Solid State Physics student laboratory

Kronig-Penney Model

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Introduction

In this student laboratory, various calculations of the electronic bandstructure of a one-dimensional crystal are performed with the Kronig-Penney (KP) model.[1] 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.

Details of the Kronig-Penney model

The KP model is a single-electron problem. The electron moves in a one-dimensional crystal of length L. The periodic potential that the electrons experience in the crystal lattice is approximated by the following periodical function.

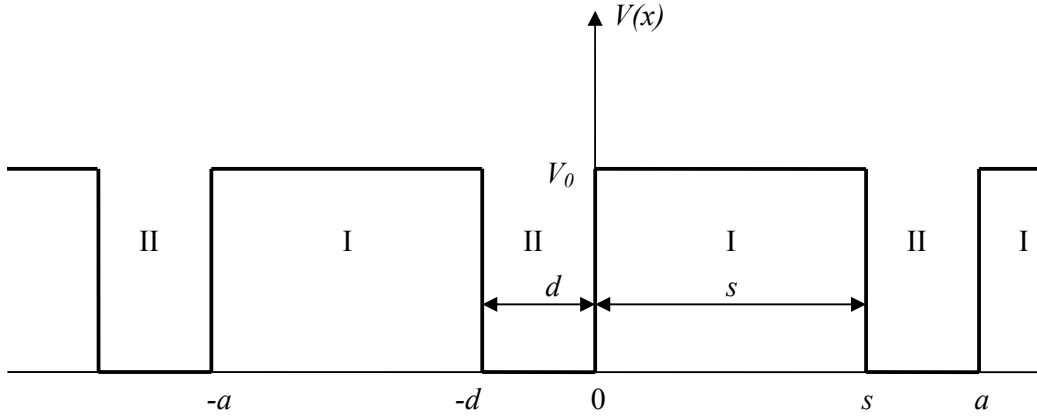[1] R. de L. Kronig and W. G. Penney, Proc. Roy. Soc. (London) **A 130** (1931) 499.

Figure 1: Potential for the electron in the Kronig-Penney model.

The regions denoted II correspond to the positively charged ions of the crystal lattice. The regions denoted I represent the empty spaces between the ions. It is the choice of this oversimplified potential that makes an analytical solution possible. The lattice parameter is $a = d + s$.

The KP potential is defined by three paramters, e.g., V_0, a, and d. The choice of zero on the energy axis has no influence on the physics of the problem.

The single-electron problem is described by the Schrödinger equation.

$$H\psi = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V[x]\right)\psi = E\psi.$$ (1)

Equation (1) can be given separately for regions I and II:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi = 0 \quad \text{(region I)}$$

(2)

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0 \qquad \text{(region II)}$$

The general solutions are

$$\psi_I = A\exp[i\beta x] + B\exp[-i\beta x], \quad \beta = \left(\frac{2m(E-V_0)}{\hbar^2}\right)^{\frac{1}{2}}$$

(3)

$$\psi_{II} = C\exp[i\alpha x] + D\exp[-i\alpha x], \quad \alpha = \left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}}$$

The coefficients *A, B, C, D* are complex constants determined by the boundary conditions and the normalizing

$$\int_0^L \psi^*\psi \, dx = 1.$$

(4)

The boundary conditions are that both ψ and $d\psi/dx$ are continuous functions of x:

$$A + B = C + D$$
$$\beta(A - B) = \alpha(C - D).$$

(5)

Further relations between the coefficient can be obtained from Bloch's theorem. Each stationary solution of the Schrödinger equation for a periodical potential can be written in the form

$$\psi_k[x] = u_k[x]\exp[ikx]$$

(6)

where $u_k[x]$ has the same periodicity as the potential. From equation (6), it also follows that

$$\psi_k[x+a] = \exp[ika]\,\psi_k[x] \tag{7}$$

which means that a translation by *a* only results in a phase shift of exp[*ika*]. The same translation symmetry is valid for the derivative of the wave function.

