1) Consider a one-dimensional wire with the following energy dispersion:

\[ E(k) = U_0 + \frac{\hbar^2 k^2}{2m} \]

1a) Use the finite difference scheme and show that the Schrödinger equation can be written in the following form:

\[ E\psi_j = \left( U_0 + 2t \right) \psi_j - t\psi_{j-1} - t\psi_{j+1} \]

where \( t = \frac{\hbar^2}{2ma^2} \) and \( a \) is the lattice constant.

**Solution:**

The 1D wave equation is:

\[-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + U_0 \psi(x) = E\psi(x)\]

If we plug \( \psi(x) = e^{ikx} \) into this equation, we will just get back \( E(k) = U_0 + \frac{\hbar^2 k^2}{2m} \), but let’s look carefully at the solution on a grid.

At node, \( j \):

\[-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} \bigg|_{x_j} + U_0 \psi(x_j) = E\psi(x_j)\]

The order second partial differential operator can be written in finite difference form as:

\[ \frac{d^2 \psi}{dx^2} \bigg|_j = \frac{1}{a^2} (\psi_{j-1} - 2\psi_j + \psi_{j+1}) \]

Inserting this in the 1D wave equation:

\[-\frac{\hbar^2}{2m} \left( \frac{1}{a^2} (\psi_{j-1} - 2\psi_j + \psi_{j+1}) \right) + U_0 \psi(x_j) = E\psi(x_j)\]

or

\[ \left(-t\psi_{j-1} + 2t\psi_j - t\psi_{j+1}\right) + U_0 \psi_j = E\psi_j \]
where  \( t = \hbar^2 / 2m^*a^2 \).

Finally:

\[
E\psi_j = (U_0 + 2t)\psi_j - t\psi_{j-1} - t\psi_{j+1}
\]

1b) Show that a plane wave of the form \( \psi(x) = \exp(ikx) \) must satisfy the following "numerical dispersion":

\[
E(k) = U_0 + 2t\left[1 - \cos(ka)\right].
\]

**Solution:**

\[
E\psi_j = (U_0 + 2t)\psi_j - t\psi_{j-1} - t\psi_{j+1} \tag{*}
\]

\( \psi(x) = \exp[ikx] \), so

\[
\psi_j = \exp[ikx_j], \\
\psi_{j-1} = \exp[ik(x_j - a)], \\
\psi_{j+1} = \exp[ik(x_j + a)]
\]

Insert in (*)

\[
E \exp[ikx_j] = (U_0 + 2t)\exp[ikx_j] - t\exp[ik(x_j - a)] - t\exp[ik(x_j + a)]
\]

\[
E = (U_0 + 2t) - t\exp[-ika] - t\exp[ika]
\]

\[
E = (U_0 + 2t) - 2t\cos(ka)
\]

\[E(k) - U_0 = 2t\left[1 - \cos(ka)\right]\]

Note what has happened. We started with the dispersion,
\[ E(k) - U_0 = \frac{\hbar^2 k^2}{2m^*}, \]

solved it on a grid, and got a different answer! This is “discretization error.” When the grid is fine enough, we should get the same answers.

1c) Show that when the lattice constant, \( a \), is sufficiently small, the numerical dispersion reduces to the parabolic dispersion:

\[ E(k) - U_0 = \frac{\hbar^2 k^2}{2m^*} \]

Solution:

Recall the Taylor series expansion: \( \cos x \approx 1 - \frac{x^2}{2} + \frac{x^4}{24} - \frac{x^6}{720} + \ldots \)

When \( x \) is small: \( \cos x \approx 1 - \frac{x^2}{2} \)

When \( a \) is small (i.e. when the grid is fine):

\[ \cos(ka) = 1 - \frac{(ka)^2}{2} \]

\[ E - U_0 = 2t \left( \frac{k^2 a^2}{2} \right) = \frac{\hbar^2 k^2}{2m^*} \]

1d) Derive the group velocity and effective mass using the numerical dispersion and compare them with the parabolic results. Also, sketch by hand the energy dispersion, group velocity and effective mass as function of \( k \). Comment if they agree well with the continuum Schrödinger case.

