EEE352: Properties of Electronic Materials

Homework set #2
(due Wednesday, February 7th, 2007)

1. A beam of electrons with number density of 1×10^{15} electrons/m is incident from the left on the step potential energy

$$V(x)=\begin{cases} 0 & x<0 \\ -V_0 & x\geq 0 \end{cases}$$

(The constant V_0 is positive, so this is a "down-step" rather than an "up-step" potential)

   (a) Write down the form of the spatial function $\psi_E(x)$ in each region of this potential, defining all wavenumbers and/or decay constants. Don't forget to impose asymptotic conditions for $x\to\pm\infty$.

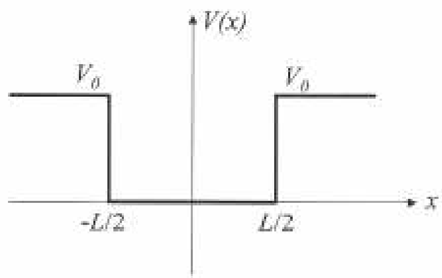
   (b) Obtain expression for the transmission and reflection coefficients for this potential, expressing your results in terms of the quantities you introduced in part (a).

   (c) Evaluate $T(E)$ and $R(E)$ for an incident beam of kinetic energy 100 eV and a step of magnitude $V_0=50eV$.

   (d) Evaluate the incident and transmitted fluxes for the conditions of part c. Be sure to show units.

   (e) Sketch $\psi_E(x)$, being careful to clearly show any differences in the nature of the spatial function or in its amplitude or wavelength between the regions.

2. A beam of particles of mass m is incident from the left on the potential well shown in the figure below. Suppose that the energy of the particles is greater than the height of the walls, i.e. $E>V_0$.



   (a) Write down the TISE and its general solution in each region, defining appropriate wavenumbers and arbitrary constants as needed. If you can set one or more of these arbitrary constants to zero at this point, do so and explain why.

   (b) Evaluate the reflected and transmitted probability current densities in each region. Be sure to indicate the direction and magnitude of each current density and label it as reflected, transmitted, etc.

(c) List the conditions that you would use to relate the pieces of the function $\psi_E(x)$ in each region to one another. Do you have enough conditions to uniquely determine all of the arbitrary constants in these solutions? If not, discuss the physical significance of the one (or ones) you cannot determine from these conditions.

(d) Define the probability of transmission into the region $x \geq L/2$, explain the physical significance of this quantity and relating it to the current densities of part c.

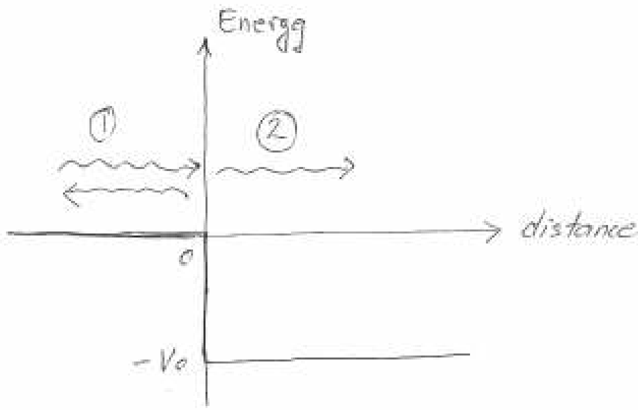
Calculate the expression for the transmission coefficient as a function of k_2, where is the wavenumber in the region $-L/2 \leq x \leq L/2$. Under what conditions on k_2 is $T(E)=1$. Consider an energy E such that this condition is satisfied. At this energy, what is the value of the reflection coefficient $R(E)$ for this system? Why?

(e) Compare the description given by quantum and classical physics of the motion of a microscopic particle with this potential.

3. Using the graphical solution method described in class:
   (a) Calculate the eigenvalues of a finite potential well with height V_0 = 0.8 eV and width L = 20 nm. For the effective electron mass use the value appropriate for *GaAs* material, i.e. $m = 6\times10^{-32}$ kg.
   (b) Calculate the corresponding infinite well results and compare them to the finite well case.
   (c) Plot the transmission coefficient as a function of the energy, for energies larger than 0.8 eV. What is the reason for the existence of the transmission coefficient maxima?

