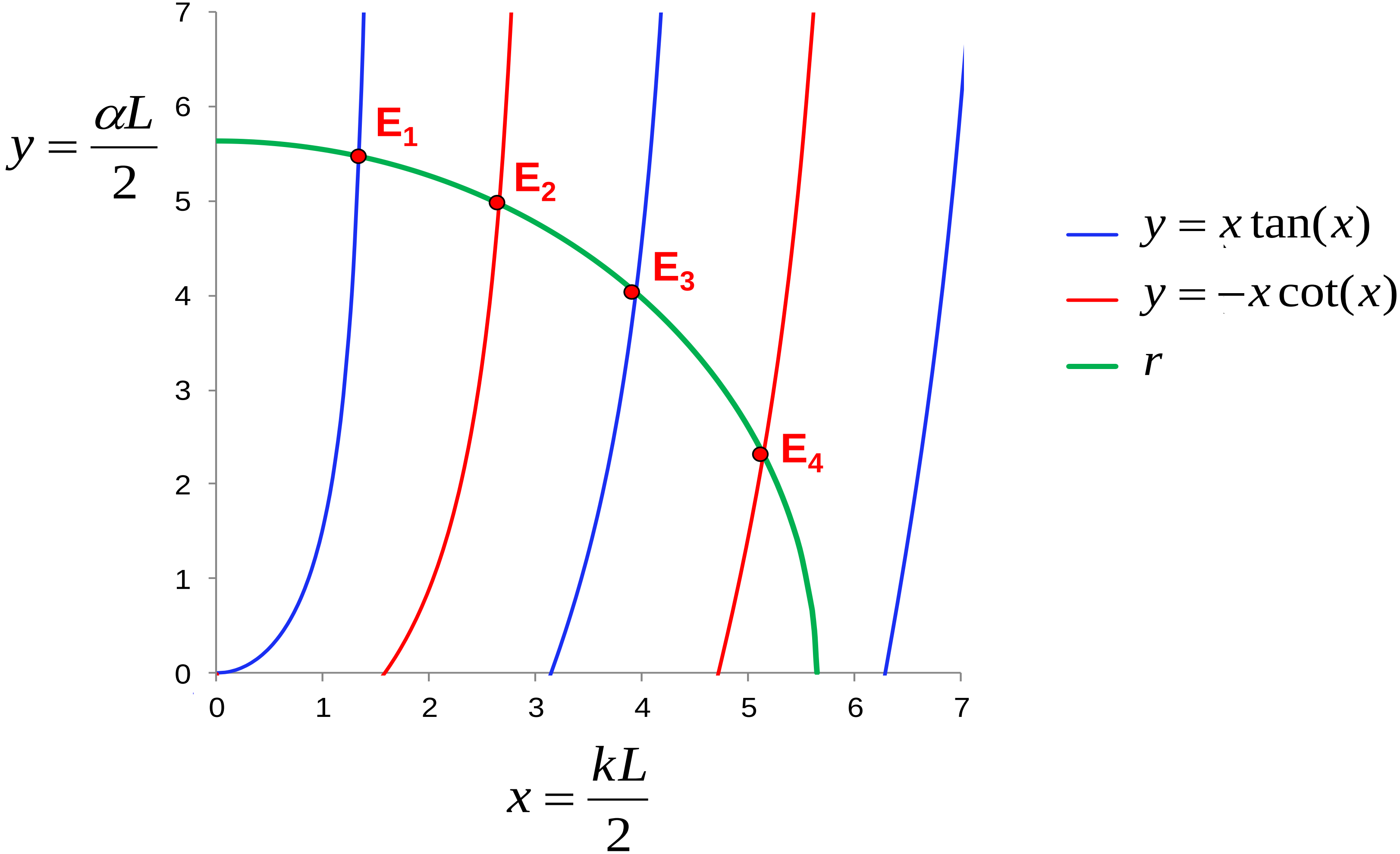
For graphical solution:

$$x = \frac{kL}{2} \qquad y = \frac{\alpha L}{2} \qquad r^2 = \frac{mL^2}{2\hbar^2} V_0$$

