

## Homework 2

2.1) a. When  $\vec{k} = 0$ ,  $g_0(\vec{0}) = 4$ ,  $g_1(\vec{0}) = g_2(\vec{0}) = g_3(\vec{0}) = 0$  b/c each of these has  $2(+1) + 2(-1) = 0$ , while  $g_0(\vec{0}) = 4(+1) = 4$ .

This makes the matrix:

$$H = \begin{pmatrix} E_s^A & 0 & 0 & 0 & -4V_0 & 0 & 0 & 0 \\ 0 & E_p^A & 0 & 0 & 0 & 4V_2 & 0 & 0 \\ 0 & 0 & E_p^A & 0 & 0 & 0 & 4V_2 & 0 \\ 0 & 0 & 0 & E_p^A & 0 & 0 & 0 & 4V_2 \\ -4V_0 & 0 & 0 & 0 & E_s^B & 0 & 0 & 0 \\ 0 & 4V_2 & 0 & 0 & 0 & E_p^B & 0 & 0 \\ 0 & 0 & 4V_2 & 0 & 0 & 0 & E_p^B & 0 \\ 0 & 0 & 0 & 4V_2 & 0 & 0 & 0 & E_p^B \end{pmatrix}$$

We are looking for non-trivial solutions to

$H\Psi = E\Psi$ , so we are interested in the allowed  $E$

$$\Rightarrow \det(H - IE) = 0$$

$H - IE$  is a block matrix that looks like:

$$H - IE = \begin{pmatrix} A_1 & A_2 \\ A_2 & A_3 \end{pmatrix}, \quad \text{where } A_1 = \begin{pmatrix} E_s^A - E & 0 \\ E_p^A - E & 0 \\ 0 & E_p^A - E \\ 0 & E_p^A - E \end{pmatrix} \quad A_2 = \begin{pmatrix} -4V_0 & 0 \\ 4V_2 & 0 \\ 0 & 4V_2 \\ 0 & 4V_2 \end{pmatrix}$$

$$A_3 = \begin{pmatrix} E_s^B - E & 0 \\ E_p^B - E & 0 \\ 0 & E_p^B - E \\ 0 & E_p^B - E \end{pmatrix}$$

This is useful because

$$\det(H - IE) = \det(A_1 A_3 - A_2 A_2)$$

just like a normal matrix. These multiplications are easy because these are all diagonal matrices, the diagonal elements just multiply, so we have:

$$\det(H - IE) = \det \begin{pmatrix} (E_s^A - E)(E_s^B - E) - 16V_0^2 & 0 & 0 & 0 \\ 0 & (E_p^A - E)(E_p^B - E) - 16V_2^2 & 0 & 0 \\ 0 & 0 & (E_p^A - E)(E_p^B - E) - 16V_2^2 & 0 \\ 0 & 0 & 0 & (E_p^A - E)(E_p^B - E) - 16V_2^2 \end{pmatrix} = 0$$

The determinant is just the product of the diagonal elements, b/c the matrix is diagonal, and because we have  $\det = 0$ , this can be satisfied if any of the diagonal elements are 0.

The allowed energies, therefore, are found by setting each diagonal to 0. 3 of the diagonals are the same, so this leaves 2 equations:

$$\textcircled{1} E^2 - E(E_s^A + E_s^B) + E_s^A E_s^B - 16V_{so}^2 = 0, \quad \textcircled{2} E^2 - E(E_p^A + E_p^B) + E_p^A E_p^B - 16V_z^2 = 0,$$

with solutions:

$$\textcircled{1} E = \frac{E_s^A + E_s^B}{2} \pm \sqrt{\frac{E_s^{A2} + E_s^{B2} + 2E_s^A E_s^B - 4E_s^A E_s^B + 64V_{so}^2}{4}} = \frac{E_s^A + E_s^B}{2} \pm \sqrt{\left(\frac{E_s^A - E_s^B}{2}\right)^2 + (4V_{so})^2}$$

$$\textcircled{2} E = \frac{E_p^A + E_p^B}{2} \pm \sqrt{\frac{E_p^{A2} + E_p^{B2} + 2E_p^A E_p^B - 4E_p^A E_p^B + 64V_z^2}{4}} = \frac{E_p^A + E_p^B}{2} \pm \sqrt{\left(\frac{E_p^A - E_p^B}{2}\right)^2 + \left(\frac{4}{3}V_{pp\sigma} - \frac{8}{3}V_{pp\pi}\right)^2}$$

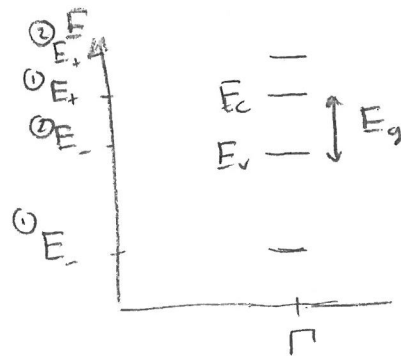
Putting in the #s for GaAs, we get

$$\textcircled{1} E_- = -21.7 \text{ eV}, E_+ = -6.9 \text{ eV}$$

$$\textcircled{2} E_- = -9.1 \text{ eV}, E_+ = -3.7 \text{ eV}$$

From the rest of the band structure we can see that  $E_c$  corresponds to  $\textcircled{1} E_+$ , and  $E_v$  corresponds to  $\textcircled{2} E_-$ .

This looks like:



From  $V_z$  as before  
(and  $V_o = V_{so}$ ).

This means we know for sure that  $E_c(\Gamma) = \textcircled{1} E_+ = \frac{E_s^A + E_s^B}{2} + \sqrt{\left(\frac{E_s^A - E_s^B}{2}\right)^2 + (4V_{so})^2}$ , which comes entirely from  $|s\rangle$  overlaps because only  $E_s^i$  and  $V_{so}$  terms are involved.

b. Likewise,  $E_v = \textcircled{2} E_- = \frac{E_p^A + E_p^B}{2} - \sqrt{\left(\frac{E_p^A - E_p^B}{2}\right)^2 + \left(\frac{4}{3}V_{pp\sigma} - \frac{8}{3}V_{pp\pi}\right)^2}$ , only

$E_p^i$  and  $V_{pp}$  terms are involved, showing that the valence band edges comes entirely from p-orbital energies and p-orbital overlaps.

