EE207:2018 Assignment-1 Solutions

Q1

The three planes available are (001), (110) and (112). Hence, we need to find the angle of the plane (112) from the two reference planes.

$cos\theta1 = (0+0+2)/(1*\sqrt{(1+1+4)}) = \sqrt{2/3}$, and
$cos\theta2 = (1+1+0)/(\sqrt{2}*\sqrt{(1+1+4)}) = \sqrt{1/3}$.
Which gives θ1 = 35.26 from (001), and θ2 = 54.73 from (110) plane. **(2 marks)**

Q2

(a) The intercepts of the plane (231) on x,y and z axis can be calculated as reciprocal of the plane indices. Hence x:y:z = 1/2:1/3:1 or 3:2:6. **(1 mark)**

(b) We can find miller indices with its intercepts on the axes or taking a vector product of any two non-linear vectors in the plane.

i) In this case, x,y and z intercepts of the plane are ∞,a and a, respectively.
Hence the miller indices can be written as (1/∞ 1/a 1/a) ≡ (011). **(1 mark)**

ii) Similarly, here the x, y and z intercepts are a, a and a, respectively;
Giving the miller indices as (1/a 1/a 1/a) ≡ (111). **(1 mark)**

iii) Here the x, y and z intercepts are a/2, a/2 and a/2, respectively; which are a multiple of the the intercepts in previous case. Hence both represent the same plane, namely (111). **(1 mark)**

Q3

we know that a vector G in the reciprocal lattice can be expressed as a linear combination of its primitive vectors.
$G = k_1b_1 + k_2b_2 + k_3b_3$

From the definition of b1, we can see that:
$b_i * a_j = 2\pi\delta_{ij}$

We let R be a vector in the direct lattice, which we can express as a linear combination of its primitive vectors.
$R = n_1a_1 + n_2a_2 + n_3a_3$

From this we can see that:
$G * R = 2\pi(k_1 n_1 + k_2 n_2 + k_3 n_3)$

From our definition of the reciprocal lattice, G must satisfy the identity $e^{iG*R} = 1$.

Any vector K satisfying the relation $e^{iG*K} = 1$ will be reciprocal to G. And hence K=R.
This proves that the reciprocal of the reciprocal lattice is the direct lattice. **(2 marks)**

Now, we know that

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$
$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)}$$
$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)}$$

The basis for the BCC and FCC lattice can be written as the following.
BCC:
a1 = a/2 (x+y-z); a2 = a/2 (-x+y+z); a3 = a/2 (x-y+z).

FCC:
a1 = a(x+y); a2 = a(y+z); a3 = a(x+z).

Now taking BCC primitive vectors and finding reciprocal gives

$$b1 = 2\pi/a\left(\frac{(-x+y+z)\times(x-y+z)}{(x+y-z)*(-x+y+z)\times(x-y+z)}\right) = a'(x+y)$$
$$b2 = 2\pi/a\left(\frac{(x-y+z)\times(x+y-z)}{(-x+y+z)*(x-y+z)\times(x+y-z)}\right) = a'(y+z)$$
$$b3 = 2\pi/a\left(\frac{(x+y-z)\times(-x+y+z)}{(x-y+z)*(x+y-z)\times(-x+y+z)}\right) = a'(x+z)$$

These are same as the basis vectors of the FCC crystal.
Hence, it proves that the BCC and FCC are reciprocal lattice pairs. **(2 marks)**

Solution 4:

Inter-planar spacing is given by $d_{hkl} = \hat{n} \cdot \frac{1}{h}\overrightarrow{a_1} = \hat{n} \cdot \frac{1}{k}\overrightarrow{a_2} = \hat{n} \cdot \frac{1}{l}\overrightarrow{a_3}$. (1.5 Marks)

Here, $\overrightarrow{a_i}$ are the primitive unit vectors of real space lattice, $\hat{n}$ is the unit vector perpendicular to the plane (hkl).