symmetric | antisymmetric

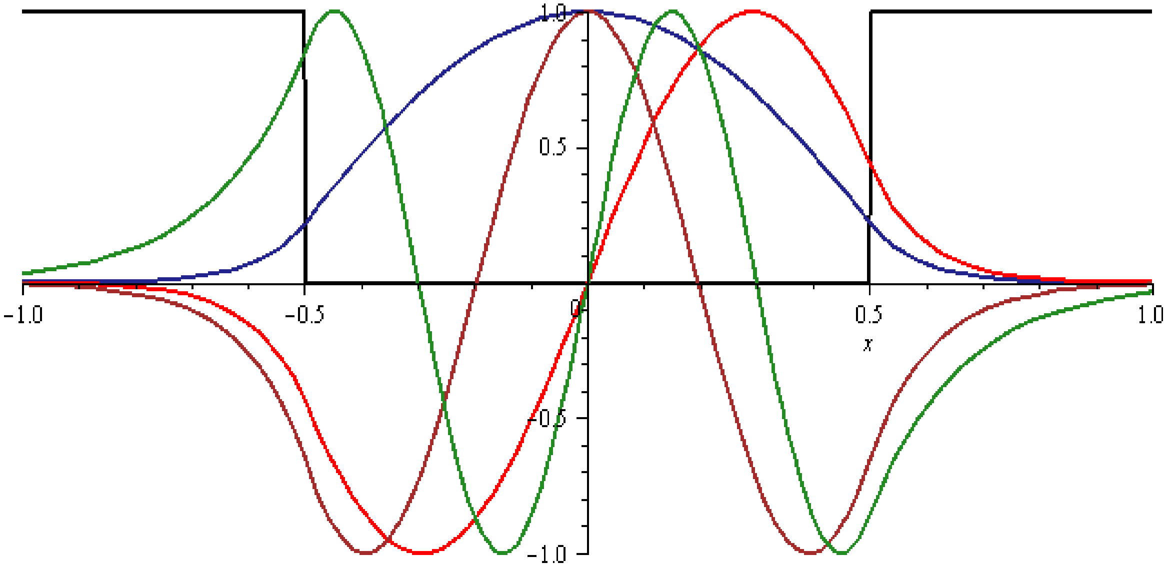
$$y = x\tan(x) \qquad x^2 + y^2 = r^2 \qquad y = -x\cot(x)$$

The Finite Square Well (7)



The Finite Square Well (8)

$$V_0 = \frac{75\hbar^2}{mL^2}$$

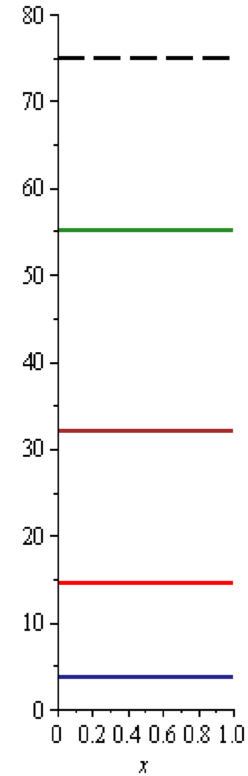


***n* = 4**

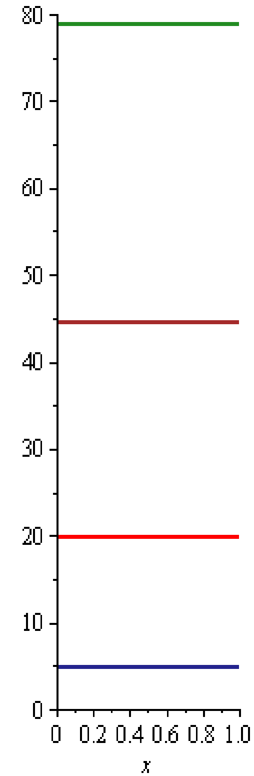
***n* = 3**

***n* = 2**

***n* = 1**



Energy Diagram



Infinite Well

Two Coupled Wells (1)

- Can solve:
  - Using approximate technique
  - Exact: semi-analytically (this is a long derivation)

Approximate technique assumptions:

- Identical Wells
  - Thus identical wavefunctions
- Treat the wavefunctions as separate

Two coupled wells (2)

The total wavefunction of the system is: $\psi = c_1\psi_1 + c_2\psi_2$

The Energy in the system is: $E = \dfrac{\int \psi^* H \psi}{\int \psi^* \psi} \Rightarrow \dfrac{\int \psi H \psi}{\int \psi^2}$

Thus: $E = \dfrac{\int (c_1\psi_1 + c_2\psi_2) H (c_1\psi_1 + c_2\psi_2)}{\int (c_1\psi_1 + c_2\psi_2)^2}$

$$= \frac{c_1^2 \int \psi_1 H \psi_1 + 2c_1c_2 \int \psi_1 H \psi_2 + c_2^2 \int \psi_2 H \psi_2}{c_1^2 \int \psi_1^2 + 2c_1c_2 \int \psi_1\psi_2 + c_2^2 \int \psi_2^2}$$

Two coupled wells (3)

We then simplify the notation, using:

$$H_{ij} = \int \psi_i H \psi_j \qquad S_{ij} = \int \psi_i \psi_j$$

So: $$E = \frac{c_1^2 H_{11} + 2c_1 c_2 H_{12} + c_2^2 H_{22}}{c_1^2 S_{11} + 2c_1 c_2 S_{12} + c_2^2 S_{22}}$$

Next we treat, c_1 and c_2 as variables and solve for minimum E

Two coupled wells (4)

$$\frac{\partial E}{\partial c_1} = \frac{2c_1H_{11} + 2c_2H_{12}}{c_1^2S_{11} + 2c_1c_2S_{12} + c_2^2S_{22}}$$

$$- \frac{c_1^2H_{11} + 2c_1c_2H_{12} + c_2^2H_{22}}{\left(c_1^2S_{11} + 2c_1c_2S_{12} + c_2^2S_{22}\right)^2}\left(2c_1S_{11} + 2c_2S_{12}\right) = 0$$

$$= \frac{2c_1H_{11} + 2c_2H_{12}}{c_1^2S_{11} + 2c_1c_2S_{12} + c_2^2S_{22}}$$

$$- \frac{2c_1S_{11} + 2c_2S_{12}}{c_1^2S_{11} + 2c_1c_2S_{12} + c_2^2S_{22}} E = 0$$

Two coupled wells (5)

Further simplifying:

$$c_1 H_{11} + c_2 H_{12} - \left(c_1 S_{11} + c_2 S_{12}\right)E = 0$$

$$\boxed{c_1\left(H_{11} - ES_{11}\right) + c_2\left(H_{12} - ES_{12}\right) = 0}$$

Similarly using $\dfrac{\partial E}{\partial c_2} = 0$ we calculate:

$$\boxed{c_1\left(H_{21} - ES_{21}\right) + c_2\left(H_{22} - ES_{22}\right) = 0}$$

Two coupled wells (6)

Thus, the determinate:

$$\begin{bmatrix} H_{11} - ES_{11} & H_{12} - ES_{12} \\ H_{21} - ES_{21} & H_{22} - ES_{22} \end{bmatrix} = 0$$

Now we go back to our assumptions…

We assume identical wavefunctions:

$$S_{11} = S_{22} = 1 \qquad H_{11} = H_{22}$$

$$S_{12} = S_{21} \Rightarrow 0 \qquad H_{12} = H_{21} < 0$$

Two coupled wells (7)