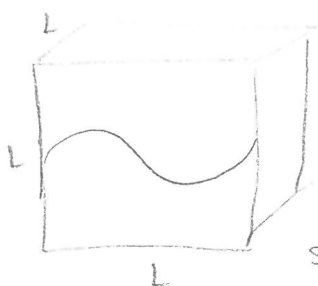
For other compound semiconductors the numbers are different but the trend is the same, the conduction band edge is usually "s-like" and the valence band edge is usually "p-like". As conducting electrons exist in the s-like conduction band, and s orbitals are isotropic, conduction band electrons are also isotropic. As holes exist mostly in the p-like valence band, and p-orbitals are anisotropic, we can also say that holes are anisotropic as well.

2.1 c.) Following the logic from part b, we know that the lowest energy band in compound semiconductors comes from the lowering of energy (banding) of s orbitals. This also makes sense intuitively as the s orbitals overlap more and produce a stronger splitting, in addition to the fact that s orbitals are lower energy to start out with. So between these two arguments, it is clear the bottom band comes from s orbitals.

ZnSe and Ge are both in the same period, but they differ mainly in the ionic nature of the bonds. ZnSe is much more ionic than Ge, and as ionic bonds are relatively isotropic, there will be a smaller dependence on  $\vec{k}$ , which encodes the direction of the electron. This makes the band energy more constant vs.  $\vec{k}$ , resulting in a narrower band.

2.2) a. For an electron allowed to move in d-dimensions,

$\psi = \prod_{j=1}^d e^{ik_j x_j}$ , and in each dimension  $\psi$  must follow periodic boundary conditions over a length  $L$ : So  $e^{ik_j(x_j+L)} = e^{ik_j x_j} \Rightarrow e^{ik_j L} = e^{i2\pi n_j} \Rightarrow k_j = \frac{2\pi n_j}{L}$



$\vec{k}$ -space is now quantized, where the allowed  $\vec{k}$  are  $\vec{k} = \frac{2\pi}{L}(n_1, n_2, \dots, n_d)$ .  $\leftarrow$  if we allow  $n$  to be negative, then we can make this  $2\pi$  instead of  $\frac{\pi}{2}$ .

We want the density of states vs.  $E$ , but we know  $E$  vs.  $k$  so it suffices to find DOS vs.  $k$ .

In a small shell of width  $dk$ , the number of states in the shell will be  $\frac{(\text{Surface area of } d\text{-dimensional shell}) \cdot (\text{thickness of shell})}{\text{volume per state}}$ .  $\nearrow dk \cdot g_s g_v \nearrow$  Spin and valley degeneracy

$S_d = \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} k^{d-1}$  the thickness is just  $dk$ , and the  $\frac{\text{volume}}{\text{state}} = (\Delta k)^d$ .

$\Delta k$  is the distance in  $k$ -space between allowable values, so the volume per state is just  $(\Delta k)^d$  for example in 3D, as this is the volume of a cube with length  $\Delta k$ . In  $d$  dimensions this becomes  $(\Delta k)^d$ .

Note that this is the volume per 1 point, because although each volume contains many vertices, it also touches many neighbors, and in the end  $(\Delta k)^d$  is the primitive unit cell volume.

Finally,  $\Delta k = \frac{2\pi}{L}$  so  $\text{Volume}_{\text{point}} = \left(\frac{2\pi}{L}\right)^d$ .

Putting this together,

# of states between  $k$  and  $k+dk = g_d \frac{2\pi^{\frac{d}{2}} k^{d-1}}{\Gamma(\frac{d}{2})} dk \cdot \frac{L^d}{(2\pi)^d} = dN$

In the end, we want  $g(E) = \frac{\text{\# of states}}{(\text{unit } E)(\text{unit } V)}$ .

The unit  $V$  is easy, just the real space volume in consideration,  $L^d$ .

$\frac{\text{\# of states}}{\text{unit } E} = \frac{dN}{dE} = \frac{dN}{dk} \frac{dk}{dE}$ . We have  $\frac{dN}{dk}$  from

For a parabolic band,  $E = E_c + \frac{\hbar^2 k^2}{2m^*}$  so  $\frac{dE}{dk} = \frac{\hbar^2 k}{m^*} \Rightarrow \frac{dk}{dE} = \frac{m^*}{\hbar^2 k}$ , so:

$g(E) = \frac{2\pi^{\frac{d}{2}} k^{d-1}}{\Gamma(\frac{d}{2}) (2\pi)^d} \cdot \frac{m^*}{\hbar^2 k} \cdot \frac{1}{L^d} g_d$ . Also, from  $k = \left[ \frac{2m^*}{\hbar^2} (E - E_c) \right]^{1/2}$ , so plugging in:

$g_d(E) = g_d \frac{2 \cdot \pi^{\frac{d}{2}} m^*}{2^d \pi^d \hbar^2 \Gamma(\frac{d}{2})} \cdot \frac{2^{\frac{(d-1)}{2}} m^{\frac{(d-1)}{2}}}{\hbar^{(d-2)}} (E - E_c)^{\frac{(d-1)}{2}} = \boxed{\frac{g_d g_v}{2^d \pi^{\frac{d}{2}} \Gamma(\frac{d}{2})} \left( \frac{2m^*}{\hbar^2} \right)^{\frac{d}{2}} (E - E_c)^{\frac{d}{2}-1}}$

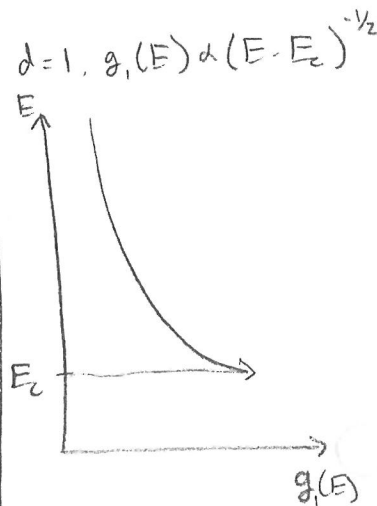
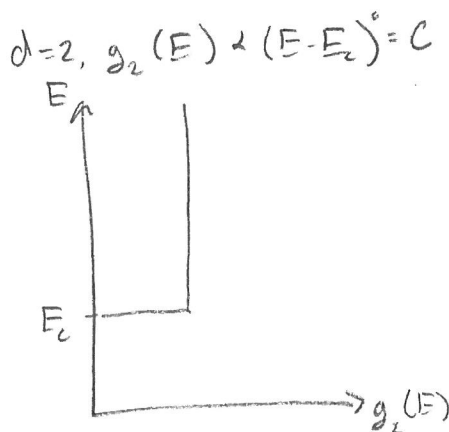
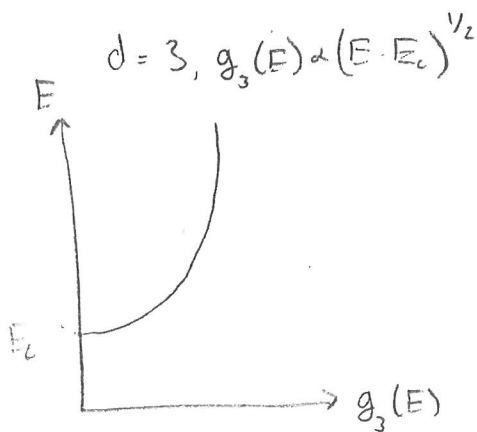
Just checking that the surface area we used was right:

$d=2 \rightarrow$  circle,  $S_2 = \text{circumference} = 2\pi k$ , the formula gives  $S_2 = \frac{2\pi k}{\Gamma(1)} = \boxed{2\pi k} \checkmark$

$d=3 \rightarrow$  sphere,  $S_3 = \text{surface area} = 4\pi k^2$ , the formula gives  $S_3 = \frac{2\pi^{3/2} k^2}{\Gamma(\frac{3}{2})}$ ,

but  $\Gamma(\frac{3}{2}) = \frac{\sqrt{\pi}}{2}$  so  $S_3 = \boxed{4\pi k^2} \checkmark$

To visualize this, we can see that  $g_d(E) = C_d (E - E_c)^{\frac{d}{2}-1}$ , so:



We can also see some important trends in this formula:

Compound semiconductors, which often have a direct band-gap at the  $\Gamma$  point, have  $g_v = 1$  because there is only 1  $\Gamma$  point per unit cell. In Si, however,

the minimum of the conduction band is found near the  $X$  point, which means

$g_v = \text{degeneracy of } X = 3$  (I think). As  $g(E) \propto g_v$ , Si will therefore

have a larger DOS for comparable other parameters.  $\rightarrow$  actually Si's  $\begin{pmatrix} +x \\ -x, y, -y \\ +z, -z \end{pmatrix}$

We can also see that  $g(E) \propto (m^*)^{\frac{d}{2}}$ , which makes sense because if the effective mass is larger than the band is 'fatter'  $\rightarrow$  so there will be more  $k$  values that given a small range of  $E$ -values.



This affects both Si and compound semiconductors equally, depending on how the numbers work out. For Si, which has a larger  $m^*$  at the conduction band minimum, this means it will again have a larger density of states.

## b. Baskett 2.6:

(a) This is very similar to before, all we need to change is  $\frac{dE}{dk}$ ,  $\rightarrow$  and do it with  $d=3$ !

Around the area of interest,  $E = E_0 + CK$ , where  $C$  is a constant, so  $\frac{dE}{dk} = C = \text{const.}$

Before, we had  $g_3(E) = \frac{dN}{dk} \frac{dk}{dE} \frac{1}{L^3} = g_s g_v \frac{2\pi^{\frac{3}{2}}}{\Gamma(\frac{3}{2}) (2\pi)^3} \frac{k^2}{C}$ , also  $k = \frac{(E - E_0)}{C}$

$$\Gamma(\frac{3}{2}) = \frac{\pi^{\frac{1}{2}}}{2}, \text{ so } g_3(E) = \frac{g_s g_v (E - E_0)^2}{2\pi^2 C^3}$$

(b) To get linear dispersion, we can note that it is true classically that  $p = mv$ ,

and  $E = pv$ , so extending this to quantum we can say  $p = \hbar k$ , so  $E = \hbar v k$ .

Then  $\frac{dE}{dk} = \hbar v = \frac{\hbar p}{m^*} = \frac{\hbar^2 k}{m^*}$ , so  $m^* = \hbar^2 k \left( \frac{dE}{dk} \right)^{-1}$ . In the case above, this

would be  $m^* = \frac{\hbar^2 k}{C}$ .

If you use  $e \rightarrow \frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2} \rightarrow m^* \rightarrow \infty$

Actually mass is undefined, from this point of view.

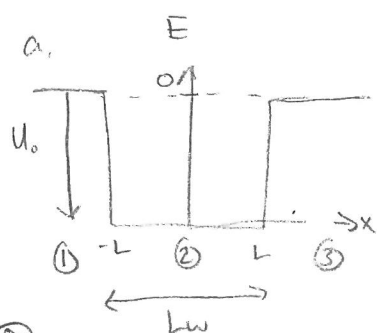
c. This is basically the same problem as part b., with  $C = \hbar v$ . Using the result of part b, with  $C = \hbar v$ , we get (and  $E_0 = 0$ )

$g_s(E) = \frac{g_s g_v}{2\pi^2 (\hbar v)^3} E^2$ . Now that we are talking about waves, there is no spin or valley degeneracy, and instead there is polarization degeneracy because there can be a number of different independent polarizations that all have the same energy.

So replacing  $g_s g_v \rightarrow g_p$ , and also making the substitution  $E = \hbar v k = \hbar \omega$ :

$$g(\omega) = \frac{g_p \hbar^2 \omega^2}{2\pi^2 \hbar^3 v^3} = \boxed{\frac{g_p \omega^2}{2\pi^2 \hbar v^3}}$$

2.3) a.



We have  $-\frac{\hbar^2}{2m^*} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi = E\psi$

In ① and ③  $V(x) = 0$ ,  $\psi(x) = Ae^{ikx} + Be^{-ikx}$

$K' = \sqrt{\frac{2m^* E}{\hbar^2}}$  but for  $\psi = 0$  as  $x \rightarrow \infty$ ,  $B = 0$  in ① and  $A = 0$  in ③

In ②:  $V(x) = -U_0 \Rightarrow \frac{\partial^2 \psi}{\partial x^2} + \frac{2m^*}{\hbar^2} (E + U_0) \psi = 0 \Rightarrow \psi(x) = C \cos Kx + D \sin Kx$

where  $K = \sqrt{\frac{2m^* (E + U_0)}{\hbar^2}}$  and  $E < 0$ .

