PROBLEM SET #5
"Periodic potential"
due on 5/16/2021

Physics–172 / Applied Physics–272
Introduction to Solid State Physics
Spring quarter, 2022

Instructor: *Aharon Kapitulnik* — aharonk@stanford.edu
Class Assistant: *David Saykin* — saykind@stanford.edu
Departments of Applied Physics and of Physics, Stanford University

Comment. Note that since these lecture notes are part of a manuscript, much of the language used here follows that of a book, with reference to chapters, sections, etc. In addition, some material in the notes may be more advanced, or will not directly be related to discussions in class. Please view these parts as stimulating extensions, where you are welcome to contact us about questions and relevant references.

Problem 5.1 (Nearly free electrons— **4 points**)**.** Consider one–dimensional periodic potential of triangular form as small perturbation.

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + \frac{\hbar^2 q^2}{m} v_a(x), \qquad v_a(x) = \sum_{n=-\infty}^{\infty} \left[1 - \frac{4}{a}|x - na|\right] \theta\left(2 - \frac{4}{a}|x - na|\right).$$

How does small periodic potential change spectrum of free electrons (no calculation is needed to answer this part of the problem)? Find the width of energy band gaps Δ_n up to the first order in potential strength $q^2 \ll 1/a^2$.

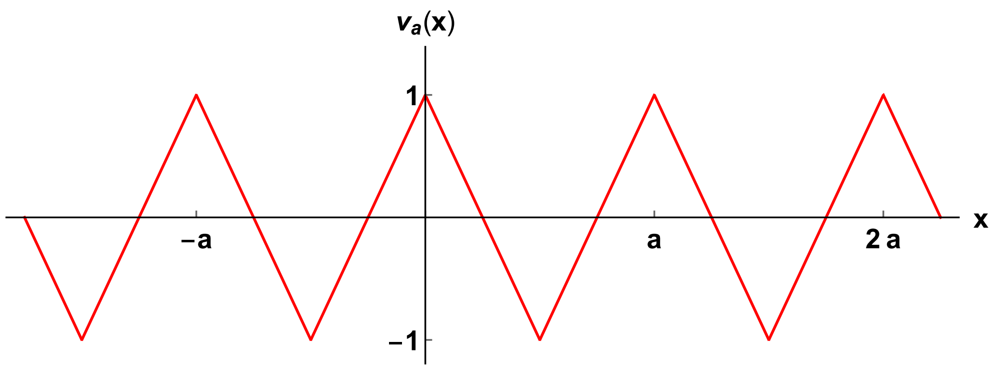

Figure 1: Triangle periodic potential.

Problem 5.2 (δ–Kronig–Penny model— **7 points**)**.** Consider a one dimensional crystal for which the potential is a periodic array of delta-functions,

$$V(x) = \frac{\hbar^2 q}{m} \sum_{n=-\infty}^{\infty} \delta(x - na).$$

where a is the lattice constant.

1. (Exact solution — **4 points**) Compute the energies for this model. Draw a picture of the band structure for positive and negative values of q.
2. (Tight–binding limit — **3 points**) If qa is large and negative, there is a tightly bound Wannier state $w_n(x)$ associated with each delta function. Find zero–order Wannier functions and calculate the width of the energy band within tight–binding approximation. Also, deduce the band width from exact solution you found before and compare the two.

   Hint. Read Chapter 10 in [1] to learn how to derive tight–binding approximation in 1D.

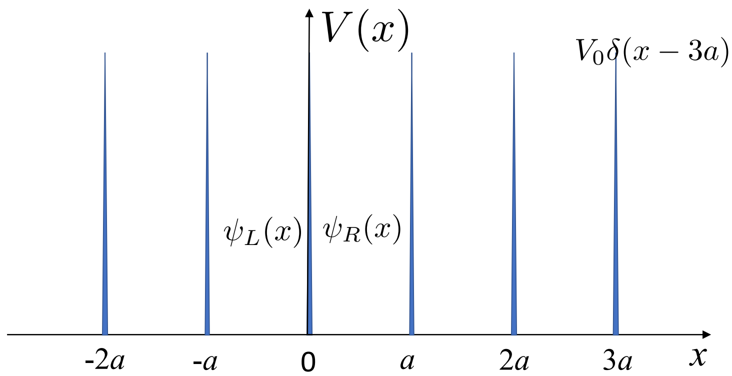

Figure 2: The δ-function Kronig-Penny Model

Problem 5.3 (Tight–binding chain— **4 points**). Consider one–dimensional chain of nodes with alternating hopping amplitudes between nearest neighbors t_1, $t_2 \in \mathbb{R}$. Such system is known in the literature as Su-Schrieffer-Heeger model.

$$\mathcal{H} = \sum_{i=-\infty}^{\infty} t_1 c^{+}_{2i+1} c_{2i} + t_2 c^{+}_{2i+1} c_{2i+2} + \text{h.c.}$$

Here h.c. stands for hermitian conjugate and c_i are fermionic annihilation operators on site i.

1. (**3 points**) Compute the spectrum.
2. (**1 point**) Imagine that you have one electron per node. Is it a metal or an insulator?

References

[1] Neil Ashcroft and David Mermin. *Solid state physics.* Harcourt College Publishers, 1976.