Then, the determinate simplifies

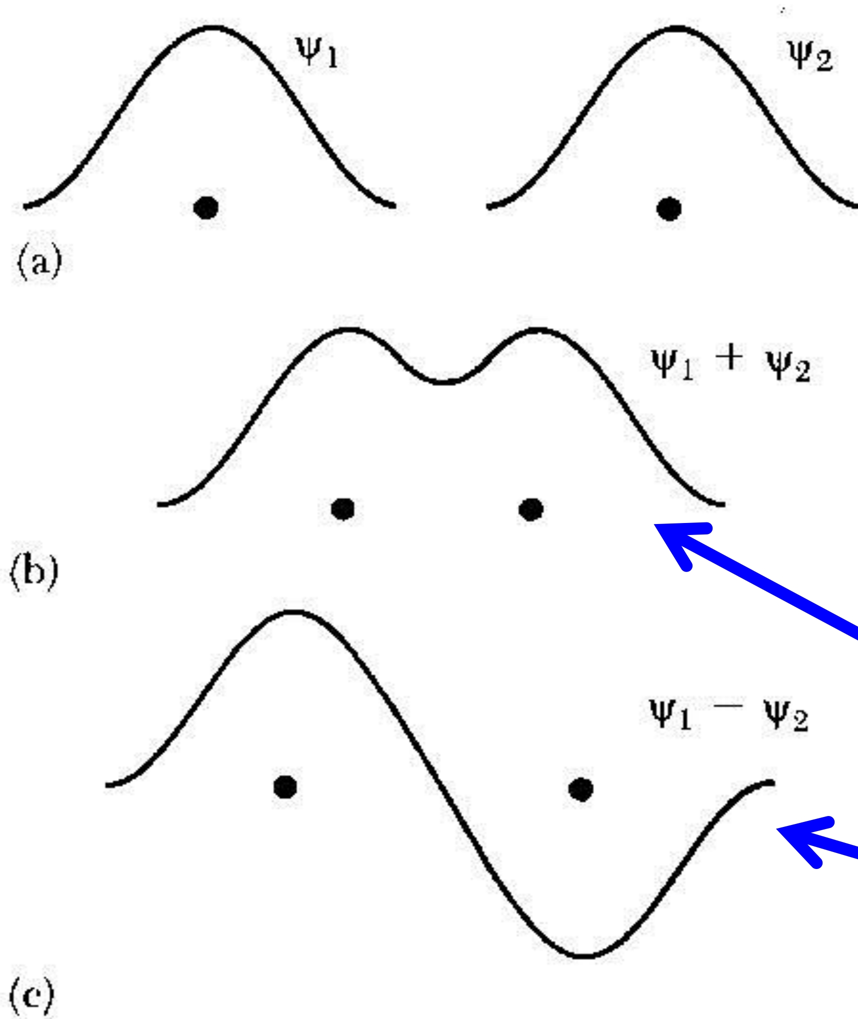
$$(H_{11}-E)^2-H_{12}^2=0$$

And the solutions are: $E=H_{11}\pm|H_{12}|$

$$E_+=H_{11}-|H_{12}| \qquad \rightarrow c_1=c_2 \qquad \text{bonding}$$

$$E_-=H_{11}+|H_{12}| \qquad \rightarrow c_1=-c_2 \qquad \text{Anti-bonding}$$

Two Coupled Wells (8)