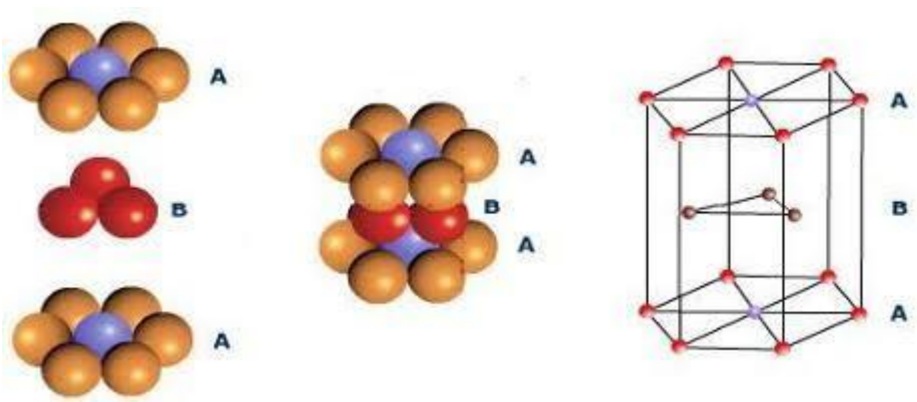
From a Tutorial-1 problem, we know that the reciprocal lattice vector, $\boldsymbol{G} = h\boldsymbol{b_1} + k\boldsymbol{b_2} + l\boldsymbol{b_3}$ is normal to the plane (hkl). (1.5 marks)

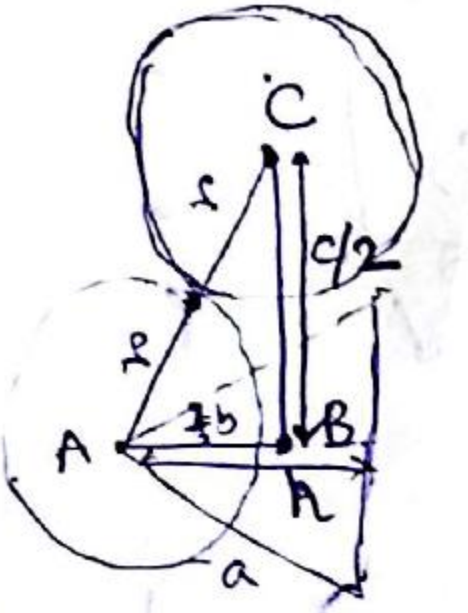
Hence, $\hat{n} = \frac{\boldsymbol{G}}{|\boldsymbol{G}|}$.

Therefore, $d_{hkl} = \frac{\boldsymbol{G}}{|\boldsymbol{G}|} \cdot \frac{1}{h}\overrightarrow{a_1} = \frac{\boldsymbol{b_1} \cdot \overrightarrow{a_1}}{|\boldsymbol{G}|} = \frac{2\pi}{|\boldsymbol{G}|}$ (1 Marks)

Solution 5:

(a)





$2r = a$ $\quad$ (1) $\quad$ (1 Marks)

And $AC^2 = AB^2 + BC^2$ $\quad$ (2)

From Fig. $AB = \frac{2}{3}h$, where $h = \frac{\sqrt{3}a}{2}$. Hence, $AB = \frac{a}{\sqrt{3}}$

$BC = \frac{c}{2}$ and $AC = 2r = a$ $\quad$ (2Marks)

Hence, from (2) $a^2 = \left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2$. This gives $\frac{c}{a} = \sqrt{\frac{8}{3}}$ $\quad$ (1 Marks)

(b) Condition: Density remains same after hcp to bcc transformation.

No. of atoms in one HCP unit cell = $\left(12 * \frac{1}{6}\right) + \left(\frac{1}{2} * 2\right) + 3 = 6$

No. of atoms in one BCC unit cell = $\left(8 * \frac{1}{8}\right) + 1 = 2$ $\quad$ (1 Marks)

Densities are same. Hence

$$\left(\frac{mass}{volume}\right)_{hcp} = \left(\frac{mass}{volume}\right)_{bcc}$$

Let mass of each Na atom be m

Hence, $mass_{hcp} = 6m$ and $mass_{bcc} = 2m$

And, $volume_{hcp} = 6 * \left(\frac{1}{2} * \left(a_{hcp}\right) * \left(\frac{\sqrt{3}}{2} a_{hcp}\right) * c\right)$ and $volume_{bcc} = a_{bcc}^3$

Hence,

$$\frac{2m}{a_{bcc}^3} = \frac{6m}{\frac{3}{2}\sqrt{3}a_{hcp}^2 c}$$

Using $\frac{c}{a_{hcp}} = \sqrt{\frac{8}{3}}$, we get $a_{bcc} = a_{hcp} 2^{\frac{1}{6}}$. (1 Marks)