Solution:

Group velocity: \( v_g = \frac{1}{\hbar} \frac{\partial E}{\partial k} = \frac{2at}{\hbar} \sin(ka) \)
Effective mass: \[ m^* = \hbar^2 \left( \frac{\partial^2 E}{\partial k^2} \right)^{-1} = \frac{\hbar^2}{2a^2 t \cos(ka)} \]

**Sketches:**

**Dispersion:** (k from 0 to \(\pi/a\))

**Group velocity:**

**Effective mass:**

**Comments:** The dispersion \( E(k) \) agrees with the continuum solution near \( k = 0 \). The group velocity does not go to zero at large values of \( k \) for the
continuum solution. Effective mass is constant, independent of energy, in the continuum solution.

1e) If an electric field is applied along the $x$ direction, describe the motion of the particle (i.e. velocity and acceleration) when $ka = 0, \pi/2$ and $\pi$.

**Solution:**

Force = mass times acceleration

Force due to an electric field: $F_e = -qE_x$. If the electric field is positive, then the force is always in the negative $x$-direction, but the sign of the acceleration will depend on the sign of the effective mass.

$ka = 0:$

$v_g = \frac{2at}{h} \sin(ka) = 0$

$m^* = \frac{\hbar^2}{2a^2t\cos(ka)} > 0$ so the acceleration is in the negative $x$-direction.

Note: We can also see this directly from the plots (slope of $E(k)$ and curvature).

$ka = \pi/2:$

$v_g = \frac{2at}{h} \sin(ka) > 0$

$m^* = \frac{\hbar^2}{2a^2t\cos(ka)} \to \infty$ so the acceleration is zero

$ka = \pi:$

$v_g = \frac{2at}{h} \sin(ka) = 0$

$m^* = \frac{\hbar^2}{2a^2t\cos(ka)} < 0$ so the acceleration is positive

2) Use the BandStructure Lab tool on nanoHUB.org to explore the bandstructure of GaAs. Follow the steps outlined below, and then answer the questions.

a) Choose a bulk material from the “Geometry” option.

b) Specify the “Material” as GaAs
c) Click on the “2 Electronic Structure” tab to move to the next screen  
d) Set the Tight Binding model to sp3d5s* and check the Spin-Orbit coupling box  
   (Note that some of the options given here are preset as defaults; you need to leave  
   them unchanged.)

e) Press the “3 Analysis” button to proceed.  
f) Leave all preset options unchanged. Press the “4 Advanced User” option to take you  
   to the next menu options.  
g) Press “Simulate” on the bottom of this screen to start the simulation.

You should be able to answer the following questions.

- What is the crystal structure of GaAs?  **Answer:** Zinc Blende  
- How many atoms are there in the unit cell of GaAs?  **Answer:** 8  
- Use the “Bulk Central” band plot to locate the Gamma, L, and X point  
  **Answer:**

![Graph showing band structure](image)

What are the corresponding energies at these points?  
**Answer:** Gamma = 1.42 eV, L = 1.71 eV, and X = 1.91 eV
• Obtain the band gap information from the plot you used for the previous sub-parts.

\textbf{Answer:}

\[ E_G = E_C - E_V \]
\[ E_C = 1.421 \text{ eV} \]
\[ E_V = -0.003 \text{ eV} \]
\[ E_G = 1.42 \text{ eV} \]

Alternatively, from “Bandgap/Bandedge information”: 1.42421 eV

• On the same plot you will notice bands below the 0 eV mark. What are these bands called and how are they classified?

\textbf{Answer:} The heavy hole, light hole, and split off valence bands.

• You will notice an energy split in the bands below 0 eV at the Gamma point. You will notice the so-called “split-off” band. How much is the energy split on the plot?

\textbf{Answer:}

-0.33 eV

• From the effective mass table information, write down the effective masses at the gamma and L point conduction bands. What quantitative difference do you see between these masses?