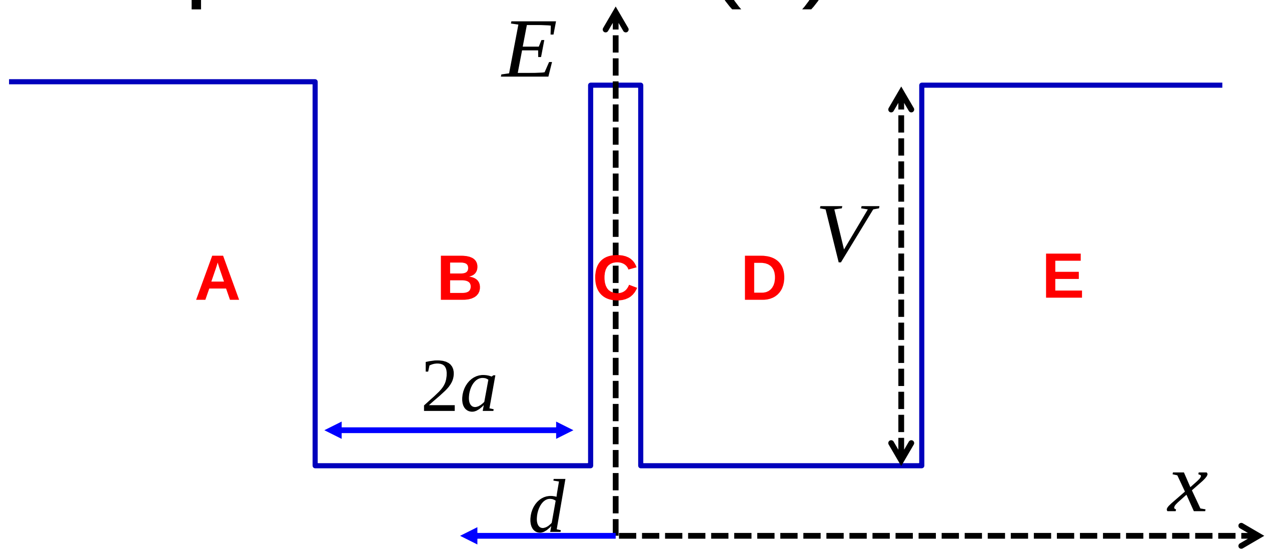


(a) Wave functions of electrons bound to two ion cores at large separation. (b) One linear combination of wave function for electrons bound to ion cores is $\psi_1 + \psi_2$ – called bonding. (c) The other one is the $\psi_1 - \psi_2$ state –called anti-bonding state.

$$c_1 = c_2$$

$$c_1 = -c_2$$

Two Coupled Wells (9)



$$\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2}\left(V(x) - E\right)\psi = 0 \qquad \psi \sim e^{\pm\alpha x}$$

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \qquad \psi \sim \sin(\beta x + \phi)$$

Two Coupled Wells (10)

A $\psi(x) = Ae^{\alpha x}$

B $\psi(x) = B\sin(\beta x + \phi_2)$

C $\psi(x) = C_1 e^{\alpha x} + C_2 e^{-\alpha x}$

D $\psi(x) = D\sin(\beta x + \phi_1)$

E $\psi(x) = Ee^{-\alpha x}$

Note:

$$\psi \ and \ \frac{d\psi}{dx}$$

are both continuous

Two Coupled Wells (11)

At Outside Boundaries:

$$\left.\begin{array}{c} Ee^{-\alpha(d+a)} = D\sin(\beta d + \beta a + \phi_1) \\ -\alpha Ee^{-\alpha(d+a)} = \beta D\cos(\beta d + \beta a + \phi_1) \\ \hline -\dfrac{\beta}{\alpha} = \tan(\beta d + \beta a + \phi_1) \\ \\ Ae^{\alpha(-d-a)} = B\sin(-\beta d - \beta a + \phi_2) \\ \alpha Ae^{\alpha(-d-a)} = \beta B\cos(-\beta d - \beta a + \phi_2) \\ \hline \dfrac{\beta}{\alpha} = \tan(-\beta d - \beta a + \phi_2) = -\tan(\beta d + \beta a - \phi_2) \end{array}\right\} \phi_1 = -\phi_2$$

Two Coupled Wells (12)

Then, if: $\phi_1 = -\phi_2$

$$Ae^{-\alpha(d+a)} = -B\sin(\beta d + \beta a + \phi_1)$$

$$Ee^{-\alpha(d+a)} = D\sin(\beta d + \beta a + \phi_1)$$

$$\frac{A}{E} = -\frac{B}{D}$$

Two Coupled Wells (13)

At Inside Boundaries:

$$C_1 e^{\alpha(d-a)} + C_2 e^{-\alpha(d-a)} = D\sin(\beta d - \beta a + \phi_1)$$

$$\alpha C_1 e^{\alpha(d-a)} - \alpha C_2 e^{-\alpha(d-a)} = \beta D\cos(\beta d - \beta a + \phi_1)$$

$$\frac{\beta}{\alpha} = \tan(\beta d - \beta a + \phi_1)\left(\frac{C_1 e^{\alpha(d-a)} - C_2 e^{-\alpha(d-a)}}{C_1 e^{\alpha(d-a)} + C_2 e^{-\alpha(d-a)}}\right)$$

$$C_1 e^{\alpha(-d+a)} + C_2 e^{-\alpha(-d+a)} = A\sin(-\beta d + \beta a - \phi_1)$$

$$\alpha C_1 e^{\alpha(-d+a)} - \alpha C_2 e^{-\alpha(-d+a)} = \beta A\cos(-\beta d + \beta a - \phi_1)$$

$$\frac{\beta}{\alpha} = \tan(-\beta d + \beta a - \phi_1)\left(\frac{C_1 e^{\alpha(-d+a)} - C_2 e^{-\alpha(-d+a)}}{C_1 e^{\alpha(-d+a)} + C_2 e^{-\alpha(-d+a)}}\right)$$