Solution to HWK #2

Problem #1



(a) $\Psi_1(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}$ $\qquad k_1 = \sqrt{\frac{2mE}{\hbar^2}}$

$\Psi_2(x) = A_2 e^{ik_2 x}$ $\qquad k_2 = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$

(b) continuity + smoothness of the wave function accross a boundary

$$\Psi_1(0) = \Psi_2(0) \Rightarrow A_1 + B_1 = A_2 \qquad (1)$$

$$\left.\frac{d\Psi_1}{dx}\right|_{x=0} = \left.\frac{d\Psi_2}{dx}\right|_{x=0} \Rightarrow k_1(A_1 - B_1) = k_2 A_2$$

$$A_1 - B_1 = \frac{k_2}{k_1} A_2 \qquad (2)$$

Adding equations (1) and (2) gives:

$$2A_1 = \left(1 + \frac{k_2}{k_1}\right) A_2 = \frac{k_1 + k_2}{k_1} A_2$$

$$A_1 = \frac{k_1 + k_2}{2k_1} A_2$$

Subtracting (2) from (1) gives:

$$2B_1 = A_2\left(1 - \frac{K_2}{K_1}\right) = A_2\,\frac{K_1 - K_2}{K_1}$$

$$B_1 = A_2\,\frac{K_1 - K_2}{2K_1}$$

Reflection coefficient

$$R = \left|\frac{B_1}{A_1}\right|^2 = \left|\frac{A_2\,\frac{K_1 - K_2}{2K_1}}{A_2\,\frac{K_1 + K_2}{2K_1}}\right|^2 = \left|\frac{K_1 - K_2}{K_1 + K_2}\right|^2$$

$$T = \frac{k_2}{k_1}\left|\frac{A_2}{A_1}\right|^2 = \frac{K_2}{K_1}\left|\frac{2K_1}{K_1 + K_2}\right|^2 = \frac{4K_1K_2}{|K_1 + K_2|^2}$$

$R + T = 1$ as it should be.

(c) $R(E)$ and $T(E)$ for $E = 100\,eV$ and $V_0 = 50\,eV$

$$R = \left|\frac{K_1 - K_2}{K_1 + K_2}\right|^2 = \left|\frac{\sqrt{E} - \sqrt{E+V_0}}{\sqrt{E} + \sqrt{E+V_0}}\right|^2 = \left|\frac{\sqrt{100} - \sqrt{150}}{\sqrt{100} - \sqrt{150}}\right|^2$$

$$R = \left|\frac{12.25 - 10}{12.25 + 10}\right|^2 = 0.0102 = 1.02\,\%$$

$$T = \frac{4K_1K_2}{|K_1 + K_2|^2} = \frac{4\sqrt{E}\sqrt{E+V_0}}{|\sqrt{E} + \sqrt{E+V_0}|^2} = \frac{4\sqrt{100}\sqrt{150}}{|\sqrt{100} + \sqrt{150}|^2}$$

$$T = \frac{4 \cdot 10 \cdot 12.25}{(22.25)^2} = 0.9898 = 98.98\,\%$$

(d) Incident and Transmitted fluxes

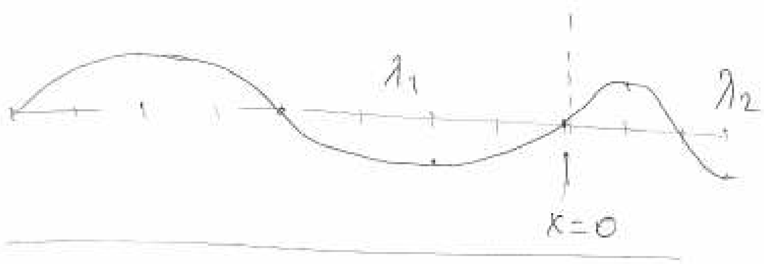
Incident flux = 10^{15} electrons/m

Reflected flux = 0.0102×10^{15} electrons/m

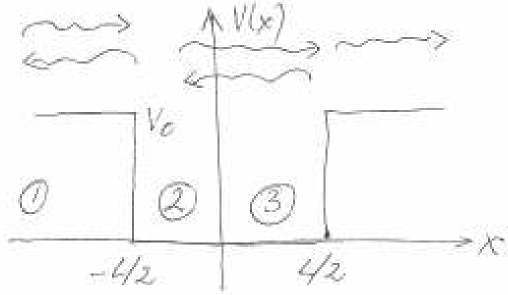
Transmitted flux $= 0.9898 \times 10^{15}$ electrons/m

(e) $k = \sqrt{\frac{2mE}{\hbar^2}}$ $\qquad E\uparrow \quad k\uparrow \implies k_2 > k_1$

