PHY 555: Solid-State Physics I

Homework #1

Due: 05/09/2025

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)*** Read the two articles in the Lecture 1 folder on the class website (`https://marivifs-teaching.github.io/PHY555-2024/`), *More is different* by Phil Anderson, and *The Joy of Condensed Matter* by Inna Vishik. In 1-3 sentences, write why you are interested in solid-state physics.

2. ***(10 points)*** In class we have been discussing periodic potentials as models of a solid. Why is periodicity expected and important in solids?

Analytical

3. ***(15 points)*** In class we discussed that the solution of the Kronig-Penney model was given by (see Sec. I.2 of Grosso and Parravicini for derivation)

$$\frac{\beta^2 - q^2}{2q\beta}\sinh(\beta b)\sin(qw) + \cosh(\beta b)\cos(qw) = \cos(ka) \tag{1}$$

with $q = \sqrt{2mE/\hbar^2}$, $\beta = \sqrt{2m(V_0 - E)/\hbar^2}$, and $a = b + w$.

   (a) Show that taking $b \to 0$ and $V_0 \to \infty$ such that $V_0 b$ is constant gives the simplified expression

$$P\frac{\sin(qa)}{qa} + \cos(qa) = \cos(ka). \tag{2}$$

   where $P = \frac{mV_0 ba}{\hbar^2}$.

   (b) What is the energy dispersion when P goes to zero?

   (c) What is the energy dispersion when P goes to infinity?

Computational

4. ***(50 points)*** Consider again the Kronig–Penney model (before taking the barriers to delta-like functions) discussed in class, with solutions given by Eq. (1). Work in atomic units ($\hbar = m = 1$).

   (a) **Numerical solver (20 pts).** Write a program that, for each k in the first Brillouin zone ($-\pi/a \le k \le \pi/a$), finds all energies E in a user-defined window that satisfy Eq. (1). Implement a robust strategy to locate roots of

$$F(E,k) \equiv \frac{\beta^2 - q^2}{2q\beta}\sinh(\beta b)\sin(qw) + \cosh(\beta b)\cos(qw) - \cos(ka) = 0,$$

with $q = \sqrt{2E}$ and $\beta = \sqrt{2(V_0 - E)}$ (note: always choose $E < V_0$). *Hint:* Scan E on a fine mesh to bracket sign changes of F, then refine each bracket with a root-finder (e.g., Brent). Return the lowest few bands present in the chosen energy window.

(**b**) **Dispersion and basic descriptors (10 pts).** Using $w = 10$ Bohr, $b = 0.01$ Bohr, $V_0 = 100$ Ha (so $a = w + b$), plot the band structure $E_m(k)$ for $k \in [-\pi/a, \pi/a]$ over $E \in [0, 1]$ Ha. Mark the zone center ($k = 0$) and boundary ($k = \pm\pi/a$), and report: (i) the first band gap at $k = \pi/a$, and (ii) the effective mass of the bottom of the first band at $k = 0$, obtained from a quadratic fit $E(k) \approx E_0 + \frac{k^2}{2m^*}$ (so $m^* = 1/ \left.\frac{d^2E}{dk^2}\right|_{k=0}$ in a.u.).

(**c**) **Parameter trends (10 pts).** Vary one parameter at a time around the values in (b): (i) $w \in \{8, 10, 12\}$ Bohr, (ii) $b \in \{0.005, 0.01, 0.02\}$ Bohr, (iii) $V_0 \in \{50, 100, 200\}$ Ha. Provide a physical explanation for how the bandwidths and the first gap change with the parameters.

(**d**) **Density of states (10 pts).** The DOS is

$$D(E) = \sum_{m,k} \delta(E - E_m(k)) .$$

Approximate it by replacing each δ with a Gaussian of width $\sigma = 0.01$ Ha and sampling k uniformly in the first BZ. Plot $D(E)$ over $[0, 1]$ Ha for the parameters in (b). Comment on the 1D van Hove divergences (where $dE/dk = 0$).