So we have:  $\left\{ \begin{array}{l} \text{① } \psi(x) = Ae^{K'x} \\ \text{② } \psi(x) = C \cos Kx + D \sin Kx \\ \text{③ } \psi(x) = Be^{-K'x} \end{array} \right\}$

We will look for even solutions, and then odd solutions, as  $[\pi, \hbar] = 0$

Even:  $D = 0$ , and  $B = A$ , so:  $\left\{ \begin{array}{l} \text{① } \psi(x) = Ae^{K'x} \\ \text{② } \psi(x) = C \cos Kx \\ \text{③ } \psi(x) = Ae^{-K'x} \end{array} \right\} \rightarrow \left\{ \begin{array}{l} \psi'(x) = AK'e^{K'x} \\ \psi'(x) = -CK \sin Kx \\ \psi'(x) = -AK'e^{-K'x} \end{array} \right.$

Equating value and derivative at the boundary:  $Ae^{-K'L} = C \cos KL$   
 $AK'e^{-K'L} = -CK \sin(-KL) = CK \sin KL$

Dividing these:  $K \tan KL = K'$

If we define  $\theta = KL$ , then we need  $K'$  in terms of  $K$ . We can see  $K^2 + K'^2 = \left( \frac{2m^* U_0}{\hbar^2} \right)$

so  $\frac{K'}{K} = \sqrt{\frac{2m^* U_0}{K^2 \hbar^2} - 1}$  and putting this into  $\tan(KL) = \frac{K'}{K} = \sqrt{\frac{2m^* U_0}{K^2 \hbar^2} - 1}$

Now we make the substitutions  $\theta = KL$ ,  $\theta_0^2 = \frac{2m^* L^2 U_0}{\hbar^2}$ , so

$$\boxed{\tan \theta = \sqrt{\frac{\theta_0^2}{\theta^2} - 1}}$$

Also  $L = \frac{Lw}{2}$ , so  $\theta = \frac{KLw}{2}$ ,  $\theta_0^2 = \frac{m^* Lw^2 U_0}{2\hbar^2}$

We can do the same thing for odd solutions:

$$\left\{ \begin{array}{l} \textcircled{1} \psi(x) = Ae^{K'x} \\ \textcircled{2} \psi(x) = D \sin Kx \\ \textcircled{3} \psi(x) = -Ae^{-K'x} \end{array} \right. \rightarrow \left\{ \begin{array}{l} \psi'(x) = AK'e^{K'x} \\ \psi'(x) = DK \cos Kx \\ \psi'(x) = -AK'e^{-K'x} \end{array} \right.$$

Boundaries:

$$Ae^{-KL} = D \sin(KL) = -D \sin KL$$

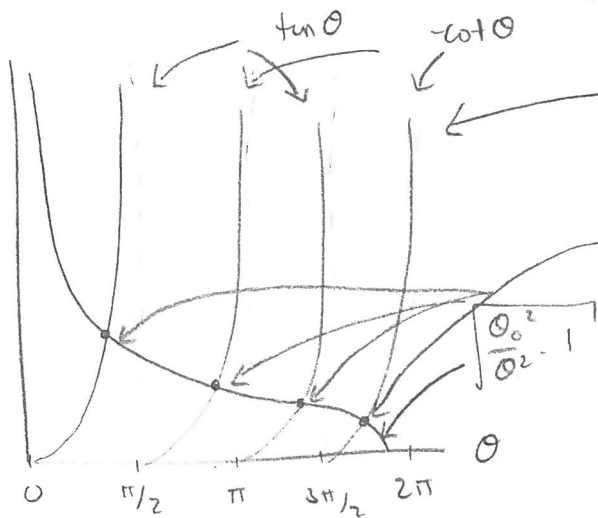
$$AK'e^{-KL} = DK \cos KL$$

Dividing:  $-\frac{K \cos KL}{\sin KL} = K'$ , again  $\frac{K'}{K} = \sqrt{\frac{2m^* U_0}{K^2 \hbar^2} - 1}$ , so  $-\cot KL = \sqrt{\frac{2m^* U_0}{K^2 \hbar^2} - 1}$

$$\text{or } \boxed{-\cot \theta = \sqrt{\frac{\theta_0^2}{\theta^2} - 1}}$$

with  $\theta$ , and  $\theta_0$  as before.

This is now a matter of finding the intersection of  $\sqrt{\frac{\theta_0^2}{\theta^2} - 1}$  and  $\tan \theta$  or  $-\cot \theta$



$\tan \theta$  and  $-\cot \theta$  make these plots, where they alternate even/odd. The allowed  $\theta$  values then come from the intersections of these 2 curves.  $\theta = \frac{KLw}{2}$ , so the allowed

$\theta$  determines the allowed  $K$ , and

$$K = \sqrt{\frac{2m^*(E+U_0)}{\hbar^2}}$$

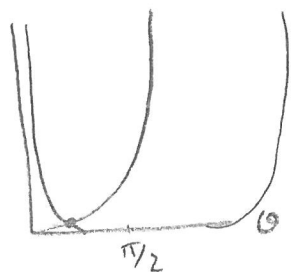
determine the energy levels.

Now we have the eigenvalues and the form of the eigenvectors, so finding the eigenvectors fully is just a matter of normalization, which requires  $\int \psi^* \psi dx = 1$ .

Note: in all of this I am measuring  $E$  down from 0.

(b) Here I measure  $E$  relative to  $0$  which is at the top of the barrier, so  $m_1$  binding energy is  $\varepsilon = -E$ .

As  $U_0 \rightarrow 0$ , there will still be 1 bound state, as the lines still make 1 intersection near  $\theta = 0$ , which by the way makes it an even state.



$\tan \theta = \sqrt{\frac{\theta_0^2}{\theta^2} - 1}$ , so  $\theta_0, \theta, k, E$ , and  $U_0$  are all small quantities.

$\tan \theta \approx \theta$ , so  $\theta = \sqrt{\frac{\theta_0^2}{\theta^2} - 1} \Rightarrow \theta^4 = \theta_0^2 - \theta^2 \Rightarrow \theta^4 + \theta^2 - \theta_0^2 = 0$

This is just a quadratic eqn:  $\theta^2 = \frac{-1 \pm \sqrt{1 + 4\theta_0^2}}{2} = \frac{-1}{2} + \frac{1}{2}\sqrt{1 + (2\theta_0)^2}$

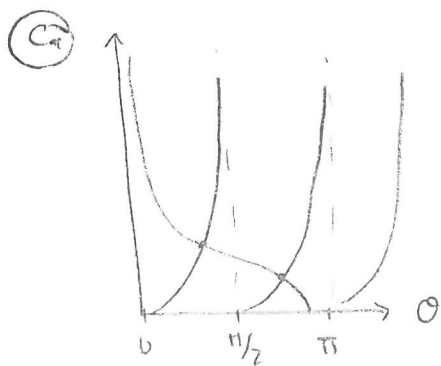
Taylor expanding to 2nd order in  $\theta_0^2$  (4th order in  $\theta_0$ ):

$$\theta^2 = \frac{1}{2} \left( -1 + 1 + \frac{(2\theta_0)^2}{2} - \frac{(2\theta_0)^4}{8} \right) = \theta_0^2 - \theta_0^4$$

Putting everything in terms of  $E$ :  $E + U_0 = \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2}{2m^*} \frac{4\theta^2}{L_w^2} = U_0 \frac{\theta^2}{\theta_0^2}$

so  $E + U_0 = U_0(1 - \theta_0^2) \Rightarrow E = -U_0\theta_0^2$

As I said before,  $\varepsilon = -E = \boxed{\theta_0^2 U_0}$



The number of bound states will be the number of multiples of  $\frac{\pi}{2}$  that  $\sqrt{\frac{\theta_0^2}{\theta^2} - 1}$  crosses before it reaches  $0$ .