$k = \frac{2\pi}{\lambda} \quad k\uparrow \quad \lambda\downarrow \quad \lambda_2 < \lambda_1$



Problem #2



(a) $\psi_1(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}$ $\qquad k_1 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$

$\psi_2(x) = A_2 e^{ik_2 x} + B_2 e^{-ik_2 x}$ $\qquad k_2 = \sqrt{\frac{2mE}{\hbar^2}}$

$\psi_3(x) = A_3 e^{ik_3 x}$

$$\begin{cases} \psi_1(-L/2) = \psi_2(-L/2) \\ \left.\frac{d\psi_1}{dx}\right|_{x=-L/2} = \left.\frac{d\psi_2}{dx}\right|_{x=-L/2} \end{cases}$$

$$A_1 e^{-ik_1 L/2} + B_1 e^{ik_1 L/2} = A_2 e^{-ik_2 L/2} + B_2 e^{ik_2 L/2}$$

$$ik_1 (A_1 e^{-ik_1 L/2} - B_1 e^{ik_1 L/2}) = ik_2 (A_2 e^{-ik_2 L/2} - B_2 e^{ik_2 L/2})$$

$$A_1 e^{-ik_1 L/2} - B_1 e^{ik_1 L/2} = \frac{k_2}{k_1} A_2 e^{-ik_2 L/2} - \frac{k_2}{k_1} B_2 e^{ik_2 L/2}$$

$$2A_1 e^{-ik_1 L/2} = \frac{k_1 + k_2}{k_1} A_2 e^{-ik_2 L/2} + \frac{k_1 - k_2}{k_1} B_2 e^{ik_2 L/2}$$

$$2B_1 e^{ik_1 L/2} = \frac{k_1 - k_2}{k_1} A_2 e^{-ik_2 L/2} + \frac{k_1 + k_2}{k_1} B_2 e^{ik_2 L/2}$$

Thus:

$$\begin{bmatrix} A_1 \\ B_1 \end{bmatrix} = \begin{bmatrix} \frac{k_1 + k_2}{2k_1} e^{i(k_1 - k_2)L/2} & \frac{k_1 - k_2}{2k_1} e^{i(k_1 + k_2)L/2} \\ \frac{k_1 - k_2}{2k_1} e^{-i(k_1 + k_2)L/2} & \frac{k_1 + k_2}{2k_1} e^{-i(k_1 - k_2)L/2} \end{bmatrix} \begin{bmatrix} A_2 \\ B_2 \end{bmatrix}$$

Analogously:

$$\begin{bmatrix} A_2 \\ B_2 \end{bmatrix} = \begin{bmatrix} \frac{k_2+k_1}{2k_2} e^{-i(k_2-k_1)L/2} & \frac{k_2-k_1}{2k_2} e^{-i(k_1+k_2)L/2} \\ \frac{k_2-k_1}{2k_2} e^{+i(k_1+k_2)L/2} & \frac{k_2+k_1}{2k_2} e^{i(k_2-k_1)L/2} \end{bmatrix} \begin{bmatrix} A_3 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} A_1 \\ B_1 \end{bmatrix} = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} \begin{bmatrix} A_3 \\ \cancel{B_3}^{\,0} \end{bmatrix} \qquad \begin{aligned} A_1 &= m_{11} A_3 \\ A_2 &= m_{21} A_3 \end{aligned}$$

$$T = \left|\frac{A_3}{A_1}\right|^2 = \frac{1}{|m_{11}|^2} \qquad R = \left|\frac{A_2}{A_1}\right|^2 = \left|\frac{m_{21}}{m_{11}}\right|^2$$

$$m_{11} = \frac{k_1+k_2}{2k_1} e^{i(k_1-k_2)L/2} \cdot \frac{k_1+k_2}{2k_2} e^{i(k_1-k_2)L/2}$$

$$+ \quad \frac{k_1-k_2}{2k_1} e^{i(k_1+k_2)L/2} \cdot \frac{k_2-k_1}{2k_2} e^{i(k_1+k_2)L/2}$$

$$= \frac{(k_1+k_2)^2}{4k_1k_2} e^{-ik_2L} - \frac{(k_2-k_1)^2}{4k_1k_2} e^{ik_2L} =$$

$$= \frac{k_1^2+k_2^2+2k_1k_2}{4k_1k_2}\left[\cos k_2L - i\sin k_2L\right] -$$

$$- \frac{k_1^2+k_2^2-2k_1k_2}{4k_1k_2}\left[\cos(k_2L) + i\sin k_2L\right] =$$

$$= 1 - i\sin k_2L \, \frac{k_1^2+k_2^2}{\cancel{4}_{2}\, k_1k_2} = 1 - i\,\frac{k_1^2+k_2^2}{2k_1k_2}\sin k_2L$$

$$T(E) = \frac{1}{|m_{11}|^2} = \left| 1 + \left(\frac{k_1^2 + k_2^2}{2k_1k_2} \right)^2 \sin^2 k_2 L \right)^2 \Big|^{-1}$$

$$R(E) = 1 - T(E)$$

(b) Reflected and transmitted probability current densities:

— region (1) $\quad T_1(E) = \frac{k_2}{k_1} \left| \frac{A_2}{A_1} \right|^2$

$$R_1(E) = \left| \frac{B_1}{A_1} \right|^2 = R(E)$$

— region (2) $\quad T_2(E) = \frac{k_1}{k_2} \left| \frac{A_2}{A_1} \right|^2$

$$R_2(E) = \left| \frac{B_2}{A_2} \right|^2$$

- region (3) $\quad T_3(E) = \left| \frac{A_3}{A_1} \right|^2 = T(E)$

(c) we matched the wavefunction and the derivative of the wavefunction. We have all but one and that is the incident flux density.

(d) $$T(E) = \frac{1}{1 + \left(\frac{k_1^2 + k_2^2}{2k_1k_2} \right)^2 \sin^2 k_2 L}$$

$T(E) = 1$, $\sin k_2 L = n\pi$

$k_2 = \frac{n\pi}{L}$ infinite well results

$$k_{2_n} = \sqrt{\frac{2mE_n}{\hbar^2}} = \frac{n\pi}{L} \Rightarrow E_n = \frac{\hbar^2}{2m} \left(\frac{n\pi}{L} \right)^2$$

(e) Classical physics assumes that $T(E)=1$ for $E>V_0$ and quantum physics assumes that there is finite probability for reflections.

Problem #3

$V_0 = 0.8eV \quad L = 20nm \quad m^* = 6\times10^{-32} kg$

(a) infinite well results:

$$k_n L = n\pi \Rightarrow k_n = \frac{n\pi}{L} \Rightarrow E_n = \frac{\hbar^2}{2m^*}\left(\frac{n\pi}{L}\right)^2$$

(c) Transmission coefficient

$$T(E) = \frac{1}{1+\left(\frac{k_1^2+k_2^2}{2k_1k_2}\right)^2 \sin^2 k_2 L}$$

where $k_1 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$ and $k_2 = \sqrt{\frac{2mE}{\hbar^2}}$

$$T(E) = \frac{1}{1+\left(\frac{E-V_0+E}{2\sqrt{E-V_0}\sqrt{E}}\right)^2 \sin^2\left(\sqrt{\frac{2mE}{\hbar^2}}L\right)}$$

$$T(E) = \frac{1}{1+\frac{(2E-V_0)^2}{4E(E-V_0)}\sin^2\left(\sqrt{\frac{2mE}{\hbar^2}}L\right)}$$

Look at program1.f for plotting the transmission coefficient

(b) Eigenvalues for the finite well results are solutions to the transcedental equations:

1) $\tan(\xi) = \sqrt{\frac{\beta^2}{\xi^2} - 1}$ where $\beta = \frac{L}{2}\sqrt{\frac{2mV_0}{\hbar^2}}$; $\xi = \frac{L}{2}\sqrt{\frac{2mE}{\hbar^2}}$

even solutions

2. $-\coth(\xi) = \sqrt{\frac{\beta^2}{\xi^2} - 1}$ odd solutions

even

$$\tan\left(\frac{L}{2}\sqrt{\frac{2mE}{\hbar^2}}\right) = \sqrt{\frac{\cancel{\left(\frac{L}{2}\right)^2} \frac{\cancel{2m}V_0}{\cancel{\hbar^2}}}{\cancel{\left(\frac{L}{2}\right)^2} \frac{\cancel{2m}E}{\cancel{\hbar^2}}} - 1} = \sqrt{\frac{V_0}{E} - 1}$$

$$\boxed{\tan\left(\frac{L}{2}\sqrt{\frac{2mE}{\hbar^2}}\right) = \sqrt{\frac{V_0}{E} - 1}}$$

odd:

$$\boxed{-\cot\left(\frac{L}{2}\sqrt{\frac{2mE}{\hbar^2}}\right) = \sqrt{\frac{V_0}{E} - 1}}$$

