HW #2

(corrected 9/29)

1. 3-dim box:

$$E(n_1,n_2,n_3) = \frac{h^2}{8m}\left[\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2}\right]$$

a) for a cubical box $L_1 = L_2 = L_3 = L$

and $E(n_1,n_2,n_3) = \frac{h^2}{8mL^2}\left(n_1^2 + n_2^2 + n_3^2\right)$

lowest level: $n_1 = n_2 = n_3 = 1$

$E_{111} = \frac{3h^2}{8mL^2}$ obviously nondegenerate

Next level:

$n_1 = 2,\ n_2 = n_3 = 1$

$n_1 = 1,\ n_2 = 2,\ n_3 = 1$

$n_1 = n_2 = 1,\ n_3 = 2$

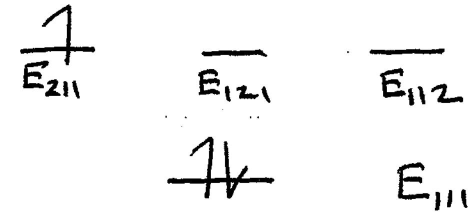
$$E_{211} = E_{121} = E_{112} = \frac{h^2}{8mL^2}\left(2^2 + 1^2 + 1^2\right)$$

$$= \frac{6h^2}{8mL^2}$$

triply degenerate

b) cubical box w/ 3 electrons inside

— draw an energy level diagram



$$E_{total} = 2E_{111} + E_{211} = 2\left(\frac{3h^2}{8mL^2}\right) + \frac{6h^2}{8mL^2}$$

$$= \boxed{\frac{12h^2}{8mL^2}}$$

c) upon distorting the box, $V = \text{constant} = L_1^2 L_3$

and $E = \frac{h^2}{8m}\left(\frac{6}{L_1^2} + \frac{6}{L_3^2}\right)$ for $L_3 > L_1$

(this is the total energy of our 3-electron system)

since $L_3 > L_1$, let's minimize L_1 to find the lowest energy: note that $L_3 = V/L_1^2$!

$$\frac{\partial E}{\partial L_1} = 0 = \frac{\partial}{\partial L_1}\left[\frac{h^2}{8m}\left(\frac{6}{L_1^2} + \frac{6}{(V/L_1^2)^2}\right)\right] = \frac{\partial}{\partial L_1}\left[\frac{h^2}{8m}\left(\frac{6}{L_1^2} + \frac{6L_1^4}{V^2}\right)\right]$$

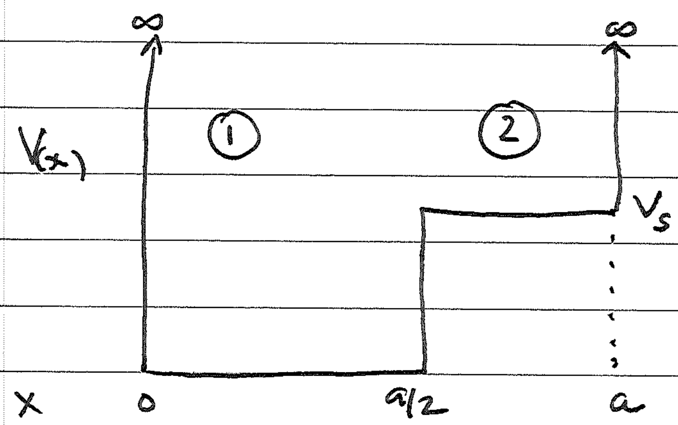
$$= \frac{h^2}{8m}\left(\frac{-12}{L_1^3} + \frac{24L_1^3}{V^2}\right)$$

or $$24L_1^6 = 12V^2$$

$$L_1^3 = \frac{1}{\sqrt{2}}V = \frac{1}{\sqrt{2}} L_1^2 L_3$$

$$\Rightarrow \boxed{\frac{L_3}{L_1} = \sqrt{2}}$$

(2)



general solutions:

$$\psi_1 = A\sin(k_1 x) + B\cos(k_1 x)$$

$$\psi_2 = C\sin(k_2 x) + D\cos(k_2 x)$$

where $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$

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

(a) b.c:

$$\psi_1(x=0) = 0$$

$$\psi_2(x=a) = 0$$

$$\psi_1(x=a/2) = \psi_2(x=a/2)$$

$$\psi_1'(x=a/2) = \psi_2'(x=a/2)$$

(b) for $x < a/2$

$$\psi_1(x=0) = 0 = A\sin(0) + B\cos(0)$$

$$\therefore\ B = 0 \qquad \text{and} \qquad \psi_1 = A\sin(k_1 x)$$

(c) for $E > V_s$ and $x > a/2$

$$\psi_2(x=a) = 0 = C\sin(k_2 a) + D\cos(k_2 a)$$

$$\text{or} \quad D = -C\tan(k_2 a)$$

$$\psi_2 = C\left[\sin(k_2 x) - \tan(k_2 a)\cos(k_2 x)\right]$$

Note: we could also have chosen $\psi_2 = C\sin\left[k_2(x-a)\right]$ which is easier.

(d) at $x = a/2$, use logarithmic matching:

$$\frac{\psi_1'(a/2)}{\psi_1(a/2)} = \frac{\psi_2'(a/2)}{\psi_2(a/2)}$$

$$\psi_1'(a/2) = Ak_1\cos(k_1 a/2) \qquad \psi_1(a/2) = A\sin(k_1 a/2)$$

$$\psi_2'(a/2) = C\left[k_2\cos(k_2 a/2) + \tan(k_2 a)\, k_2 \sin(k_2 a/2)\right]$$

$$\psi_2(a/2) = C\left[\sin(k_2 a/2) - \tan(k_2 a)\cos(k_2 a/2)\right]$$

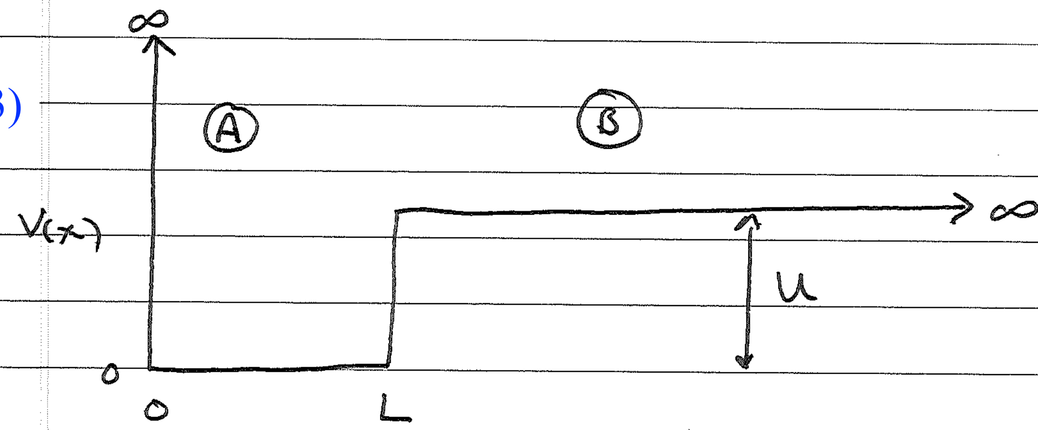
$$\therefore \quad \frac{k_1 \cos(k_1 a/2)}{\sin(k_1 a/2)} = \frac{k_2\left[\cos(k_2 a/2) + \tan(k_2 a)\sin(k_2 a/2)\right]}{\sin(k_2 a/2) - \tan(k_2 a)\cos(k_2 a/2)}$$

it's a bit messy, but only certain energies will satisfy this equation

remember $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$

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

(3)



$$\psi_A = A\sin(k_A x) \qquad \psi_B = B\sin(k_B x + \delta)$$

$$k_A = \sqrt{\frac{2mE}{\hbar^2}} \qquad k_B = \sqrt{\frac{2m(E-U)}{\hbar^2}}$$

(a) find the phase shift δ by matching at $x=L$.