By considering the wave function at the points *-d* and *s*, we obtain

$$\psi_{I,k}[-d] = \exp[ika]\,\psi_{II,k}[s]$$

$$\Leftrightarrow A\exp[-i\beta d] + B\exp[i\beta d] = (C\exp[i\alpha s] + D\exp[-i\alpha s])\exp[ika] \tag{8}$$

and from the derivatives at *-d* and *s*, we have

$$i\beta(A\exp[-i\beta d] - B\exp[i\beta d]) = i\alpha(C\exp[i\alpha s] - D\exp[-i\alpha s])\exp[ika]. \tag{9}$$

The four equations (5, 8, 9) form a homogeneous linear system of equations. In order to obtain nontrivial solutions, the system determinant must vanish. This condition leads to the final equation

$$\cos[ka] = F$$

$$F = \cos[\alpha d]\cos[\beta s] - \frac{\beta^2 + \alpha^2}{2\alpha\beta}\sin[\alpha d]\sin[\beta s]. \tag{10}$$

Equation (10) relates energies *E* and indices *k* of possible Bloch functions. *E* is contained in the equation via α and β. Equation (10) only has real solutions for k in certain energy intervals, when $|F| < 1$. These solutions correspond to wavelike solutions. For $|F| > 1$, there are no Bloch electrons. The corresponding energy intervals are denoted energy or band gaps.

Assignments

You will implement equation (10) in Matlab and investigate several physical situations with the help of the implemented functions. The Matlab help function contains a lot of information and the instructions are rather easy to read. Matlab is very popular in Sweden, both at universities and in industry. ABB, e.g., requires knowledge of Matlab for many positions. In order to make the programming part a bit easier, we have included substantial guiding.

Start by implementing the script `kpmain`, which defines global variables (electron mass, $\hbar$, V_0, a, d), constants, and sets a path to the folder where you will save your functions.

```
% kpmain
% kpmain defines global variables, constants, and sets a path

global me hbar V0 a d

me=5.68572e-32;
hbar=6.58199e-16;
path('X:/xxxx/xxxx/xxxx/xxxx',path);
```

The most important function to be implemented is $k[E]$, i.e., the wavenumber (or one-dimensional wavevector) as a function of energy. Write a function `k(E)` that calculates the real part of another function `kv(E)`, which calculates k from equation (10). Write a separate function `F(E)` that calculates F in equation (10). `kv(E)` calls `F(E)`. `F(E)` itself calls the functions `alpha(E)` and `beta(E)`, where `alpha(E)` calculates α and `beta(E)` calculates β from equation (3). As an example, possible implementations of `kv(E)` and `alpha(E)` are given below. You might wonder why the electron mass has such a strange value. The reason is the chosen system of units: the laboratory uses the units Ångström for length, Å^{-1} for wave number, and eV for energy. If you define the electron mass as it is done in the example below, your results will be given in the above units. These units are much more convenient than SI units in the context of this laboratory.

```
% k(E)
% k(E) calculates the real part of the wave vector as a function of
% energy.

function [res]=k(E)

vect=kv(E);
le=length(vect);
for j=1:1:le
     if (abs(vect(j)) ~= real(vect(j)))  % returns NaN in
          vect(j)=NaN;                    % the band gap
     end;
end;
res=vect;




% alpha:
% alpha calculates alpha = sqrt(2*me*E/hbar^2)

function [res] = alpha(E)
global me hbar

res = sqrt(2*me*E)/hbar;
```

The free-electron model

The KP model can of course be used to obtain the band structure for the case of free electrons as well. In this lab, we will model 'one-dimensional aluminum'. Aluminum has a lattice constant of 4.05 Å. For our KP model, we choose to model aluminum along a direction that cuts through atomic planes with the highest packing density, i.e., we model along the [111] direction.

We choose a in our model to be the distance between two (111) planes. Calculate this distance and define the variable a, either directly in the command window or via a script. To start with, define $d = a/2$. As we are investigating free electrons, set $V_0 = 0$.