Two Coupled Wells (14)

Moreover:

$$\frac{\beta}{\alpha} = -\tan(\beta d - \beta a + \phi_1)\left(\frac{C_1 e^{-\alpha(d-a)} - C_2 e^{\alpha(d-a)}}{C_1 e^{-\alpha(d-a)} + C_2 e^{\alpha(d-a)}}\right)$$

So:

$$\frac{C_1 e^{\alpha(d-a)} - C_2 e^{-\alpha(d-a)}}{C_1 e^{\alpha(d-a)} + C_2 e^{-\alpha(d-a)}} = \frac{C_2 e^{\alpha(d-a)} - C_1 e^{-\alpha(d-a)}}{C_2 e^{\alpha(d-a)} + C_1 e^{-\alpha(d-a)}}$$

Eliminating the denominator yields:

$$\rightarrow \left(C_1 e^{\alpha(d-a)} - C_2 e^{-\alpha(d-a)}\right)\left(C_2 e^{\alpha(d-a)} + C_1 e^{-\alpha(d-a)}\right)$$
$$= \left(C_2 e^{\alpha(d-a)} - C_1 e^{-\alpha(d-a)}\right)\left(C_1 e^{\alpha(d-a)} + C_2 e^{-\alpha(d-a)}\right)$$

Two Coupled Wells (15)

Thus:
$$C_1^2 - C_2^2 + \cancel{C_1 C_2 e^{2\alpha(d-a)}} - \cancel{C_1 C_2 e^{-2\alpha(d-a)}}$$
$$= -C_1^2 + C_2^2 + \cancel{C_1 C_2 e^{2\alpha(d-a)}} - \cancel{C_1 C_2 e^{-2\alpha(d-a)}}$$

And simplifying:
$$2C_1^2 = 2C_2^2$$

Therefore:
$$C_1 = \pm C_2$$

And we already calculated: $\dfrac{A}{E} = -\dfrac{B}{D}$

Symmetric, or Anti-symmetric cases…

Two Coupled Wells (16)

Also: $$C_1 e^{\alpha(d-a)} + C_2 e^{-\alpha(d-a)} = D\sin(\beta d - \beta a + \phi_1)$$

$$C_1 e^{-\alpha(d-a)} + C_2 e^{\alpha(d-a)} = -B\sin(\beta d - \beta a + \phi_1)$$

Thus if: $C_1 = -C_2 = C$

$$C\left(e^{\alpha(d-a)} - e^{-\alpha(d-a)}\right) = D\sin(\beta d - \beta a + \phi_1)$$

$$C\left(e^{-\alpha(d-a)} - e^{\alpha(d-a)}\right) = -B\sin(\beta d - \beta a + \phi_1)$$

So: $B = D \qquad A = -E$

$$C\left(e^{\alpha(d-a)} - e^{-\alpha(d-a)}\right) \Rightarrow C\sinh[\alpha(d-a)]$$

Two Coupled Wells (17)

Also: $$C_1 e^{\alpha(d-a)} + C_2 e^{-\alpha(d-a)} = D\sin(\beta d - \beta a + \phi_1)$$

$$C_1 e^{-\alpha(d-a)} + C_2 e^{\alpha(d-a)} = -B\sin(\beta d - \beta a + \phi_1)$$

And if: $C_1 = C_2 = C$

$$C\left(e^{\alpha(d-a)} + e^{-\alpha(d-a)}\right) = D\sin(\beta d - \beta a + \phi_1)$$

$$C\left(e^{-\alpha(d-a)} + e^{\alpha(d-a)}\right) = -B\sin(\beta d - \beta a + \phi_1)$$