$\sqrt{\frac{\theta_0^2}{\theta^2} - 1} = 0$  when  $\theta = \theta_0$ , so  $\left\lceil \frac{\theta_0}{\pi/2} \right\rceil = \text{ceil}\left(\frac{2\theta_0}{\pi}\right) = \# \text{ of bound states}$

$\text{ceil}\left(\frac{2\theta_0}{\pi}\right) = 1 + \text{floor}\left(\frac{2\theta_0}{\pi}\right) = \boxed{1 + \text{Int}\left[\frac{2\theta_0}{\pi}\right] = \# \text{ of bound states}}$

$$\frac{2\theta_0}{\pi} = \frac{2}{\pi} \frac{L_w}{\sqrt{2}\hbar} \sqrt{m^* U_0} = \frac{\sqrt{2}}{\pi} \frac{L_w(\text{nm})}{1 \text{ nm}} \sqrt{\frac{m^*}{m_0} U_0 m_0 \frac{(1 \text{ nm})^2}{\hbar^2}} = \frac{\sqrt{2}}{\pi} \frac{L_w(\text{nm})}{1 \text{ nm}} \sqrt{\frac{m^*}{m_0} U_0 (9.11 \times 10^{-31} \text{ kg}) (1 \text{ nm}^2) (2\pi)^2 / (4.136 \times 10^{-15} \text{ eV} \cdot \text{s})^2 (1 \text{ eV}^2 \cdot \text{s}^2)}$$

$1 \text{ eV} = e^2 (1.78 \times 10^{-36} \text{ kg}) = (3 \times 10^8 \text{ m/s})^2 ( ) = (3 \times 10^8 \cdot 10^9 \text{ nm/s})^2 (1.78 \times 10^{-36} \text{ kg})$   
 $= 0.1602 \text{ nm}^2 \text{ kg s}^{-2}$

so  $\frac{2\theta_0}{\pi} = \frac{\sqrt{2}}{\pi} \frac{L_w}{1 \text{ nm}} \sqrt{\frac{m^*}{m_0} \frac{U_0}{1 \text{ eV}} 0.33} = 1.63 \frac{L_w}{1 \text{ nm}} \sqrt{\frac{m^*}{m_0} \frac{U_0}{1 \text{ eV}}} \Rightarrow \boxed{N = 1 + \text{Int}\left[1.63 \left(\frac{L_w}{1 \text{ nm}}\right) \sqrt{\frac{m^*}{m_0} \frac{U_0}{1 \text{ eV}}}\right]}$



d. 2.6.4:

a. This is just like before:

$$C e^{-kL} = A \cos kL - B \sin kL$$

$$C k e^{-kL} = A k \sin kL + B k \cos kL$$

at  $x = -L$

↓

$$k = k \frac{A \sin kL + B \cos kL}{A \cos kL - B \sin kL}$$

$$D e^{-kL} = A \cos kL + B \sin kL$$

$$-D k e^{-kL} = A k \sin kL + B k \cos kL$$

at  $x = L$

$$k = k \frac{A \sin kL - B \cos kL}{A \cos kL + B \sin kL}$$

b.  $U_0 = 85 \text{ meV}$ ,  $L_w = 4 \text{ nm}$ ,  $m^* = 0.45$  (assuming heavy holes)

$$\theta_0^2 = 4.01, \text{ so } N = 1 + \text{Int} \left[ \frac{2}{\pi} (2) \right] = 2$$

So there are two bound states

To get the energies, I just solved  $\left[ \frac{\theta_0^2}{\theta^2} - 1 \right] = \tan \theta, -\cot \theta$  numerically

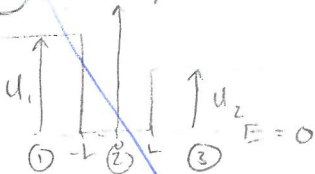
$$\Rightarrow \theta = 1.03, 1.90$$

$$U_0 + E = \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2 \theta^2 \cdot 4}{2m^* L_w^2} = \frac{\theta^2}{\theta_0^2} U_0 \Rightarrow E = U_0 \left( \frac{\theta^2}{\theta_0^2} - 1 \right) = -62 \text{ meV}, -8.7 \text{ meV}$$

but the well is "upside down" so this means the energies are 62 and 8.7 meV above the free electron energy:



(e) If you have an asymmetric well,



We can do the same thing:

$$\psi_1 = A e^{k_1 x}$$

$$\psi_2 = B \cos kx + C \sin kx$$

$$\psi_3 = D e^{-k_2 x}$$

$$\psi_1' = A k_1 e^{k_1 x}$$

$$\psi_2' = -B k \sin kx + C k \cos kx$$

$$\psi_3' = -D k_2 e^{-k_2 x}$$

$$A e^{-k_1 L} = B \cos kL - C \sin kL$$

$$A k_1 e^{-k_1 L} = B k \sin kL + C k \cos kL$$

$$k_1 = k \frac{B \sin kL + C \cos kL}{B \cos kL - C \sin kL}$$

Same thing as before, so now

$$k_2 = k \frac{B \sin kL - C \cos kL}{B \cos kL + C \sin kL}$$

$$\text{We also have } k = \frac{2m^* E}{\hbar}$$

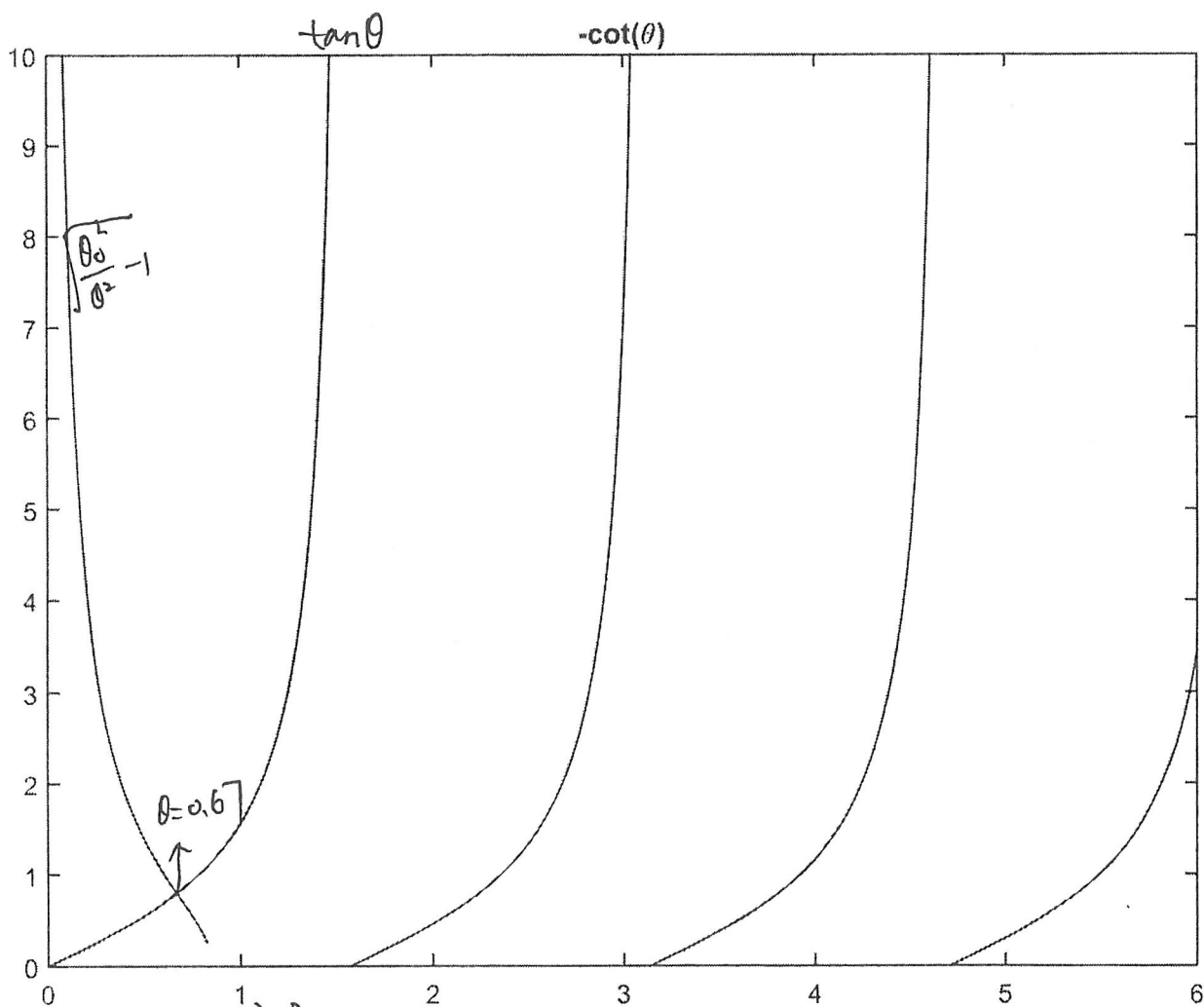
$$k_1 = \frac{\sqrt{2m^* (U_1 - E)}}{\hbar}$$

$$k_2 = \frac{\sqrt{2m^* (U_2 - E)}}{\hbar}$$

Rockett 2.6.4

light hole

1 State



$$E_1 = \frac{\hbar^2 k^2}{2m^*} - U_0$$

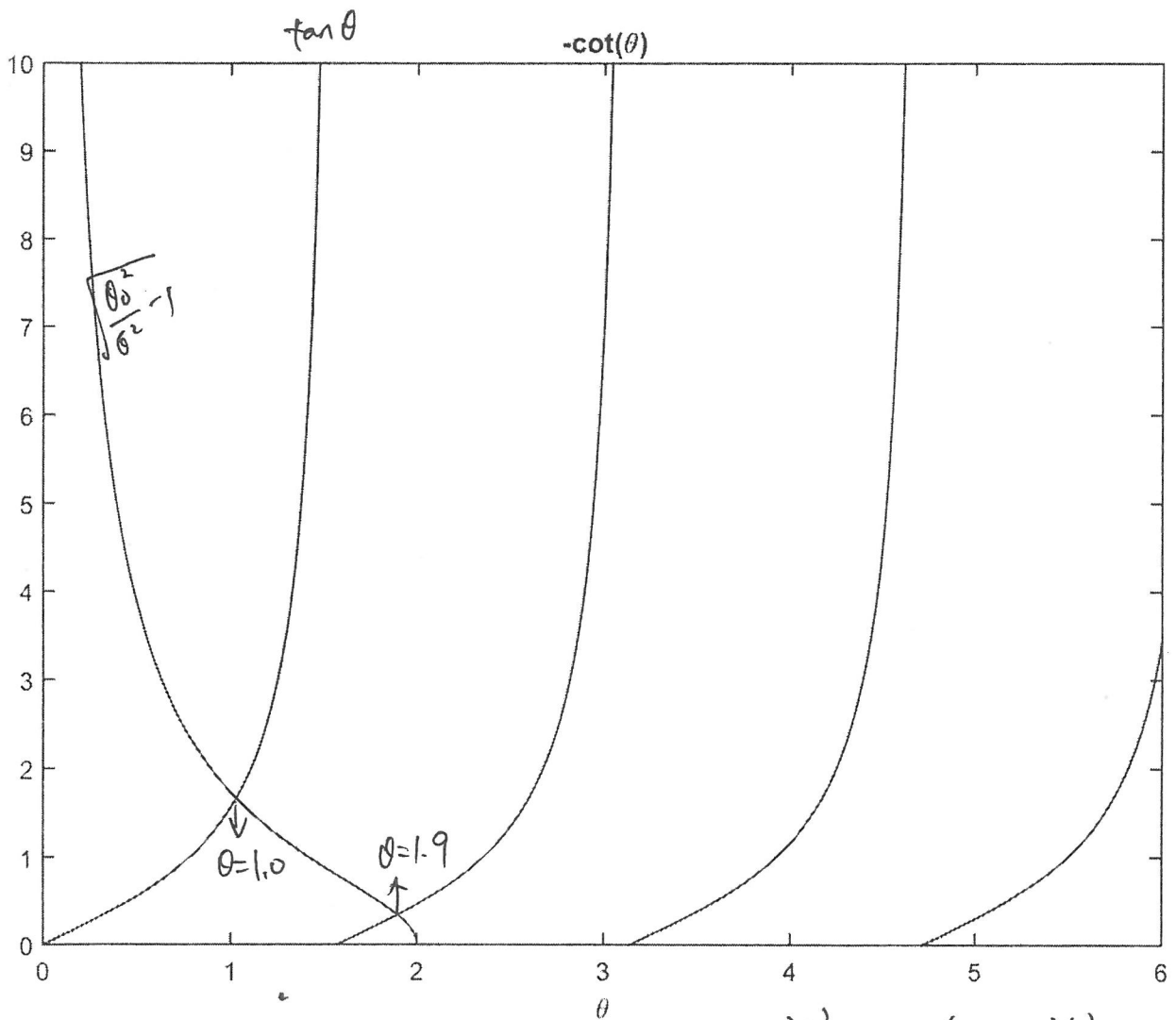
$$k = \frac{2\theta}{2\omega} = \frac{2 \times 0.67}{4 \times 10^{-9}} = 3.35 \times 10^8 \text{ m}^{-1}$$

