PHY 555: Solid-state Physics I

Homework #4

Due: 10/18/2024

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., 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 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*** Consider a 1D periodic potential that results in bands of allowed energies separated by gaps. If we "fill" an entire band with electrons how many electrons do we have in our entire crystal? How many per repeat unit? Explain.

2. ***10 points*** In the analytic and computational questions on this homework, the theme is that often the generalization of formalism between systems of 1, 2, and 3 dimensions is trivial (or at least straightforward), but the properties and physics can be quite different. Once you have completed problems 3, 4, and 5, summarize in one sentence per problem how this was illustrated.

Analytical

3. ***25 points*** In class, we derived the semiclassical velocity, which in 3D can be written as

$$\mathbf{v}(\mathbf{k}) \equiv \langle \psi_{n\mathbf{k}} | \frac{\mathbf{p}}{m} | \psi_{n\mathbf{k}} \rangle = \frac{1}{\hbar} \frac{\partial \epsilon_{n\mathbf{k}}}{\partial \mathbf{k}} = \langle u_{n\mathbf{k}} | \left(\frac{1}{\hbar} \frac{\partial H_{\mathbf{k}}}{\partial \mathbf{k}} \right) | u_{n\mathbf{k}} \rangle, \tag{1}$$

where $H_{\mathbf{k}}$ is the cell-periodic Hamiltonian (i.e., $H_{\mathbf{k}}|u_{n\mathbf{k}}\rangle = \epsilon_{n\mathbf{k}}|u_{n\mathbf{k}}\rangle$) and bold quantities indicate vectors. We related this quantity to the response of an electron to an external electric field. Actually, our derivation was incomplete, as we will explore in this problem.

Consider a Hamiltonian H with a periodic potential, whose eigenstates are Bloch states $\psi_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}$ given by $H|\psi_{n\mathbf{k}}\rangle = \epsilon_{n\mathbf{k}}|\psi_{n\mathbf{k}}\rangle$. Now we add an electric field to the Hamiltonian via the term $H' = e\mathbf{E}\cdot\mathbf{r}$, where $\mathbf{E}$ is the strength of the electric field, e is the electron charge, and $\mathbf{r}$ is the position operator.

(**a**) Using nondegenerate perturbation theory, write the change in the wavefunction $|\psi_{n\mathbf{k}}\rangle$ from this perturbation to first order in $\mathbf{E}$. We will refer to this quantity as $|\delta\psi_{n\mathbf{k}}\rangle$.

(**b**) Show that the corresponding expression for the cell periodic part can be written as

$$|\delta u_{n\mathbf{k}}\rangle = ie\hbar\mathbf{E}\cdot\sum_{n'\neq n} \frac{|u_{n'\mathbf{k}}\rangle\langle u_{n'\mathbf{k}}|\frac{1}{\hbar}\frac{\partial H_{\mathbf{k}}}{\partial \mathbf{k}}|u_{n\mathbf{k}}\rangle}{(\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}})^2}. \tag{2}$$

(**c**) Now write $\mathbf{v}(\mathbf{k})$ including the first-order-in-$\mathbf{E}$ changes in cell-periodic wavefunctions, i.e, on the right-hand-side of Eq. (1), replace $|u_{n\mathbf{k}}\rangle$ with $|u_{n\mathbf{k}}\rangle + |\delta u_{n\mathbf{k}}\rangle$ and neglect terms of order $\mathbf{E}^2$.

Show that $\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\frac{\partial \epsilon_{n\mathbf{k}}}{\partial \mathbf{k}} + \frac{e}{\hbar}\mathbf{E} \times \mathbf{B}_n(\mathbf{k})$ where

$$\mathbf{B}_n(\mathbf{k}) = i \sum_{n' \neq n} \frac{\langle u_{n\mathbf{k}} | \partial H_{\mathbf{k}} / \partial \mathbf{k} | u_{n'\mathbf{k}} \rangle \times \langle u_{n'\mathbf{k}} | \partial H_{\mathbf{k}} / \partial \mathbf{k} | u_{n\mathbf{k}} \rangle}{(\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}})^2}, \tag{3}$$

and $\times$ denotes the cross product. ***Hint:*** You may find the following vector triple product useful: $\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = \mathbf{b}(\mathbf{c} \cdot \mathbf{a}) - \mathbf{c}(\mathbf{a} \cdot \mathbf{b})$.

(**d**) The quantity $\mathbf{B}_n(\mathbf{k})$ is known as the *Berry curvature*, and is important in, e.g., the study of topological materials. Show that if we interpret the Berry curvature as a magnetic field *in reciprocal space*, the term $\frac{e}{\hbar}\mathbf{E} \times \mathbf{B}_n(\mathbf{k})$ can be written in the form of the magnetic-field part of a Lorenz force *in reciprocal space*.

4. ***20 points*** In class we discussed the Fermi energy E_F and density of states (DOS) for the free-electron gas in three dimensions.

(**a**) Determine the average energy per electron (in class denoted as E_0/N) for the 1D and 2D free electron gasses.

(**b**) Determine the DOS for the free-electron gas in one and two dimensions. Schematically plot the energy dependence of the DOS.

(**c**) To leading order in T, what is the temperature dependence of the Fermi energy in the 1D free-electron gas? What happens if we try to use the Sommerfeld expansion to linear order for the T-dependence of the Fermi energy in 2D?

(**d**) Find the T dependence of E_F for the 2D case (without using the Sommerfeld expansion) by calculating

$$N = 2\left(\frac{L}{2\pi}\right)^2 \int f(E) d^2k, \tag{4}$$

relating N to $E_\mathrm{F}(T=0)$ and solving for $E_\mathrm{F}(T)$. Show that the result is discontinuous at $T = 0$, and hence the Sommerfeld expansion does not apply.

Computational

5. ***40 points*** In class we discussed the one-dimensional nearest-neighbor tight-binding model with dispersion $E(k) = E_0 + 2\gamma\cos(ka)$. The generalization to two and three dimensions, i.e., square and cubic lattices (where a is the distance between sites) is quite simple: $E_{2\mathrm{D}}(\mathbf{k}) = E_0 + 2\gamma[\cos(k_x a) + \cos(k_y a)]$ and $E_{3\mathrm{D}}(\mathbf{k}) = E_0 + 2\gamma[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)]$. In this problem, set $E_0 = 0$, $\gamma = -0.5$ Ha and $a = 1$ Bohr.

(**a**) Write a program to calculate and plot the density of states for the 1D, 2D, and 3D tight-binding models. Use the same strategy as Homework 1, i.e., replacing the delta function with a Gaussian. Note that for, e.g., the 3D case, you will have to make a grid of $\mathbf{k} = (k_x, k_y, k_z)$ in three dimensions. Increase the number of $\mathbf{k}$ points until your DOS is converged. For each case, normalize by the number of k points N_k such that the DOS integrates to 2 total electrons. You may find that, especially in 3D, you require many $\mathbf{k}$'s and the sum takes quite long, so converge the DOS as much as you can.

(**b**) Write a program that numerically determines the Fermi energy for the 1D, 2D, and 3D tight-binding models for a given number of electrons n_e per unit cell. What is the Fermi level in each case for an occupation of 0.5 electrons per unit cell?

(**c**) For the 2D case, write a program to make a plot of the Fermi surface, i.e., the occupation in the k_x, k_y plane, for a given temperature. For 0.5, 1.0, and 1.5 electrons per unit cell, make plots for $k_B T = 0.05|\gamma|$ and $k_B T = 0.5|\gamma|$. You can neglect any T-dependence of the Fermi level.