Solution 6: The given wavefunction is $\psi(k) = \frac{1}{\sqrt{L}} e^{ikx}, x \in \left(-\frac{L}{2}, \frac{L}{2}\right)$

(a) $\left||\psi(k)^* \psi(k)|\right|^2 = \int_{-\frac{L}{2}}^{\frac{L}{2}} \left(\frac{1}{\sqrt{L}} e^{-ikx}\right)\left(\frac{1}{\sqrt{L}} e^{ikx}\right) dx = \int_{-\frac{L}{2}}^{\frac{L}{2}} \frac{1}{L} dx = \frac{1}{L}\left(\frac{L}{2} + \frac{L}{2}\right) = 1$
   Hence, the wavefunctions $\psi(k)$ are normalized $\forall\, L$. (2 Marks)

(b) For orthogonality, we need to prove that
   $\langle \psi(k1) | \psi(k1) \rangle = 1$ and $\langle \psi(k1) | \psi(k2) \rangle = 0\ for\ k1 \neq k2$. (1 Marks)

   Now, consider the inner product $\langle \psi(k1) | \psi(k2) \rangle$.

$$\langle \psi(k1) | \psi(k2) \rangle = \int_{-\frac{L}{2}}^{\frac{L}{2}} \frac{1}{\sqrt{L}} e^{-ik_1 x} * \frac{1}{\sqrt{L}} e^{ik_2 x} dx = \frac{2}{a(k_2 - k_1)} \sin\left(\frac{(k_2 - k_1)a}{2}\right)$$
$$= \frac{\sin\left(\frac{(k_2 - k_1)a}{2}\right)}{\left(\frac{(k_2 - k_1)a}{2}\right)}$$

(1 Marks)

Now, for $k_1 = k_2$, applying $\lim_{p \to 0} \frac{\sin p}{p} = 1$, $\langle \psi(k1) | \psi(k1) \rangle = 1\ \forall\, L$

And, for $k_1 \neq k_2$ and $L \to \infty$, $\langle \psi(k1) | \psi(k2) \rangle = 0$. (1 Marks)

Hence, the wavefunctions $\psi(k)$ are orthogonal for $L \to \infty$.

7.

Let us rewrite the given the given wavefunction in terms of the stationary state solutions (because they have well known properties of orthogonality and normalization).

$$\psi(x,0) = \frac{A}{\sqrt{a}}\sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}}\sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}}\sin\left(\frac{5\pi x}{a}\right)$$

$$\psi(x,0) = \frac{A}{\sqrt{2}}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{10}}\sqrt{\frac{2}{a}}\sin\left(\frac{3\pi x}{a}\right) + \sqrt{\frac{1}{10}}\sqrt{\frac{2}{a}}\sin\left(\frac{5\pi x}{a}\right)$$

$$\psi(x,0) = \frac{A}{\sqrt{2}}\phi_1 + \sqrt{\frac{3}{10}}\phi_3 + \sqrt{\frac{1}{10}}\phi_5$$

(a) To ensure normalisation: $\int_{-\infty}^{\infty}\psi^*\psi\, dx = 1$ (1 mark)

The effective limits become 0 to a. (Infinite well)

All cross terms ($\phi_i^*\phi_j$) integral go to zero by orthogonal property of stationary states.

All self terms ($\phi_i^*\phi_i$) integral become 1 by normalized property of stationary states.

$$\int_{-\infty}^{\infty}\psi^*\psi\, dx = \frac{A^2}{2} + \frac{3}{10} + \frac{1}{10} = 1 \quad \Rightarrow A = \sqrt{\frac{6}{5}}$$ (1 mark)

(b) The probability of finding the particle in one of the energy states, $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$, corresponding to the wavefunction, $\phi_n = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$, can be found out as:

$$p_n = \int_{-\infty}^{\infty}\phi_n^*\psi\, dx$$

Since $\psi(x,0) = c_1\phi_1 + c_3\phi_3 + c_5\phi_5$, the probability of finding the particles in an energy states, E_n is non-zero only for $n = 1, 3$ and 5, i.e.

$$p_i = 0 \text{ for } i \neq 1, 3 \text{ and } 5$$

Also,

$$p_1 = |c_1|^2 = 0.6$$
$$p_3 = |c_3|^2 = 0.3$$
$$p_5 = |c_5|^2 = 0.1$$

(1 mark)

To calculate the average energy we use the definition,

$$< E > = \int_{-\infty}^{\infty}\psi^*\boldsymbol{H}\psi\, dx$$

We know that $H\phi_n = E_n\phi_n$ for all stationary states, ϕ_n.