Look at program 2.f for plotting these two plots

Even:	0.576	odd	0.736
	0.3		0.429
	0.109		0.193
	0.012		0.048

Energy levels of finite well	0.012	Infinite well	0.0143
	0.048		0.0571
	0.109		0.1285
	0.193		0.2284
	0.3		0.3568
	0.429		0.5139
	0.576		0.6994
	0.736		0.9135

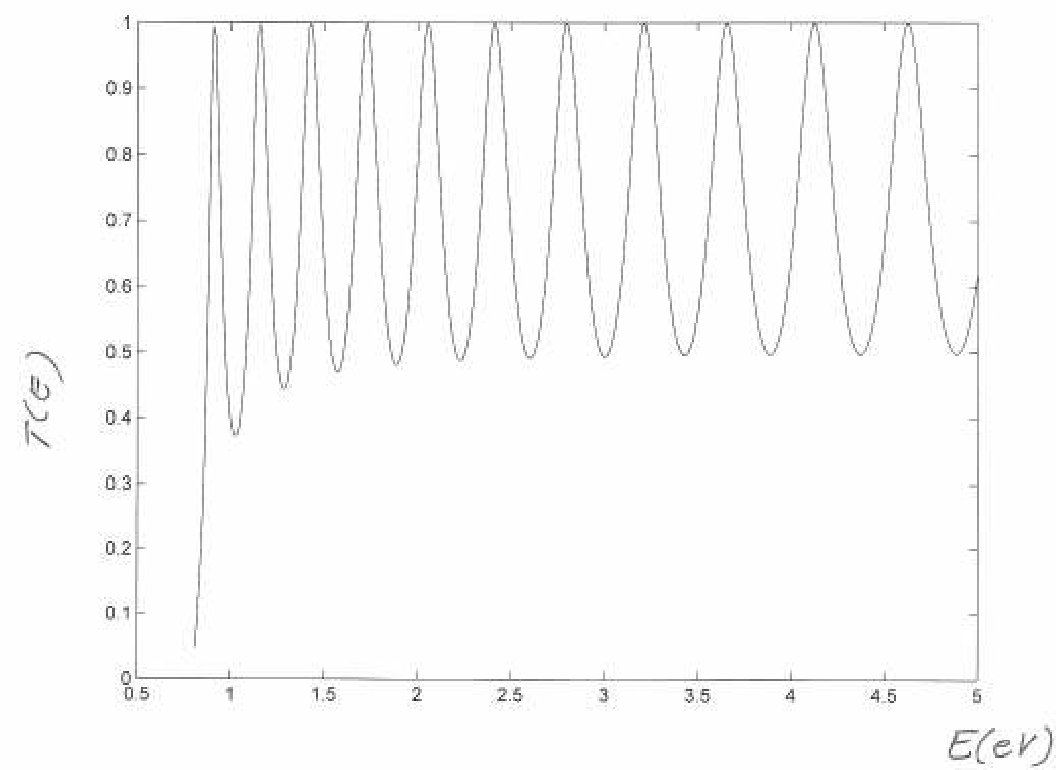
TRANSMISSION COEFFICIENT CALCULATION

```
rm = 6e-32
rl = 20e-9
vo = 0.8
h = 6.626e-34
pi=3.141592654
hb = h/2./pi
q = 1.602e-19

i = 1

for E = (vo+0.01):0.01:5
    fac1 = (2.*E-vo)^2/4./E/(E-vo)
    fac2 = rl*sqrt(2.*rm*q/hb*E/hb)
    denom = 1. + fac1*(sin(fac2))^2
    xvec(i)=E
    yvec(i)=1/denom
    i = i + 1
end

plot(xvec,yvec);
```


1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
T(E)
E(eV)

BOUND STATES IN FINITE well

```
rm = 6e-32
rl = 20e-9
vo = 0.8
h = 6.626e-34
pi=3.141592654
hb = h/2./pi
q = 1.602e-19

i = 1

for E = 0.001:0.001:(vo-0.001)
    rhs(i) = sqrt(vo/E-1)
    rlhs_factor = rl*sqrt(2.*rm*q/hb*E/hb)/2.
    rlhs1(i) = tan(rlhs_factor)
    rlhs2(i) = -cot(rlhs_factor)
    xvec(i)=E
    i = i + 1
end

plot(xvec,rhs,xvec,rlhs2);

for  i=1:1:8
    en =hb/q*hb/2./rm*(real(i)*pi/rl)^2
    i,en
end
```

infinite well results