$$\frac{\psi_A'(L)}{\psi_A(L)} = \frac{\psi_B'(L)}{\psi_B(L)}$$

$$\frac{A k_a \cos(k_a L)}{A\sin(k_A L)} = \frac{B k_B \cos(k_B L + \delta)}{B\sin(k_B L + \delta)}$$

$$k_a \cot(k_a L) = k_B \cot(k_B L + \delta)$$

$$\frac{k_A}{k_B} = \frac{\cot(k_B L + \delta)}{\cot(k_A L)} \quad \text{or} \quad \frac{k_B}{k_a} = \frac{\tan(k_B L + \delta)}{\tan(k_A L)}$$

$$\therefore \tan^{-1}\left[\tan(k_A L)\frac{k_B}{k_A}\right] - k_B L$$

now use this together with $\psi_A(L) = \psi_B(L)$

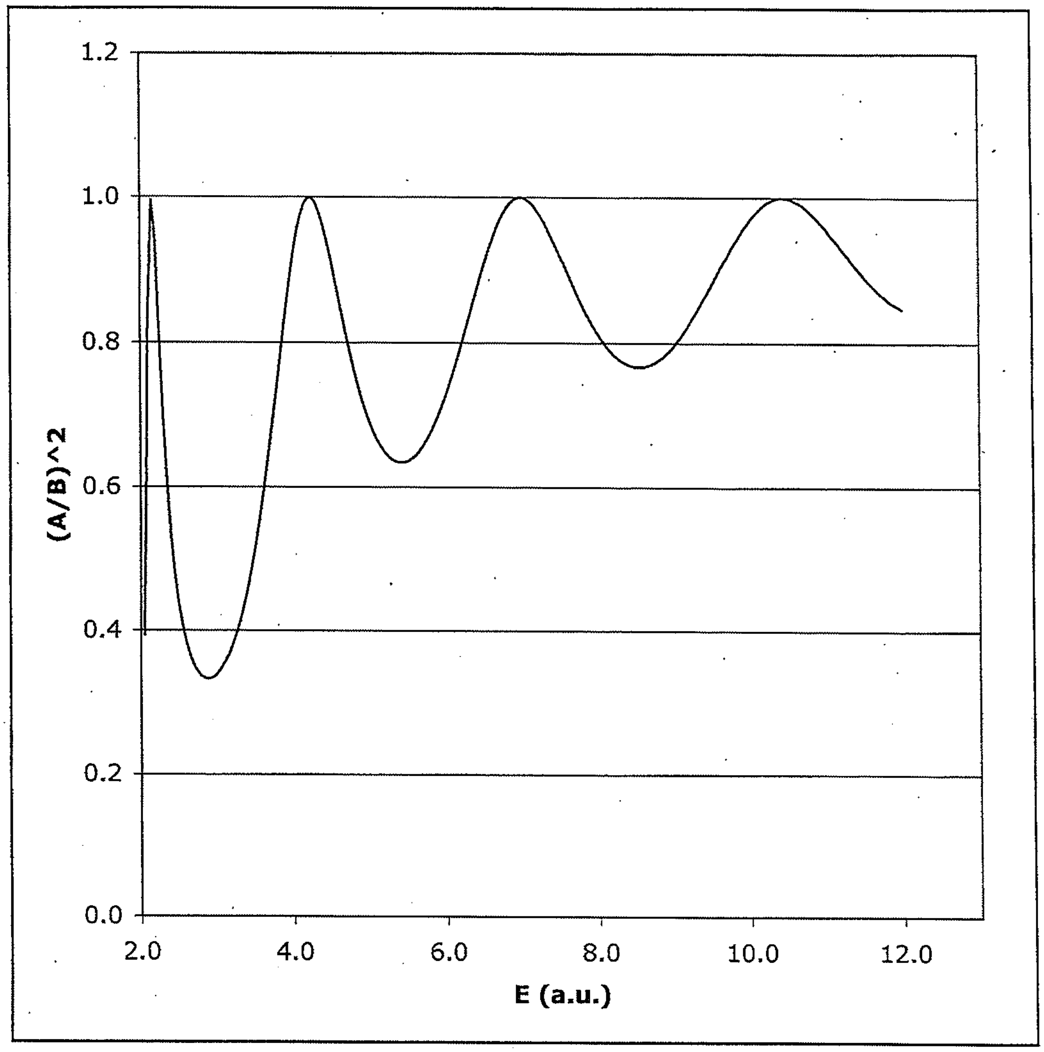
$$\frac{A}{B} = \frac{\sin(k_B L + \delta)}{\sin(k_A L)}$$

$$= \frac{\sin\left[\tan^{-1}\left(\frac{k_B}{k_A}\tan k_A L\right)\right]}{\sin(k_A L)}$$