$$\therefore E_1 = \frac{(1.055 \times 10^{-34})^2 \times (3.35 \times 10^8)^2}{2 \times (0.082 \times 9.11 \times 10^{-31})} - U_0$$

$$= 52 \text{ meV} - 85 \text{ meV} = \boxed{-33 \text{ meV}}$$

Rockett 2.6.4

heavy hole  
2 States



$$k_1 = \frac{2\theta_1}{L_w} = \frac{2 \times 1.0}{4 \times 10^{-9}} = 5 \times 10^8 \text{ m}^{-1}$$

$$E_1 = \frac{\hbar^2 k_1^2}{2m^*} - U_0 = \frac{(1.055 \times 10^{-34})^2 \times (5 \times 10^8)^2}{2 \times (0.45 \times 9.11 \times 10^{-31})} - U_0$$

$$= -64 \text{ meV}$$

$$k_2 = \frac{2\theta_2}{L_w} = 9.5 \times 10^8 \text{ m}^{-1}$$

$$E_2 = \frac{(1.055 \times 10^{-34})^2 \times (9.5 \times 10^8)^2}{2 \times (0.45 \times 9.11 \times 10^{-31})} - U_0$$

$$= -8.4 \text{ meV}$$



PROBLEM 2. Determine the energy levels for the potential well shown in Fig. 2 (p. 66).

SOLUTION. The spectrum of energy values  $E < U_1$ , which we shall consider, is discrete. In the region  $x < 0$  the wave function is

$$\psi = c_1 e^{\kappa_1 x}, \text{ where } \kappa_1 = \sqrt{[(2m/\hbar^2)(U_1 - E)]},$$

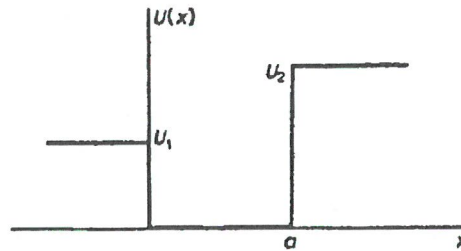


FIG. 2

while in the region  $x > a$

$$\psi = c_2 e^{-\kappa_2 x}, \text{ where } \kappa_2 = \sqrt{[(2m/\hbar^2)(U_2 - E)]}.$$

Inside the well ( $0 < x < a$ ) we look for  $\psi$  in the form

$$\psi = c \sin(kx + \delta), \text{ where } k = \sqrt{(2mE/\hbar^2)}.$$

The condition of the continuity of  $\psi'/\psi$  at the edges of the well gives the equations

$$k \cot \delta = \kappa_1 = \sqrt{[(2m/\hbar^2)U_1 - k^2]}, \quad k \cot(ka + \delta) = -\kappa_2 = -\sqrt{[(2m/\hbar^2)U_2 - k^2]}.$$

or

$$\sin \delta = k \hbar \sqrt{(2mU_1)}, \quad \sin(ka + \delta) = -k \hbar \sqrt{(2mU_2)}.$$

Eliminating  $\delta$ , we obtain the transcendental equation

$$ka = n\pi - \sin^{-1}[k \hbar \sqrt{(2mU_1)}] - \sin^{-1}[k \hbar \sqrt{(2mU_2)}] \quad (1)$$

(where  $n = 1, 2, 3, \dots$ , and the values of the inverse sine are taken between 0 and  $\frac{1}{2}\pi$ ), whose roots determine the energy levels  $E = k^2 \hbar^2 / 2m$ . For each  $n$  there is in general one root; the values of  $n$  number the levels in order of increasing energy.

Since the argument of the inverse sine cannot exceed unity, it is clear that the values of  $k$  can lie only in the range from 0 to  $\sqrt{(2mU_1/\hbar^2)}$ . The left-hand side of equation (1) increases monotonically with  $k$ , and the right-hand side decreases monotonically. Hence it is necessary, for a root of equation (1) to exist, that for  $k = \sqrt{(2mU_1/\hbar^2)}$  the right-hand side should be less than the left-hand side. In particular, the inequality

$$a \sqrt{(2mU_1)} \cdot \hbar > \frac{1}{2}n\pi - \sin^{-1} \sqrt{(U_1/U_2)}, \quad (2)$$

which is obtained for  $n = 1$ , is the condition that at least one energy level exists in the well. We see that for given and unequal  $U_1, U_2$  there are always widths  $a$  of the well which are so small that there is no discrete energy level. For  $U_1 = U_2$ , the condition (2) is evidently always satisfied.

For  $U_1 = U_2 \equiv U_0$  (a symmetrical well), equation (1) reduces to

$$\sin^{-1}[k \hbar \sqrt{(2mU_0)}] = \frac{1}{2}(n\pi - ka). \quad (3)$$

Introducing the variable  $\xi = \frac{1}{2}ka$ , we obtain for odd  $n$  the equation

$$\cos \xi = \pm \gamma \xi, \text{ where } \gamma = (\hbar a) \sqrt{(2mU_0)}, \quad (4)$$

and those roots of this equation must be taken for which  $\tan \xi > 0$ . For even  $n$  we obtain the equation

$$\sin \xi = \pm \gamma \xi, \quad (5)$$

and we must take those roots for which  $\tan \xi < 0$ . The roots of these two equations determine the energy levels  $E = 2\xi^2 \hbar^2 / ma^2$ . The number of levels is finite when  $\gamma \neq 0$ .