Plot the band structure for energies between 0 and 30 eV. You can, e.g., write in the command window:

```
E=0.1:0.1:30;
plot(k(E),E);
```

Write a function to calculate the band structure for free electrons and compare with the band structure obtained by the KP model. You can add graphs into an existing figure window by use of the command `hold on`. `hold on` can be switched off again by `hold off`. Can you observe any difference?

Nearly free electrons

Now raise the potential barrier to 0.1 eV. Why is this a low barrier – to which quantity should you compare in order to decide whether the barrier is low or high?

Can you find any energy gap between the first and second band? – Zoom into the figure in order to determine the size of the bandgap. Note that you will obtain too large a value if you plot in large steps. Steps of 0.1 eV, e.g., are too large here.

For nearly free electrons, the following can be shown (compare Kittel or Hook&Hall): The size of the first band gap is approximately $2|V_1|$, where V_1 is the first term in the Fourier development of the potential. In general, the *n*-th Fourier coefficient of a potential $U[x]$ with the period T is

$$U_n = \frac{1}{T} \int_c^{c+T} U[x]\exp[-in\omega x]\,dx, \quad \omega = \frac{2\pi}{T}. \tag{11}$$

In the case of the KP potential, we have

$$V_1 = \frac{1}{a} \int_c^{c+a} V[x]\exp\left[-\frac{i2\pi x}{a}\right]dx. \tag{12}$$

Calculate V_1 and compare $2|V_1|$ with the value that you obtained from your plot. When you calculate $2|V_1|$, you will see that the increase of the band gap is proportional to V_0. Set $V_0 = 0.2$ and check whether this is true for your KP model.

Band structure for stronger potential

Consider now stronger potential wells by increasing V_0 to 5 eV and reducing d to 1 Å. Plot the band structure for energies from 0 to 35 eV. Have the band gaps increased in size? By which factor has the first gap increased?

Surface states

Inside the band gap, no real solutions exist for $k[E]$. However, solutions with imaginary k can be obtained. Imaginary k means that the wave function cannot be delocalized over the whole crystal because its amplitude would grow to infinity in one direction. The wavefunction with imaginary k can be written as

$$\psi = A \exp\left[-|k|x\right] + B \exp\left[+|k|x\right] \tag{13}$$

Such a solution to the Schrödinger equation can exist as a surface state. For the left side of a one-dimensional crystal, e.g., the choice $B = 0$ yields a wave function that has the value A at the crystal surface and decays exponentially inside the crystal.

Plot the imaginary part of $k[E]$. To this end, implement a function imk(E) that calculates the imaginary part of the wave vector. Comment on your results. (You can compare your results to Figure 12 on page 196 in the textbook by Kittel, seventh edition). Over how many atomic layers does a surface state extend in the center of the first bandgap?

Group velocity

Study the group velocity as a function of k in the first band. Define a function `vg(E)` for this purpose. The group velocity is defined as

$$v_g = \frac{\mathrm{d}\omega}{\mathrm{d}k}, \quad \omega = \frac{E}{\hbar} \tag{14}$$

What is the maximum v_g, expressed in percents of the velocity of light?
Can you give a physical explanation for this behaviour of v_g when approaching the boundary of the Brillouin zone?

Effective mass

Calculate the effective mass normalized to the mass of a free electron as a function of the energy and discuss the results. Give a physical interpretation of the change in sign of the effective mass. The effective mass is defined as

$$m^* = \left(\frac{1}{\hbar^2} \frac{\mathrm{d}^2 \varepsilon}{\mathrm{d}k^2} \right)^{-1}. \tag{15}$$

Laboratory report

The report should be a self-consistent piece of work. This means that your report should be independent of this instruction. However, you can closely follow the order employed in this instruction, i.e., start with an introduction into the KP model and then introduce the different special cases and present and discuss your results. Please include your Matlab code in an appendix.