$$< E > = |c_1|^2E_1 + |c_3|^2E_3 + |c_5|^2E_5$$
$$= \left(\frac{6}{10}\times 1^2 + \frac{3}{10}\times 3^2 + \frac{1}{10}\times 5^2\right)\times\frac{\pi^2\hbar^2}{2ma^2}$$
$$\frac{29}{10}\frac{\pi^2\hbar^2}{ma^2}$$

(1 mark)

(c) The time dependent Schroedinger equation looks like:

$$\boldsymbol{H}\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)$$

Separation of variables technique results in solutions of the form,

$\psi(x,t) = \Sigma_n c_n(t)\phi_n(x)$, where $\phi_n(x)$ are the well-known stationary states
We need to find the $c_n(t)$,

$$i\hbar\frac{\partial}{\partial t}\left(\Sigma_n c_n(t)\phi_n(x)\right) = \boldsymbol{H}\left(\Sigma_n c_n(t)\phi_n(x)\right),$$

Now, $\boldsymbol{H} = \frac{\boldsymbol{p}^2}{2m} + V$, assuming time unvarying V,

$$i\hbar\left(\frac{\partial}{\partial t}\left(\Sigma_n c_n(t)\right)\right)\phi_n(x) = \Sigma_n c_n(t)\boldsymbol{H}\phi_n(x)$$

$$i\hbar\Sigma_n\left(\frac{\partial}{\partial t}c_n(t)\right)\phi_n(x) = \Sigma_n c_n(t)E_n\phi_n(x)$$

Since the ϕ_n are orthogonal, their coefficients on the LHS and the RHS must be the same,

$$i\hbar\frac{\partial}{\partial t}c_n(t) = c_n(t)$$

$$c_n(t) = c_n(0)e^{\left(-\frac{iE_nt}{\hbar}\right)}$$

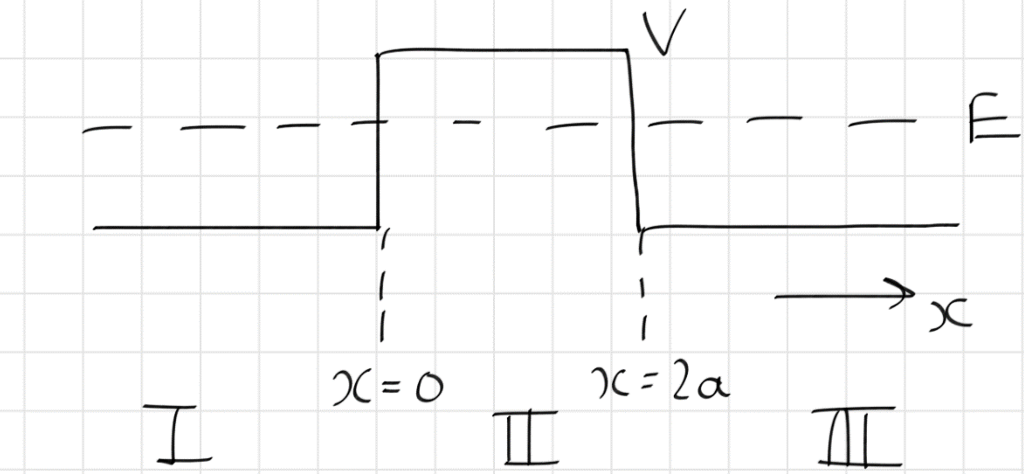
$$\Rightarrow \boldsymbol{\psi(x,t) = \Sigma_n c_n(0)e^{\left(-\frac{iE_nt}{\hbar}\right)}\phi_n(x)}$$

Given $\psi(x,0)$ as a linear combination of the stationary states ϕ_n, it is easy to get back the $\psi(x,t)$ as

$$\psi(x,t) = \sqrt{\frac{6}{5a}}\sin\left(\frac{\pi x}{a}\right)e^{\left(-\frac{iE_1t}{\hbar}\right)} + \sqrt{\frac{3}{5a}}\sin\left(\frac{3\pi x}{a}\right)e^{\left(-\frac{iE_3t}{\hbar}\right)} + \frac{1}{\sqrt{5a}}\sin\left(\frac{5\pi x}{a}\right)e^{\left(-\frac{iE_5t}{\hbar}\right)}$$ (1 mark)

For further information, please refer to this document.