So: $B = -D$ $\qquad A = E$

$$C\left(e^{\alpha(d-a)} + e^{-\alpha(d-a)}\right) \Rightarrow C\cosh[\alpha(d-a)]$$

Two Coupled Wells (18)

$$\alpha^2 = \frac{2m(V_0 - E)}{\hbar^2} \qquad \beta^2 = \frac{2mE}{\hbar^2} \qquad \beta^2 + \alpha^2 = \frac{2mV}{\hbar^2}$$

symmetric

$$\frac{\beta}{\alpha} = \tan(\beta(d-a)+\phi_1)\tanh(\alpha(d-a))$$

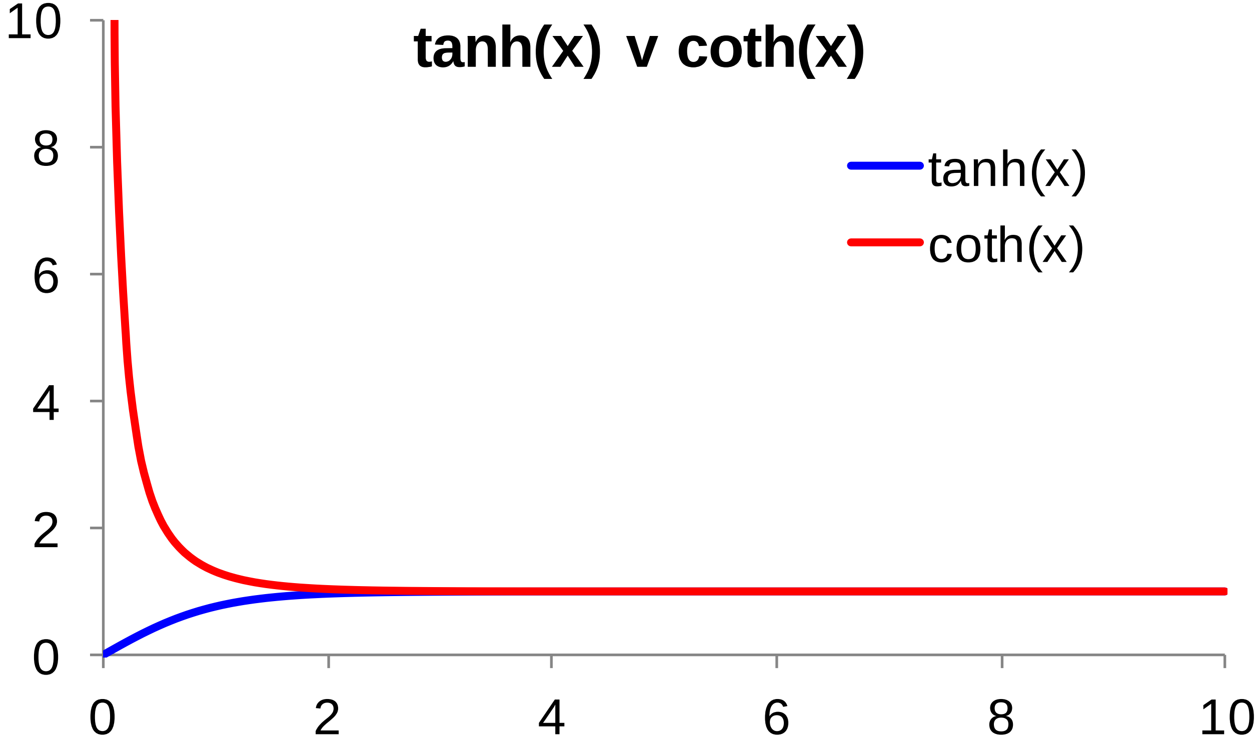
antisymmetric

$$\frac{\beta}{\alpha} = \tan(\beta(d-a)+\phi_1)\coth(\alpha(d-a))$$

Two Coupled Wells (19)

The difference in the modes is based on:

$$\tanh\left(\alpha\left(d-a\right)\right) \qquad \coth\left(\alpha\left(d-a\right)\right)$$



Relevant when:

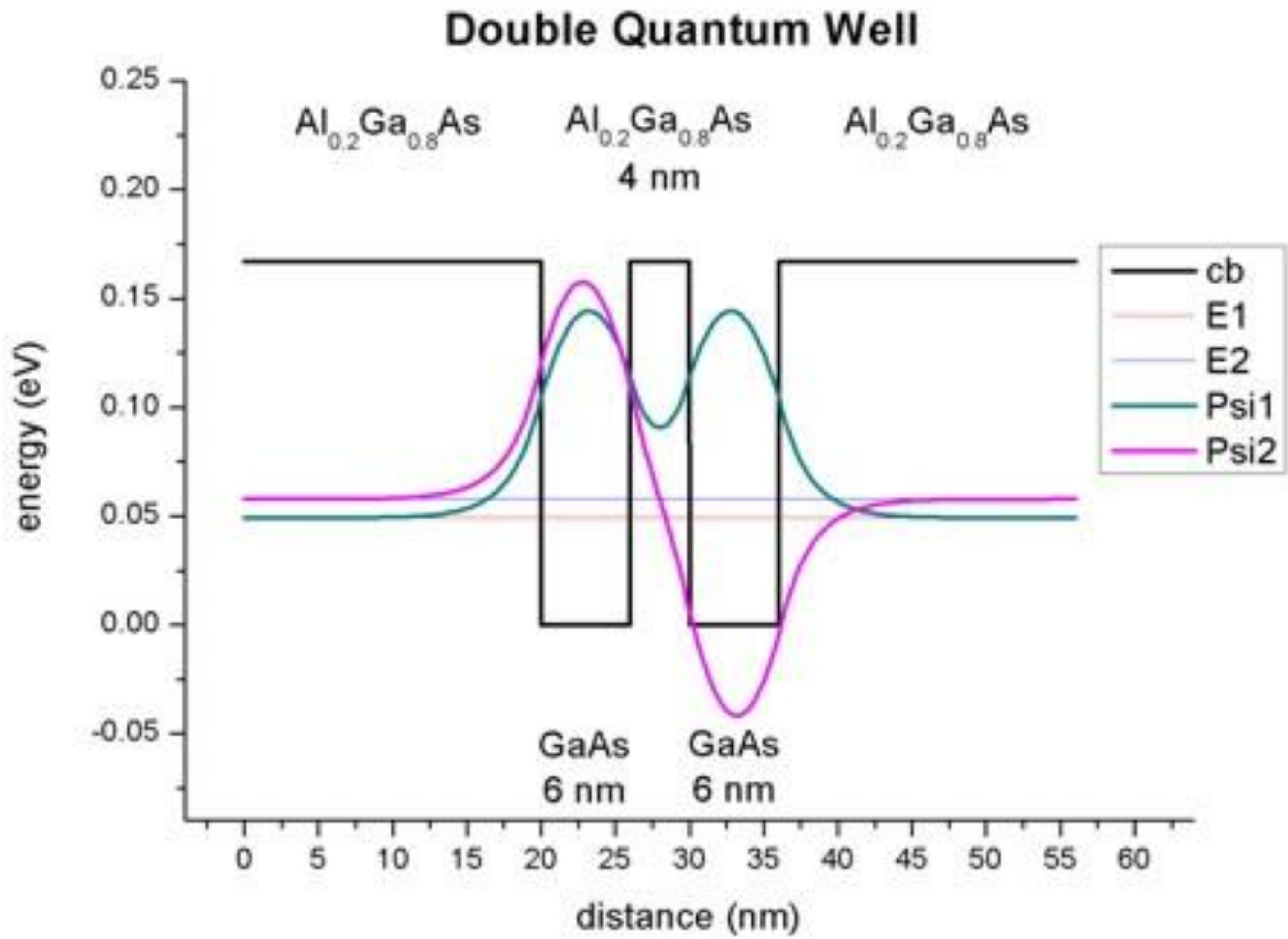
$$x < 2$$

Or: $d - a < \dfrac{2}{\alpha}$

Separation:

$$2\left(d-a\right) < \frac{4}{\alpha}$$

Two Coupled Wells (20)



Two Coupled Wells (21)