

PHY 555: Solid-state Physics I

Homework #2

Due: 09/21/2022

Homework is due by the end of the due date specified above. **Late homework will be subject to 3 points off per day past the deadline, please contact me if you anticipate an issue making the deadline.** It should be turned in via blackboard. For the conceptual and analytical parts, turn in a scan or picture of your answers (please ensure that they are legible) or an electronic copy if done with, e.g., $\text{\LaTeX}$. For the computational part, turn in your source code and a short description of your results (including plots). The description can be separate (e.g., in $\text{\LaTeX}$ or word), or combined (e.g., in a jupyter notebook). Let me know if you are not sure about the format.

Conceptual

1. **5 points** Explain why crystal momentum $\hbar k$ does not correspond to the true momentum of electrons in a periodic potential, but is still a useful quantity.
2. **5 points** We discussed how $\frac{1}{\hbar} \frac{dE(k)}{dk}$ corresponds to a “semiclassical” velocity of electrons. What is meant by semiclassical, and why is it an appropriate label for this expression?
3. **5 points** Argue that the “overlapping band” situation shown in Fig. 1 is not possible for an electron in a one-dimensional periodic potential. (*Hint*: What type of differential equation is the Schrödinger equation in 1D? How many solutions does it have for a given energy? What do the band dispersions we have analyzed look like with respect to $\pm k$?) What does this imply about the locations of band extrema for 1D potentials?

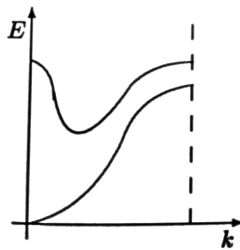


Figure 1: Impossible bands in 1D periodic potential.

Analytical

4. **15 points** Show that for wavefunctions in Bloch form, i.e., $\psi_k(x) = u_k(x)e^{ikx}$, the expectation value of the kinetic energy operator can be written as

$$\langle \psi_k | \frac{p^2}{2m} | \psi_k \rangle = \langle u_k | \frac{(p + \hbar k)^2}{2m} | u_k \rangle \quad (1)$$

5. **30 points** We discussed in class that the electronic structure is given by the Bloch wavefunctions evaluated at k 's in the first Brillouin zone. At a given k , say k_0 , there are an infinite number of solutions to the Schrödinger equation, labeled by n , at increasing energies E_{nk_0} . Because the eigenfunc-

tion ψ_{nk_0} form a complete set we can actually use them to represent the wavefunction and energies at any other k .

- (a) Consider the expansion the crystal wavefunction in terms of Bloch functions of the form:

$$\psi_k(x) = \sum_n c_{nk} \left[e^{i(k-k_0)x} \psi_{nk_0}(x) \right]. \quad (2)$$

Show that if we know the wavefunctions (ψ_{nk_0}) and energies (E_{nk_0}) at k_0 , we can determine the wavefunction and energies at any other k . **Hint:** It is sufficient to show that the matrix elements of the Hamiltonian with respect to the basis functions in the square brackets in Eq. (2) can be determined if ψ_{nk_0} and E_{nk_0} are known.

- (b) Consider a given energy state n and k -point k . Assume that this state is nondegenerate. Treat $\hbar(k - k_0)p/m$ as a perturbing potential and write the energy E_{nk} up to second order in $k - k_0$ using nondegenerate perturbation theory.
- (c) Consider the case where k_0 is a band extremum. Show that the energy versus k can be written as a quadratic dispersion around k_0 , with an “effective mass” different from the free-electron mass.

Computational

6. **40 points** Consider the Mathieu potential discussed in I.5.2 of Grosso and Parravicini, where $V(x) = 2V_1[1 - \cos(2\pi x/a)]$. We will solve for the band structure of an electron in this potential using a plane wave basis.

- (a) Show (analytically) that the matrix elements between plane waves for the Mathieu potential are of the tridiagonal form

$$\langle W_{k_m} | H | W_{k_n} \rangle = \left[\frac{\hbar^2(k + h_n)^2}{2m} + 2V_1 \right] \delta_{mn} - V_1 \delta_{m,n+1} - V_1 \delta_{m,n-1} \quad (3)$$

where δ is the Kronecker delta function, and $W_{kn} = \frac{1}{\sqrt{L}} e^{i(k+h_n)x}$ and $h_n = 2\pi n/a$.

- (b) Write a program to calculate the retarded Green's function from the continued-fraction expression:

$$G_{00,k}(E) = \frac{1}{E - \alpha_0(k) - \frac{V_1^2}{E - \alpha_1(k) - \frac{V_1^2}{E - \alpha_2(k) - \frac{V_1^2}{\dots}}} - \frac{V_1^2}{E - \alpha_{-1}(k) - \frac{V_1^2}{E - \alpha_{-2}(k) - \frac{V_1^2}{\dots}}}}, \quad (4)$$

where $\alpha_n(k) = 2V_1 + (\hbar^2/2m)(k + 2\pi n/a)^2$. Note that a small imaginary number should be added to the energy ($E \rightarrow E + i\eta$) to obtain the retarded version. You will have to choose a finite number of fractions to include, make sure it is large enough that the quantities in the following parts are converged.

- (c) For parameters $V_1 = 5(\hbar^2/2m)(\pi/a)^2$ and $a = 5$ Bohr, plot the real and imaginary parts of $G_{00,k}(E)$ as a function of energy for fixed $k = \pi/a$ (use $\eta = 0.01$ Ha). You should see a series of poles of the real part and peaks of the imaginary part. The poles and peaks will be at the same energies, which correspond to the allowed energies for the given k point.
- (d) From the poles or the peaks of $G_{00,k}$, plot the band dispersion $E(k)$ in the first Brillouin Zone over the energy range from 0 to 10 Ha. To do this, you will need to identify the peak/pole

energies at each k (note that α_n depends on k), and plot them for a mesh of k points in the first Brillouin zone.

- (e) Using the imaginary part of the Green's function, plot the *total* density of states over the energy range from 0 to 10 Ha. Note that you will need to sum over diagonal elements of G , i.e., $\sum_k \sum_m G_{mm,k}$. You can obtain $G_{mm,k}$ by shifting the indices of α in Eq. (4), i.e., for $m = 1$,

$$G_{11,k}(E) = \frac{1}{E - \alpha_1(k) - \frac{V_1^2}{E - \alpha_2(k) - \frac{V_1^2}{E - \alpha_3(k) - \frac{V_1^2}{\dots}}} - \frac{V_1^2}{E - \alpha_0(k) - \frac{V_1^2}{E - \alpha_{-1}(k) - \frac{V_1^2}{\dots}}}}, \quad (5)$$

Taking $m = 0 - 4$ in your sum should give you a converged DOS.