8.



$$Be^{-ik_1x} + Ae^{ik_1x} \qquad Ce^{k_2x} + De^{-k_2x} \qquad Fe^{-ik_1x}$$

(1 mark)

Let the incident wave be from region I Be^{-ik_1x} and the transmitted wave in region III be Fe^{-ik_1x}

$$k_1 = \frac{\sqrt{2mE}}{\hbar} \quad ; \quad k_2 = \frac{\sqrt{2m(V-E)}}{\hbar}$$

Continuity of wavefunctions at the region boundaries give

$$A + B = C + D \; ; \; Ce^{2k_2a} + De^{-2k_2a} = Fe^{-2ik_1a}$$

(1/2 mark)

Since the barrier height is finite the wavefunction derivatives are also continuous.

$$ik_1(A-B) = k_2(C-D) \quad \text{(½ mark)}$$

$$k_2\left(Ce^{2k_2a} - De^{-2k_2a}\right) = -ik_1Fe^{-2ik_1a}$$

Transmission Coefficient, $T = \frac{|F|^2}{|B|^2}$

$$B = \frac{1}{2}\left(A+B-(A-B)\right)$$

$$= \frac{1}{2}\left(C+D + \frac{ik_2}{k_1}(C-D)\right)$$

$$= \frac{1}{2}\left(\left(1+\frac{ik_2}{k_1}\right)C + D\left(1-\frac{ik_2}{k_1}\right)\right)$$

$$C = \frac{1}{2}e^{-2k_2a}\left(Ce^{2k_2a} + De^{-2k_2a} + Ce^{2k_2a} - De^{-2k_2a}\right)$$

$$= \frac{1}{2}e^{-2k_2a}\left(Fe^{-2ik_1a} - \frac{ik_1}{k_2}Fe^{-2ik_1a}\right)$$

$$= \tfrac{1}{2}e^{-2k_2a}\left(1 - ik_1/k_2\right)Fe^{-2ik_1a}$$

Similarly for D,

$$D = \frac{1}{2}e^{2k_2a}\left(Ce^{2k_2a} + De^{-2k_2a} - \left(Ce^{2k_2a} - De^{-2k_2a}\right)\right)$$

$$= \frac{1}{2}e^{2k_2a}\left(1 + \frac{ik_1}{k_2}\right)Fe^{-2ik_1a}$$

Putting C & D back into equation for B,

$$B = \frac{1}{4}Fe^{-2ik_1a}\left[e^{-2k_2a}\left(1+i\frac{k_2}{k_1}\right)\left(1-\frac{ik_1}{k_2}\right) + e^{2k_2a}\left(1-i\frac{k_2}{k_1}\right)\left(1+\frac{ik_1}{k_2}\right)\right]$$

$$\left|\frac{B}{F}\right| = \left|\frac{1}{4}\left[e^{-2k_2a}\left(2+i\left(\frac{k_2}{k_1}-\frac{k_1}{k_2}\right)\right) + e^{2k_2a}\left(2+i\left(\frac{k_1}{k_2}-\frac{k_2}{k_1}\right)\right)\right]\right|$$

$$\left|\frac{B}{F}\right| = \left|\cosh(2k_2a) - \frac{i}{2}\left(\frac{k_2}{k_1}-\frac{k_1}{k_2}\right)\left(\sinh(2ka)\right)\right|$$

$$\frac{1}{T} = \left|\frac{B}{F}\right|^2 = 1 + \frac{1 \times V^2}{4E(V-E)}\sinh^2(2k_2a)$$ (1 mark)

