Periodic Potentials

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Exercise Background

(*We will utilize the Periodic Potential Lab installed on nanoHUB for this exercise*)

In this exercise, various calculations of the electronic band structure of a one-dimensional crystal are performed with the Kronig-Penney (KP) model. This model has an analytical solution and therefore allows for simple calculations. More realistic models always require extensive numeric calculations, often on the fastest computers available. The electronic band structure is directly related to many macroscopic properties of the material and therefore of large interest. Nowadays, hypothetical (nonexistent) materials are often investigated by band structure calculations – and if they show attractive properties, researchers try to prepare these materials experimentally. The KP model is a strongly simplified one-dimensional quantum mechanical model of a crystal. Despite of the simplifications, the electronic band structure obtained from this model shares many features with band structures that result from more sophisticated models.

Exercise Objectives

The exercise will enable you to learn the following:

1. Understand the concept of energy bands and energy gaps, their variations as a function of the size of the periodic potentials and energy

Relevant Literature

The following text-books may be helpful for further study:

1. D. K. Ferry, *Quantum Mechanics: An Introduction for Device Physicists and Electrical Engineers* (Institute of Physics Publishing, London, 2001).

2. D.M. Kim, *Introductory Quantum Mechanics for Semiconductor Nanotechnology* Wiley-VCH (2010).

3. P. Yu, M. Cardona, *Fundamentals of Semiconductors: Physics and Materials Properties*, Springer; (4th ed. edition, 2010).

Exercise: Periodic potentials

1a) Write down in not more than 5 sentences, the essential idea contained in the Kronig Penney model.

1b) The real Columbic potential is approximated in the Kronig Penney model through a step potential representation. Assuming that the electron moves in a one-dimensional crystal of lattice parameter "a", approximate the periodic potential experienced by an electron through a rough sketch and clearly mark out the regions corresponding to the positively charged ions of the lattice and the empty spaces between the ions. How many parameters define the KP model?

1c) Write down the Schrödinger equation applicable for each region and the general solutions obtained from them. What boundary conditions would you use to connect the coefficients in your solutions to the Schrodinger equation? Derive the conditions explicitly.

1d) We will use the Periodic Potential Lab under the ABACUS suite. You can invoke it by using of the two links supplied in the question. (www.nanohub.org/tools/abacus) /https://nanohub.org/tools/kronig_penney

Follow the steps outlined and supply answer to the questions presented.

- Choose the potential type as "step" (potential type tab)
- Set the maximum barrier height (U) to 2eV, the minimum to zero and energy of particle over barrier as 0 eV (energy details tab)
- Set the width of single periodic cell to 12A (well geometry tab)
- Use "a" equal to 8A (well geometry tab)
- Set the effective mass to unity.

I. Launch the tool for U = 2eV. Estimate the band-gap between the first and second energy bands. You should choose the "Allowed Bands" option from the drop down menu to answer this question.

II. Repeat part 1 with U = 4eV. Did the band gap between the first and second bands become larger or smaller than part 1? Give a physical reason for your answer.

III. Did the bands become wider (bandwidth) or narrower than in part 1?

IV. Use the drop down menu to look at the effective mass, you might notice certain values are negative; provide a physical interpretation of the change in sign of the effective mass.

For the next two sub questions, set the energy of particle over barrier as 5 eV

V. Now set the width of the single periodic cell to 100A and the width of the barrier to 2A. Perform the simulation and observe the wave function probability plot. Can you explain the nature of the plot on your screen?

VI. What difference do you see in the wave function probability plot when you change the width of the barrier to 94A? Can you reconcile the results with the simple expression you use to obtain energy levels for a particle in the box problem?

VII. From the plots obtained, what conclusions would you draw about the transmission as you modulated the width of the barrier (the energy height is kept constant). Does your answer depend on the "energy of the particle over barrier" parameter that can be altered through the energy details tab?

VIII. Suppose you have been provided with the energy levels present within a single step potential well, you are now required to line up 3 such single step potentials and compute the energy levels, do you expect to observe a change in the allowed energy levels present in any potential well? Which physical concept does this point to?

How does the above thought experiment relate to the Kronig Penny model, if you have a large number of potential wells instead of three that you use above?