\textbf{Answer:}

Gamma: 0.0655 \( m_0 \)

L: longitudinal: 1.5605 \( m_0 \) transverse: 0.0949 \( m_0 \)

3) Derive an expression for the density-of-states in energy for a 1D semiconductor for states near the center of the band at \( k_x = 0 \). Assume a valley degeneracy of \( g_V \).

3a) Assume a parabolic dispersion near \( k_x = 0 \).

\textbf{Solution:}

\[ E(k_x) = E_C + \frac{\hbar^2 k_x^2}{2m} \]
We proceed as follows.

In k-space: \( N_{1D}(k)dk = \left( \frac{L}{2\pi} \times 2 \right) dk \)

Equate to energy space: \( D^+_1(E)dE = N_{1D}(k)dk / L \)

(Note that we are only considering +k states as in the figure below.)

\[
D^+_1(E)dE = \frac{1}{\pi} dk
\]

\[
D^+_1(E) = \frac{1}{\pi} \frac{dk}{dE} = \frac{1}{\pi \hbar v}
\]

where the group velocity is: \( v(k) = \frac{dE}{\hbar dk} \)

The above expression is valid for any band structure, but we need to multiply by 2 to include the –k states. (See figure below.)

\[
D_{1D}(E) = \frac{2}{\pi \hbar v}
\]

For a parabolic energy band: \( E = E_c + \frac{\hbar^2 k^2}{2m^*} \) and \( v = \frac{1}{\hbar} \frac{dE}{dk} = \sqrt{\frac{2(E - E_c)}{m^*}} \)

The DOS becomes:

\[
D^i_{1D}(E) = g_V \frac{1}{\pi \hbar} \sqrt{\frac{2m^*}{(E - \varepsilon_i)}}
\]

where we have now included a valley degeneracy, \( g_V \) and a subband index, \( i \) and a subband energy, \( \varepsilon_i \).

Fig. Both + and –k states contribute to \( D_{1D}(E) \).
3b) Assume a linear dispersion near $k_x = 0$.

$$E(k_x) = E_C + \hbar v_F |k_x|$$

**Solution:**

The general expression from 3a) still applies: $D_{1D}(E) = \frac{2}{\pi \hbar} \frac{1}{v}$

But here, the group velocity is constant, independent of $k$: $v(k) = v_F$

So the answer is:

$$D_{1D}(E) = \frac{2}{\pi \hbar} \frac{1}{v_F} \textbf{ Independent of energy!}$$

(We have not included a valley degeneracy or subband index, but these could be included if necessary.

4) Assume a nonparabolic, 1D energy bandstructure described by the so-called Kane dispersion as:

$$E(k_x)[1 + \alpha E(k_x)] = \frac{\hbar^2 k_x^2}{2 m^*(0)}.$$  

where

$$\frac{1}{m^*(0)} = \frac{1}{\hbar^2} \frac{d^2 E(k_x)}{dk_x^2} \bigg|_{k_x=0}.$$  

4a) Sketch (or produce a Matlab plot) of $E(k)$ vs. $k$ for two cases: i) $\alpha = 0$ and ii) $\alpha > 0$. If you are producing a Matlab plot, the energy range should be from 0 to 1 eV, and you can assume $\alpha = 0.5$ eV.

**Solution:**
4b) For this bandstructure, derive an expression for the velocity, \( v_x(E) \) as a function of energy, \( E \).

Solution:

\[
\begin{align*}
v & = \frac{1}{\hbar} \frac{dE}{dk} \\
E(k_x)[1+\alpha E(k_x)] & = \frac{\hbar^2 k_x^2}{2m^*(0)} \\
\frac{dE}{dk_x}[1+2\alpha E] & = \frac{\hbar^2 k_x}{m^*(0)} \\
\frac{1}{\hbar} \frac{dE}{dk_x} & = \frac{\hbar k_x}{m^*(0)[1+2\alpha E]} \\
\text{Finally:} & \\
v & = \frac{\hbar k_x}{m^*(E)} \\
m^*(E) & = m^*(0)[1+2\alpha E]
\end{align*}
\]

This looks like the parabolic expression, but with the effective mass replaced by an energy-dependent effective mass.

