Please complete the following questions. You are allowed to work in groups but remember to show your own work.

Problem 1. (Nearly Free Electron Model Revisited)
In class, we considered the nearly free electron model as next step up from the free electron gas. We briefly discussed the 1D model where

$$V(x) = A\cos\left(\frac{2\pi x}{a}\right)$$

and we will now work through some of the details we skipped.

(a) How is the dispersion relation different between the nearly- and the free electron model? Explain what physically leads to this difference.

(b) Make a sketch of the 1st Brillouin zone of the dispersion relations for both models (use the same plot but different colors for both) to show the differences between the two models.

(c) Now focus on the boundary of the 1st BZ. In your own words, explain what we mean by there being a degeneracy at the boundaries. What does this degeneracy tell us about k and $k' = k + G$, the crystal momenta for the two dispersions that intersect at the boundary?

(d) Now, consider the potential given above, repeat the degenerate perturbation theory method we used in class to find the eigenvalue equation for this potential at the BZ boundary. Recall that we defined

$$V_G = \langle k|V|k'\rangle = \frac{1}{a}\int_0^a e^{i(k'-k)x}V(x)\,dx$$

and you might find it useful to know $\int_0^a e^{in\pi x/a}\,dx = 0$ for even n.

(e) Show that the energy eigenvalues are

$$E_\pm = \frac{\hbar^2 k^2}{2m} \pm \frac{A}{2}$$

Explain how this represents a band gap in the dispersion relation. What is the width of the band gap?

(f) Use the eigenvalues you obtained above to show that the corresponding eigenstates are

$$|\psi_\pm\rangle = \frac{1}{\sqrt{2}}(|k\rangle \pm |k'\rangle)$$

In other words, find the eigenvectors of the matrix. In your own words, explain why these eigenstates physically makes sense.

(g) In real space, we can write these eigenstates as plane waves

$$\psi_\pm = \frac{1}{\sqrt{2}}\left(e^{ikx} \pm e^{ik'x}\right)$$

Show that ψ_+ and ψ_- represent standing waves at the boundary of the BZ (*hint:* how are k and k' related here see part (d)). How does the shape band structure tell you that this must be the case?

(h) In your own words, explain how the electron probability densities $|\psi_\pm|^2$ explain the opening of the band gap at the BZ boundary. A picture helps.

Problem 2. (Dirac Comb Potential)

A possible periodic potential we can use to model a 1D lattice of N atoms with lattice constant a is equally spaced dirac-delta functions:

$$V(x) = U \sum_n \delta(x - na)$$

(a) Argue that the Schrodinger equation away from the atoms will have a plane wave solution of the

$$\psi(x) \sim e^{\pm iqx}$$

where the wavenumber q is given by

$$q = \frac{\sqrt{2mE}}{\hbar}$$

(*Hint:* what does the potential look like away from the lattice sites?)

(b) Explain why we can say that the solution to this periodic potential has the form

$$\psi(x) = e^{ikx} u(x)$$

for some function $u(x)$ and show that

$$\psi(x) = e^{ika} \psi(x + a).$$

(c) (*Extra Credit*:) Consider the two zero potential segments around the lattice site at $x = 0$:

$$\text{Region I:} \quad -a < x < 0$$
$$\text{Region II:} \quad 0 < x < a$$

If we write a generic solution at each region as follows,

$$\psi_I(x) = Ae^{iqx} + Be^{-iqx}$$
$$\psi_{II}(x) = Ce^{iqx} + De^{-iqx}$$

show that the (i) periodicity of $\psi(x)$ (ii) continuity at $x = 0$ of $\psi(x)$ and (iii) the discontinuity of $\psi'(x)$ at $x = 0$ gives the following transendeltal form of the dispersion relation:

$$\cos(ka) = \cos(qa) + \frac{mUa}{\hbar^2} \frac{\sin(qa)}{qa} \tag{1}$$

(d) Use your favorite graphing software to plot the dispersion relation above (Eq. 1). You can set all constants but U to 1. Remember that there is an E hidden in q! Sketch the dispersion relation in the reduced zone scheme for $U = 0$. In your sketch, show what happens when you set $U > 0$. (desmos can plot implicit equations. Dont try to solve for E it's not possible!)

(e) Interpret your plot above. What happened when U went from zero to non-zero and why? What forms as the strength of the potential potential is not neglected?

Problem 3. (1D Semiconductor)

Suppose we have a one-dimensional semiconductor with valence and conduction bands given by

$$E_v = 2t_v \left[\cos(ka) - 1\right]$$
$$E_c = E_{gap} - 2t_c \left[\cos(ka) - 1\right]$$

with Fermi level set somewhere within the bandgap.

(a) In your own words, explain the idea of effective mass. What property of the band structure leads to a different mass? What does it mean for the effective mass to be negative?

(b) Find expressions for the group velocity and effective mass for electrons in the conduction band and holes in the valence band.

(c) If we say that the Fermi level is very far away from both bands, give an argument as to why we can approximate our populations of conducting electrons and holes to be at low k. Give expressions for E_v and E_c for low k.

(d) Write down expressions for the density of states for both electrons and holes in this low k limit.

(e) Calculate the electron density in the conduction band and the hole density in the valence band. (Use the approximation that $n_{FD}^{(e,h)} \approx e^{\beta(-E^{(e,h)} \pm E_F)}$ when E_F is far away from the bands to help you calculate your integral)

(f) Find an expression for the Fermi energy if this semiconductor is an intrinsic semiconductor.