UNIVERSITÄT SIEGEN
FESTKÖRPERPHYSIK

Solid state physics (*winter term 2015/2016*)

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Exercise sheet 7

Electrons in a Periodic Potential

In this exercise we will study a simple model for a one-dimensional crystal lattice, which was introduced by Kronig and Penney in 1931. In the original model the atomic potentials are taken to be rectangular, with the minima corresponding to the atomic cores. Here we will consider a simplified version of this problem which still displays the essential physics behind the model. We will consider a potential of the form:

$$V(x) = V_0 \sum_{-\infty}^{\infty} \delta(x - an)$$

Where the $\delta(x - an)$ being Dirac delta function distributions located at the centre of the atomic cores and $V_0 > 0$.

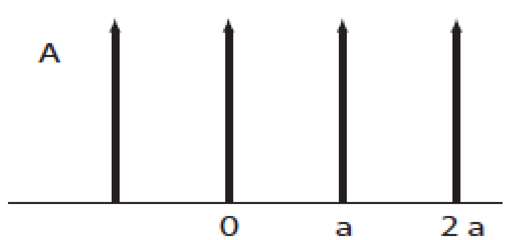

Figure 1 Kronig-Penney potential V (x)

a) Using Bloch's proposed solution for the wave function in a periodic potential,

$$\Psi(x) = u(x)e^{ikx} \text{ and } u(x+a) = u(x),$$

Show that the energy of the Kronig-Penny potential for a given k obeys the equation:

$$cos\lambda = \frac{v}{2\beta} sin\beta + cos\beta$$

Where

$$\lambda = ka, \beta = a\sqrt{\frac{2mE}{\hbar^2}} \text{ and } v = 2mV_0\frac{a}{\hbar^2}$$

Hint. Firstly, find the solution to the Schrödinger equation in the finite interval (na, na+a). Then, make use of the fact that the wave function has to be continuous everywhere. Lastly, the integration of the Schrödinger equation over the interval (na−η, na+η) in the limit of η → 0 yields another boundary condition for the derivative of the wave function.

b) Starting from part (a), discuss the two limits v << 1 and v >> 1 and show that there you recover the nearly free electron approximation and the tight binding approximation, respectively.

c) Calculate the density of states of the Kronig-Penney model. What is the behavior of the density of states at the band boundaries?

Hint. The number of states per unit cell in the interval (E, E + dE) is given through ρ(E)dE. Consider first a finite Kronig-Penney potential of length Na with periodic boundary conditions (N is the number of unit cells) such that the states can be indexed by discrete k-values. $\rho(E) = \frac{Na}{\pi}\left|\frac{dk}{dE}\right|$ *and the derivative can be calculated using the result of part a.*

Please return on 09/12/2015