Corrections to HW5, problems 15.5 and 15.6

A. 15.5: Decaying waves

As we saw in this chapter, in one dimension, a periodic potential opens a band gap such that there are no plane-wave eigenstates between energies $\epsilon_0(G/2) - |V_G|$ and $\epsilon_0(G/2) + |V_G|$ with G a reciprocal lattice vector. However, at these forbidden energies, decaying (evanescent) waves still exist. Assume the form

$$\psi(x) = e^{-\kappa x}[Ae^{ikx} + Be^{i(k-G)x}] \ ,$$

with $0 < \kappa \ll k$ and κ real. Using first order degenerate perturbation theory (as in problem 15.1), find κ as a function of energy for $k = G/2$. For what range of V_G and E is your result valid?

B. 15.6: Kronig-Penney Model*

Consider electrons of mass m in a so-called "delta-function comb" potential in one dimension

$$V(x) = aU \sum_n \delta(x - na) \ .$$

(a) Argue using the Schroedinger equation that in-between delta functions, an eigenstate of energy E is always of plane wave form $e^{iq_E x}$, with

$$|q_E| = \sqrt{2mE}/\hbar \ .$$

Using Bloch's theorem, conclude that we can write an eigenstate with energy E as

$$\psi(x) = e^{ikx} u_E(x) \ ,$$

where $u_E(x)$ is a periodic function defined as

$$u_E(x) = e^{-ikx}\left[A\sin(q_E x) + B\cos(q_E x)\right] \qquad 0 < x < a \ ,$$

and $u_E(x) = u_E(x+a)$ defines u outside of this interval.

(b) Using continuity of the wave function at $x = 0$ derive

$$B = e^{-ika}[A\sin(q_E a) + B\cos(q_E a)] \ ,$$

and using the Schroedinger equation to fix the discontinuity in slope at $x = 0$ derive

$$q_E A - e^{-ika} q_E [A\cos(q_E a) - B\sin(q_E a)] = \frac{2maUB}{\hbar^2} \ .$$

Solve these two equations to obtain

$$\cos(ka) = \cos(q_E a) + \frac{mUa}{\hbar^2 q_E}\sin(q_E a) \ .$$

The left-hand side of this equations is always between -1 and 1, but the right-hand side is not. Conclude that there must be values of E for which there are no solutions of the Schroedinger equation – hence concluding that there are gaps in the spectrum.

(c) For small values of the potential U show that this result agrees with the predictions of the nearly free electron model (i.e., determine the size of the gap at the zone boundary).