5) For parabolic energy bands, the 2D density of states is

\[
D_{2D}(E) = \frac{m^*}{\pi \hbar^2} \Theta(E - E_c) .
\]

Assume a non-parabolic band described by the so-called Kane dispersion,
\[ E(k)[1 + \alpha E(k)] = \frac{\hbar^2 k^2}{2m^*(0)}, \]
and derive the corresponding density of states.

**Solution:**

Begin by repeating the derivation in the class notes:

\[
N_{2D}(k)dk = \left( \frac{A}{(2\pi)^2} \times 2 \right) dk_x dk_y
\]

\[
D_{2D}(E)dE = N_{2D}(k)2\pi kdk / A
\]

\[
D_{2D}(E)dE = \left( \frac{1}{2\pi^2} \right)2\pi kdk = \frac{1}{\pi} kdk
\]

Now, we need to be careful and get \( kdk \) from the non-parabolic dispersion.

\[
E(k)[1 + \alpha E(k)] = \frac{\hbar^2 k^2}{2m^*(0)} = E + \alpha E^2
\]

\[
\frac{\hbar^2 kdk}{m^*(0)} = dE(1 + 2\alpha E)
\]

\[
kdk = \frac{m^*(0)}{\hbar^2} dE(1 + 2\alpha E)
\]

Now insert this in the DOS expression to find:

\[
D_{2D}(E)dE = \frac{m^*(0)(1 + 2\alpha E)}{\pi\hbar^2} dE
\]

\[
D_{2D}(E) = \left[ \frac{m^*(E)}{\pi\hbar^2} \right]
\]

\[
m^*(E) \equiv m^*(0)(1 + 2\alpha E)
\]

We see that the result is just like the parabolic band case, except for the energy dependent effective mass. Since the mass increases with energy, the 2D DOS is not constant with energy as it was for parabolic bands.
This can be qualitatively understood from the figure in part 4a). States are equally spaced in k-space, but a faller E(k) (as in the nonparabolic case) puts a larger number of states in the same energy range.

We can also see this effect in a numerically computed 2D DOS for Si:

![Graph showing 2D DOS](image)

(sp^3d^5s* tight binding calculation by Yang Liu, Purdue University, 2007)

But if we look as MUCH higher energies:

![Graph showing 2D DOS](image)

(sp^3d^5s* tight binding calculation by Yang Liu, Purdue University, 2007)

So \( E(k)\left[1 + \alpha E(k)\right] = \frac{\hbar^2 k^2}{2m^*(0)} = E + \alpha E^2 \) is a way to get a little more accurate answer not too far from the band edge, but for energy way above the bottom of the conduction band, numerical bandstructure calculations are needed.

6) Consider a Si quantum well (like the inversion layer of a MOSFET) with the confining potential in the z-direction. Recall that the constant energy surfaces for the parabolic conduction band are described by ellipsoids of revolution with the long axis described by the longitudinal effective masses and the two transverse axes by the transverse effective mass. That is, for the two ellipsoids oriented along the z-axis, we have:
The confining potential in the $z$-direction will produce a set of quantized energy levels that are determined by the shape of the well (approximately triangular) and by the effective mass in the direction of confinement. Answer the following questions.

6a) For the ellipsoids with their long axes in the $z$-direction, what is $E(k)$ in the plane of the channel (the $k_x, k_y$ plane)? What is the valley degeneracy (i.e. how many ellipsoids respond to the confining potential with the longitudinal effective mass? 

Solution:

$$E(k) = \frac{\hbar^2 (k_x^2 + k_y^2)}{2m^*_x} \text{ (this is the equation of a circle)}$$

There are two of these valleys, so $g_v = 2$

6b) For the ellipsoids with their long axes perpendicular to the $z$-direction, what is $E(k)$ in the plane of the channel (the $k_x, k_y$ plane)? What is the valley degeneracy (i.e. how many ellipsoids respond to the confining potential with the transverse effective mass? 