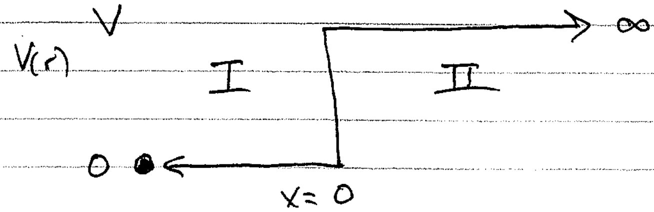
(b) see the next page for a plot of $\left(\frac{A}{B}\right)^2$

one sees resonances at about

$E = 2.15$ a.u, 4.25 a.u., 7.00 a.u., 10.45 a.u.


1.2
1.0
0.8
0.6
0.4
0.2
0.0
(A/B)^2
2.0
4.0
6.0
8.0
10.0
12.0
E (a.u.)

(4)



(a) in zone I $(x<0)$

$$H = \frac{-\hbar^2}{2m_e}\frac{d^2}{dx^2}$$

$$k = \sqrt{\frac{2m_e E}{\hbar^2}}$$

in zone II $(x>0)$

$$H = \frac{-\hbar^2}{2m_e}\frac{d^2}{dx^2} + V$$

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

(b) for $E<V$, $k' = \sqrt{\frac{2m_e(E-V)}{\hbar^2}}$ is pure imaginary

let $k' = iK$ where $K = \sqrt{\frac{2m_e(V-E)}{\hbar^2}}$

which is pure real

then $\psi_{II} = A'e^{-Kx} + B'e^{+Kx}$

but $B'e^{Kx} \to \infty$ as $x \to \infty$, which is not allowed

so $B'=0$ and $\psi_{II} = A'e^{-Kx}$

(c) for $E \leq V$ $\psi_I = Ae^{ikx} + Be^{-ikx}$

$\psi_{II} = A'e^{-Kx}$

at $x=0$ $\psi_I = \psi_{II}$ and $\psi_I' = \psi_{II}'$

$A + B = A'$ $\qquad$ $Aik - Bik = -KA'$

thus $ik(A-B) = -K(A+B)$

$$A(ik+\kappa) = B(ik-\kappa)$$

$$\frac{B}{A} = \frac{ik+\kappa}{ik-\kappa} = \frac{-(ik+\kappa)}{-ik+\kappa}$$

$$R = \frac{|B|^2}{|A|^2} = \frac{(ik+\kappa)(-ik+\kappa)}{(-ik+\kappa)(ik+\kappa)} = 1$$

for $E > V$, $\quad \psi_{II} = A'e^{ik'x} + B'e^{-ik'x}$

but in zone II there is no reflected wave,

so $\psi_{II} = A'e^{ik'x}$

at $x=0$,

$$A + B = A' \qquad \psi_I(0) = \psi_{II}(0)$$

$$ikA - ikB = ik'A' \qquad \psi_I'(0) = \psi_{II}'(0)$$

~~combining~~ $\frac{k}{k'}A - \frac{k}{k'}B = A'$

combining:

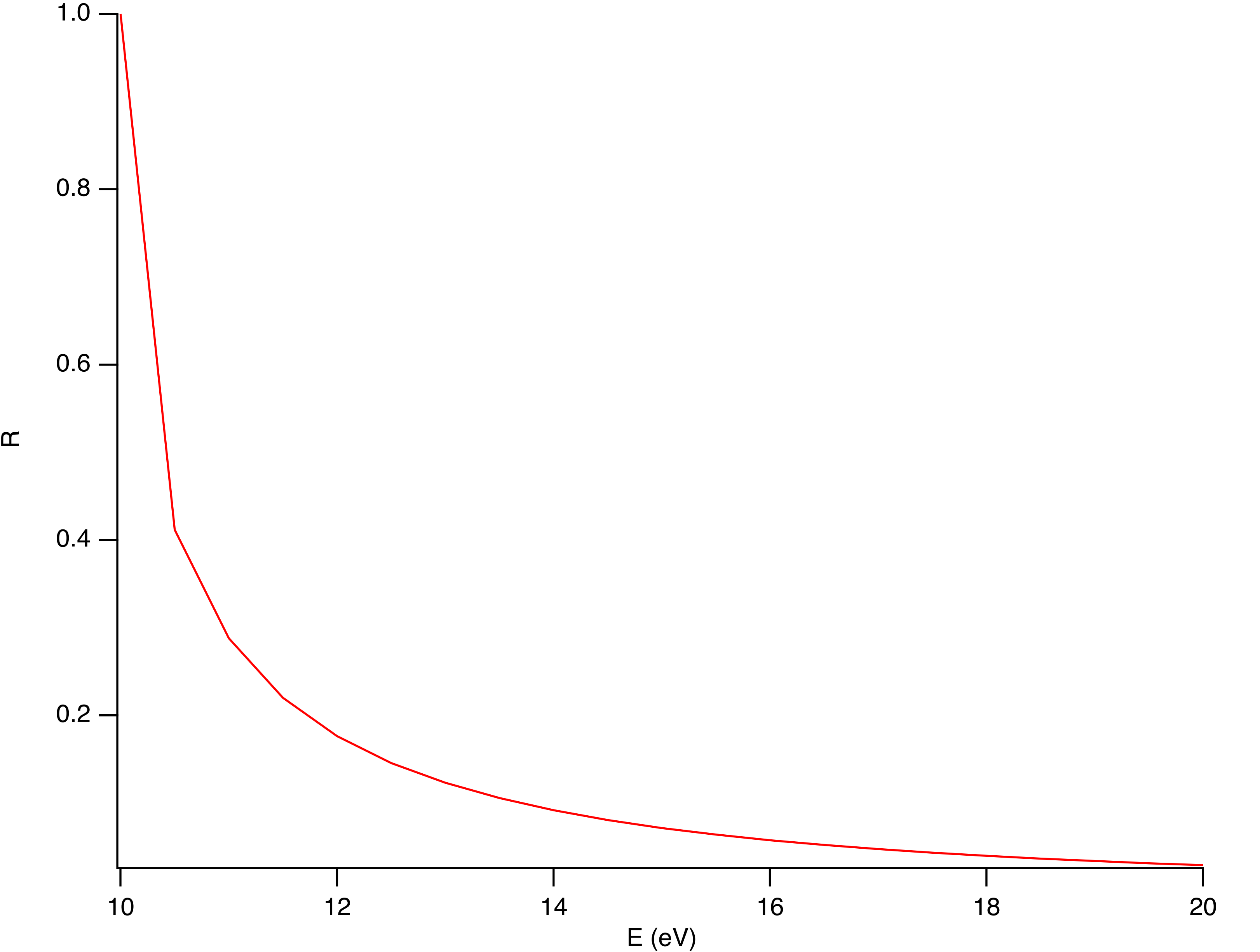
$$\left(\frac{k}{k'} - 1\right)A = \left(1 + \frac{k}{k'}\right)B$$

$$\frac{B}{A} = \frac{-(1 - k/k')}{(1 + k/k')}$$

$$R = \frac{|B|^2}{|A|^2} = \frac{(1-k/k')^2}{(1+k/k')^2} = \left(\frac{k'-k}{k'+k}\right)^2$$

$$= \left[\frac{\sqrt{E-V} - \sqrt{E}}{\sqrt{E-V} + \sqrt{E}}\right]^2$$

independent of m.



1.0
0.8
0.6
0.4
0.2
R
10
12
14
16
18
20
E (eV)