When V = E,

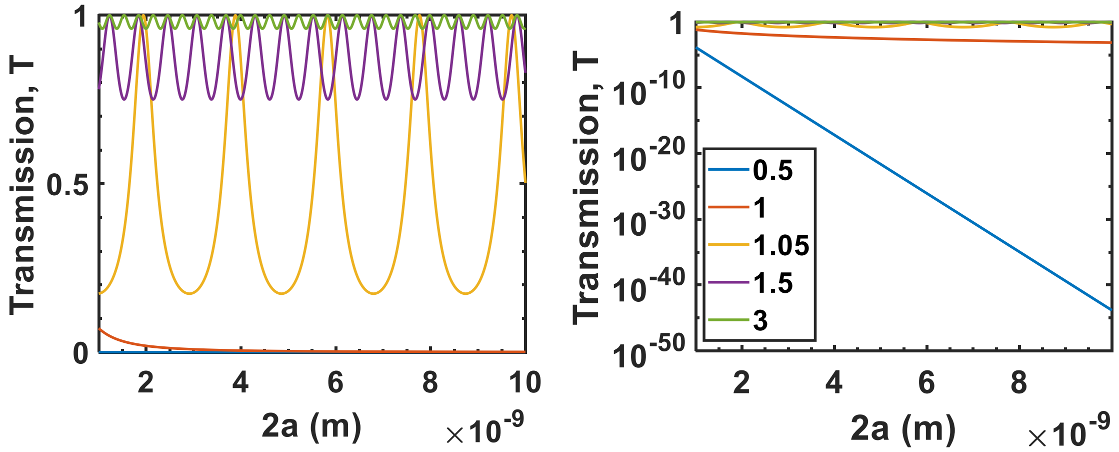
Using the limit of sinh(x) when x -> 0, we get,

$$\frac{1}{T} = 1 + \frac{1}{4} \times \frac{2mV(2a)^2}{\hbar^2}$$

Plots:

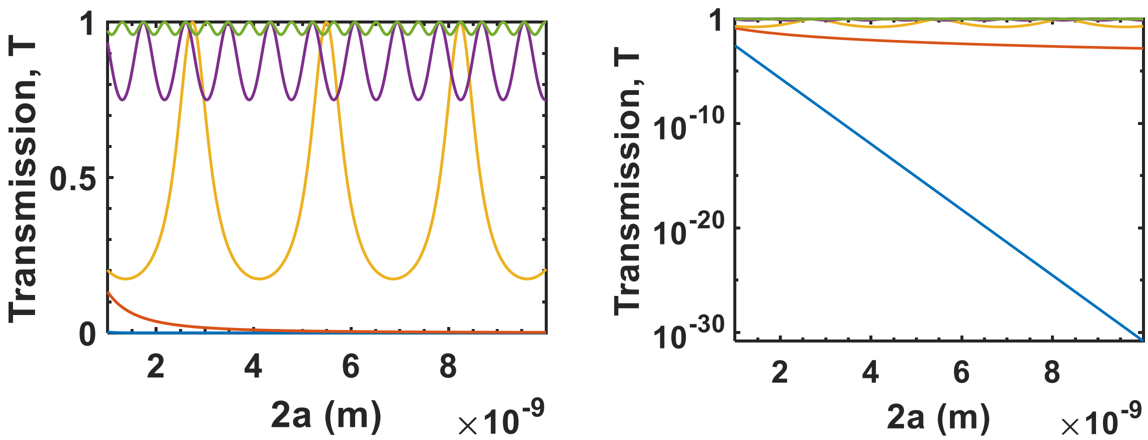
For m = m0, E/V is given in the legend. Linear and log scale plots

3



For m = 0.5m0, linear and log scale plots

2



Observations and Conclusions:

3

1. For lighter particles, quantum effects are more prominent, for E < V case, the transmission of lighter particles is more than the heavier particle. This is a scenario more away from the classical case.

1

2. For E > V, the transmission is not 1. It is oscillating as a function of barrier width. The peaks (or even the wavelength) of oscillation is not aligned for the two particles. This is because the particles have different de-Broglie wavelengths (because they have different masses). The transmission peaks are governed by the particles wavelength and the barrier width.

1

3. As energies go much beyond V, the particles approach T ~ 1 for all widths. This is the classical situation. However, in the quantum regime, slightly higher E than V, can result in significantly lower T depending on the barrier width.

2

Matlab code

```
clear all;
close all;

q = 1.6e-19;
V = 2*q;

EbyV = [0.5, 1, 1.05, 1.5, 3];

twoa = [1:0.01:10]*1e-9;

m0 = 9.1e-31;
m = m0*[1, 0.5];

h = 6.626e-34;
hbar = h/(2*pi);

i = 1;

for mthis = m
    for EbyVthis = EbyV
        k = (2*mthis*V*(1 - EbyVthis))^0.5/hbar;
        if (EbyVthis == 1)
            T = 1./(1 + 0.25*2*mthis*V*twoa.^2/hbar^2);
        else
            T = 1./(1 + 0.25*(1/((EbyVthis)*(1-EbyVthis)))*(sinh(k*twoa)).^2);
        end
        figure(i)
        plot(twoa, T)
        hold on
    end
    i = i+1;
end
```