Solid State Theory
Exercise 3

Problem 3.1 The Kronig-Penney model

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,

$$V(x) = V_0 \sum_{n=-\infty}^{\infty} \delta(x - an). \tag{1}$$

with the $\delta(x - an)$ being Dirac delta distributions located at the center of the atomic cores and $V_0 > 0$. This is our version of the so-called Kronig-Penney potential which is shown in Fig. 1A.

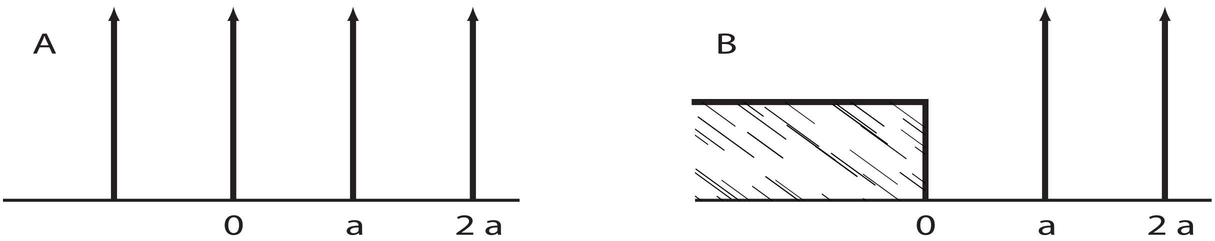

Figure 1: Kronig-Penney potential $V(x)$ (A) and interface between a constant potential $U(x)$ and a Kronig-Penney potential (B).

(a) Using Bloch's ansatz for the wave function in a periodic potential,

$$\Psi(x) = u(x)\mathrm{e}^{ikx} \quad \text{and} \quad u(x+a) = u(x)\,, \tag{2}$$

show that the energy in the Kronig-Penney potential for a given k obeys the equation

$$\cos\lambda = \frac{v}{2\beta}\sin\beta + \cos\beta, \tag{3}$$

where $\lambda = ka$, $\beta = a\sqrt{2mE/\hbar^2}$ and $v = 2mV_0a/\hbar^2$. In general, this equation can only be solved graphically or numerically. Show that the resulting band structure has band gaps (i.e., intervals where there exists no solution to Eq. (3)). Discuss the special cases where $v \to 0$ and $v \to \infty$.

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 Schödinger equation over the interval $(na - \eta, na + \eta)$ in the limit of $\eta \to 0$ yields another boundary condition for the derivative of the wave function.

(b) Starting from Eq. (3), discuss the two limits $v \ll 1$ and $v \gg 1$ 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 $\rho(E)dE$. 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. Convince yourself that

$$\rho(E) = \frac{Na}{\pi}\left|\frac{dk}{dE}\right|. \tag{4}$$

The derivative dk/dE can be calculated using Eq. (3).

(d) Consider now the potential

$$U(x) = \begin{cases} U_0 & x \leq 0, \\ V_0 \sum_{n=1}^{\infty} \delta(x-na) & x > 0, \end{cases} \tag{5}$$

which is shown in Fig. 1B.

Show that for $E < U_0 < \infty$ there is one additional state in every band gap which decays exponentially on both sides of $x = 0$. Show that the energy of this state is given by the solution of

$$\beta \cot \beta = \frac{u}{v} - \sqrt{u - \beta^2} \tag{6}$$

with $u = 2mU_0a^2/\hbar^2$.

Hint: The solution for $x > 0$ is given as in part a, but exponentially decaying. Thus, the energy eigenvalues should solve Eq. (3) within the band gaps. We set

$$\lambda = \begin{cases} i\mu & s = 1, \\ i\mu + \pi & s = -1, \end{cases} \tag{7}$$

where s is the sign of the right hand side of Eq. (3) where the Bloch ansatz implies that $\mu > 0$ for the wave function not to grow exponentially.

For $x < 0$ we use the ansatz

$$\Psi(x) = Ce^{\kappa x/a} \tag{8}$$

with $\kappa = \sqrt{u - \beta^2}$. Use the continuity of the wave function and of its first derivative at $x = 0$ to find the energy.