PHY 555: Solid-State Physics I

Homework #1

Due: 06/09/2024

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)*** 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. ***(40 points)*** Consider again the Kronig-Penney model (before taking the barriers to delta-like functions) discussed in class, with solutions given by Eq. (1)

(a) Write a program that plots the energy dispersion $E(k)$ in the first Brillouin zone given inputs w, b, V_0

(**b**) For inputs: $w = 10$ Bohr, $b = 0.01$ Bohr, $V_0 = 100$ Ha, Plot the dispersion (energy versus k in the first Brillouin Zone) in the energy range from 0 to 1 Ha. Describe qualitatively how the dispersion changes when you change the inputs w, b, V_0.

(**c**) The density of states (DOS) gives the number of states at a given energy (summed over k), i.e.,

$$D(E) = \sum_{m,k} \delta(E - E_{m,k}) \tag{3}$$

A common approach to plot the DOS is to smear the delta function into a Gaussian with a finite width. Plot the DOS for the Kronig-Penney model with the same parameters and in the same energy range as (**b**) using this approach.