In particular, for a shallow well in which  $U_0 \ll \hbar^2 / ma^2$ , we have  $\gamma \gg 1$  and equation (5) has no root. Equation (4) has one root (with the upper sign on the right-hand side),  $\xi \approx 1/\gamma - 1/2\gamma^3$ . Thus the well contains only one energy level,

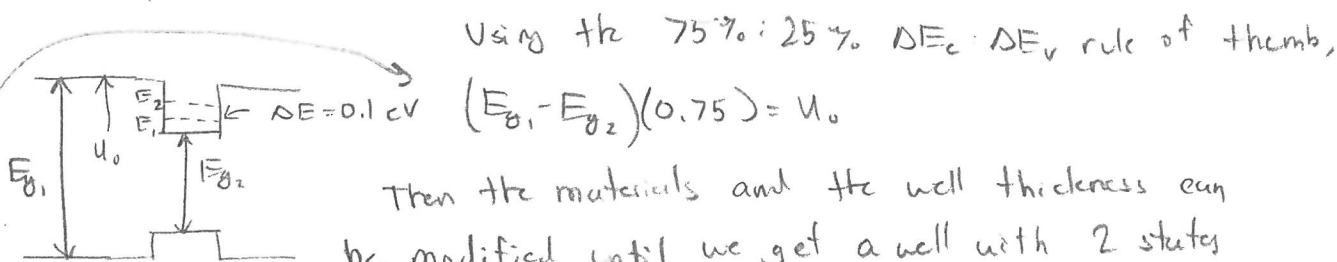
$$E_0 \approx U_0 - (ma^2/2\hbar^2)U_0^2,$$

which is near the top of the well.

2.4) First of all, as we are using intersubband transitions in a III-V quantum well, we know we will need a well with 2 bound states with an energy separation that corresponds to  $\lambda = 12.4 \mu\text{m}$

$$\Delta E (\text{eV}) = \frac{1.24}{\lambda (\mu\text{m})} = 0.1 \text{ eV}$$

This looks like:



Using the 75%:25%  $\Delta E_c : \Delta E_v$  rule of thumb,

$$(E_{c1} - E_{v2})(0.75) = U_0$$

Then the materials and the well thickness can be modified until we get a well with 2 states where  $\Delta E = 0.1 \text{ eV}$ .

The parameters chosen that turn out to work well are:

GaAs,  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ , with a 8.06 nm thickness

With these materials, GaAs is the material with the  $e^-$  band states and AlGaAs is the barrier. Because GaAs holds the  $e^-$ ,  $m^* = 0.067 m_0$

From the chart,  $E_g(\text{GaAs}) = 1.42 \text{ eV}$  and  $E_g(\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}) = 1.65 \text{ eV}$ ,

so by  $U_0 = 0.169 \text{ eV}$

With these parameters,  $\Theta_0 = 2.19$ , so  $N = 1 + \text{Int}(1.39) = 2$ , so there are exactly 2 bound states which means, at least with intersubband transitions, this material will only absorb 1 wavelength of light.

Numerically, we can solve  $\tan \Theta = \sqrt{\frac{\Theta_0^2}{\Theta^2} - 1}$  and  $-\cot \Theta = \sqrt{\frac{\Theta_0^2}{\Theta^2} - 1}$

to get  $E_2$  and  $E_1$ , and then  $\Delta E = E_2 - E_1 = \boxed{0.1 \text{ eV}}$

which is exactly what we wanted. Furthermore, the plot of  $\tan \Theta$  and  $-\cot \Theta$  vs.  $\sqrt{\frac{\Theta_0^2}{\Theta^2} - 1}$  is attached, showing that there are indeed 2 states. From the plot we can also see that if  $\Theta_0$  is slightly different, the  $\Delta \Theta$  (and therefore  $\Delta E$ ) will be approx unchanged, and in particular another state will not be introduced if  $\Theta_0$  changes a little.



Lastly, we have to make sure we can grow this.

$$a_0(\text{AlAs}) = 5.66 \text{ \AA}, a_0(\text{GaAs}) = 5.651 \text{ \AA}, \text{ so } a_0(\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}) = 5.654$$

and  $\varepsilon = \frac{a_0(\text{AlGaAs}) - a_0(\text{GaAs})}{a_0(\text{GaAs})} \approx 0.0005$

so  $t_{\text{max}} \sim \frac{0.56}{2\varepsilon} \text{ nm} = 590 \text{ nm}$ , so for our 8.06 nm layers there will be no issue of defects from strain. That 8.06 nm  $\ll$  590 nm also means that the design is robust, there is very little room for defects to occur,

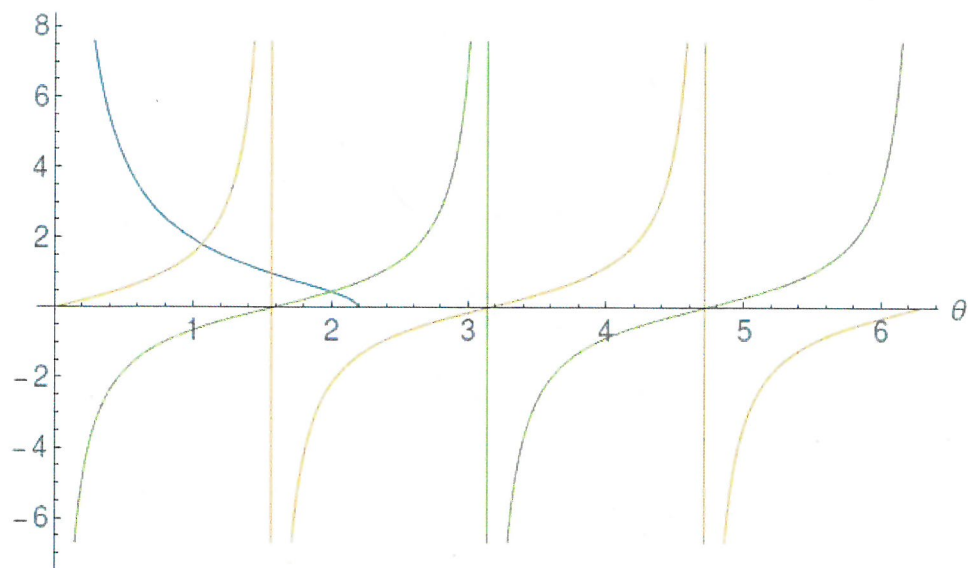


Figure 1: Graphical solution for the quantum well outlined in problem 2.4, showing the existence of two bound states and the robustness of the design to handle small changes in the parameters.