Solution:

For the ellipsoids along the y-axis:
There are two of these valleys, so $g_V = 2$

For the ellipsoids along the x-axis:

$$E(k) = \frac{\hbar^2 k_x^2}{2m_t} + \frac{\hbar^2 k_y^2}{2m_t}$$

(this is the equation of an ellipse)

There are two of these valleys, so $g_V = 2$

6c) The first set of subbands (the quantum confined states of 6a), are known as the **unprimed subbands**. What is the 2D density of states for electrons in these subbands? What is the DOS effective mass for these subbands?

**Solution:**

Since there is just one effective mass for the x- and y-directions, and it is the transverse eff. mass, so:

$$D_{2D}(E) = g_v \frac{m^*_v}{\pi \hbar^2} = 2 \frac{m^*_t}{\pi \hbar^2}$$

If we write this as:

$$D_{2D}(E) = \frac{m^*_D}{\pi \hbar^2}$$

We can identify the DOS effective mass as:

$$m^*_D = 2m^*_t$$

6d) The second set of subbands (the quantum confined states of 6b), are known as the **primed subbands**. What is the 2D density of states for electrons in these four subbands? What is the DOS effective mass for these subbands?

**Solution:**

Let’s follow Prof. Alam’s approach (slide 13, of Lecture 8).
Pick one of the 4 ellipses: (You can check that we’ll get the same answer for any one of the four.)

\[ E(k) = \frac{\hbar^2 k_x^2}{2m_x^*} + \frac{\hbar^2 k_y^2}{2m_y^*} \]

Write it in the standard form of an equation for an ellipse:

\[ 1 = \frac{k_x^2}{(2m_x^*E/\hbar^2)} + \frac{k_y^2}{(2m_y^*E/\hbar^2)} = \left(\frac{k_x}{\alpha}\right)^2 + \left(\frac{k_y}{\beta}\right)^2 \]

where

\[ \alpha = \left(\sqrt{2m_x^*E/\hbar}\right) \]
\[ \beta = \left(\sqrt{2m_y^*E/\hbar}\right) \]

The area of this ellipse in k-space is: (Multiply by valley degeneracy to get the total area for all 4 ellipses in k-space.)

\[ g_v A_k = g_v \pi \alpha \beta = g_v \pi \left(\sqrt{2m_x^*E/\hbar}\right)\left(\sqrt{2m_y^*E/\hbar}\right) \]

Equate this to the area of a circle in a transformed k-space with where the constant energy line is a circle, i.e.

\[ \frac{\hbar^2 k_{\text{eff}}^2}{2m_{D}^*} = E \]

Equating the two areas:

\[ g_v A_k = g_v \pi \left(\sqrt{2m_x^*E/\hbar}\right)\left(\sqrt{2m_y^*E/\hbar}\right) = \pi k_{\text{eff}}^2 = \pi \left(2m_{D}^*E/\hbar^2\right) \]

Solving for \( m_{D}^* \), we find:

\[ m_{D}^* = g_v \sqrt{m_x^*m_y^*} = 4\sqrt{m_x^*m_y^*} \]
So for the unprimed subbands, the DOS is:

\[ D_{2D}(E) = \frac{m_D^*}{\pi h^2} = \frac{2m_l^*}{\pi h^2} \]

and for the primed subbands:

\[ D'_{2D}(E) = \frac{m_D^*}{\pi h^2} = \frac{4\sqrt{m_l^* m_t^*}}{\pi h^2} \]

6e) Which subband do you expect to be lowest in energy? Is the \( n = 1 \) unprimed subband lower or higher in energy than the \( n = 1 \) primed subband? Explain why.

**Solution:**
This is not a rectangular quantum well (it is closer to triangular), but the same general considerations apply. A heavy effective mass in the confinement direction gives a small energy, and a light effective mass gives a higher energy. (Similar to:

\[ \varepsilon_n = \frac{\hbar^2 n^2 \pi^2}{2m^* W^2} \]

The unprimed valleys have the large effective mass in the direction of confinement, so the lowest energy is the \( n = 1 \) unprimed state. The lowest prime state energy is higher, because these four valleys respond to the confining potential with the lighter, transverse effective mass. There are two “ladders” of energy levels corresponding to the unprimed and primed valleys.