

# PHY 555: Solid-state Physics I

Homework #1

Due: 09/09/2022

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) Read the two articles in the Lecture 1 folder on the class website ([https://dreyer-research-group.github.io/phy555\\_fall2022.html](https://dreyer-research-group.github.io/phy555_fall2022.html)), *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)

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

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

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

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

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

- (b) What is the energy dispersion when  $P$  goes to zero?
- (c) What is the energy dispersion when  $P$  goes to infinity?
4. (30 points) In class we discussed the approach of relating the amplitudes of plane waves impinging on (and scattering off of) a barrier using the transfer matrix  $\mathbf{S}$  via

$$\begin{bmatrix} A_R \\ B_R \end{bmatrix} = \mathbf{S} \begin{bmatrix} A_L \\ B_L \end{bmatrix} = \begin{bmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{bmatrix} \begin{bmatrix} A_L \\ B_L \end{bmatrix} \quad (3)$$

where the subscript  $L$  ( $R$ ) indicates coefficients for plane waves on the left (right) of the barrier and  $A$  ( $B$ ) coefficients are for plane waves propagating right (left).

- (a) Show that if the total number of particles in the barrier region is constant in time, this implies that  $|A_L|^2 - |B_L|^2 = |A_R|^2 - |B_R|^2$ . What is the necessary condition on the form of the potential  $V(x)$  for this to be true? **Hint:** First show that a constant particle number in the barrier region implies that quantum mechanical current density is the same on both sides of the barrier [under the relevant constraint on  $V(x)$ ]. Then use the current density for plane waves to show the relation.
- (b) Without assuming the relations we discussed in class ( $s_{11} = s_{22}^*$  and  $s_{12} = s_{21}^*$ ), show that the following relations hold for the elements of the transfer matrix :

$$\begin{aligned} |s_{11}|^2 - |s_{21}|^2 &= 1 \\ |s_{22}|^2 - |s_{12}|^2 &= 1 \\ s_{11}^* s_{12} - s_{21}^* s_{22} &= 0 \\ s_{12}^* s_{11} - s_{22}^* s_{21} &= 0 \end{aligned} \quad (4)$$

**Hint:** One way to do this is to first show that the relation from (a) can be written as

$$\begin{bmatrix} A_L^* & B_L^* \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} A_L \\ B_L \end{bmatrix} = \begin{bmatrix} A_R^* & B_R^* \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} A_R \\ B_R \end{bmatrix}, \quad (5)$$

and then use Eq. (3) and it's Hermitian conjugate (i.e., conjugate transpose) on the right-hand-side.

- (c) Now we will make the assumption that our system is *time-reversal symmetric*, i.e., symmetric with respect to inverting time. In our case, time reversal means flipping the propagation direction of the plane waves, which just means taking their complex conjugate. If we have this symmetry, then we must have that

$$\begin{bmatrix} B_R^* \\ A_R^* \end{bmatrix} = \mathbf{S} \begin{bmatrix} B_L^* \\ A_L^* \end{bmatrix} \quad (6)$$

Use this to show that  $s_{11} = s_{22}^*$  and  $s_{12} = s_{21}^*$ . Combine this with part (b) to show that  $\det \mathbf{S} = 1$ .

**Hint:** One way to do this is to first show that Eq. (6) can be written

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} A_R^* \\ B_R^* \end{bmatrix} = \mathbf{S} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} A_L^* \\ B_L^* \end{bmatrix}, \quad (7)$$

and then compare to the *complex conjugate* (not Hermitian conjugate) of Eq. (3).

- (d) Consider the *scattering* matrix  $\bar{\mathbf{S}}$  defined by

$$\begin{bmatrix} B_L \\ A_R \end{bmatrix} = \bar{\mathbf{S}} \begin{bmatrix} A_L \\ B_R \end{bmatrix} = \begin{bmatrix} \bar{s}_{11} & \bar{s}_{12} \\ \bar{s}_{21} & \bar{s}_{22} \end{bmatrix} \begin{bmatrix} A_L \\ B_R \end{bmatrix}. \quad (8)$$

Show that  $\bar{\mathbf{S}}^\dagger \bar{\mathbf{S}} = 1$ , i.e.,  $\bar{\mathbf{S}}$  is unitary ( $^\dagger$  indicates Hermitian conjugate).

## Computational

5. (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.,

$$D(E) = \sum_{m,k} \delta(E - E_{m,k}) \quad (9)$$

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.