**Homework 6:  Bloch Electrons and Band Structure**

1. The Kronig-Penney model is very useful for understanding a myriad of interesting physical effects that occur with the application of quantum mechanics and Bloch's theorem to band structure.   It also applies remarkably well to semiconductor superlattices, and also to quantum wells in certain limits.  The model shown here in Fig. 1 consists of infinite array of potential wells of width a separated by barriers of height $V_B$ width b.  In a real solid, the wells might be associated with the binding energy of a covalent or ionic bonding region between adjacent atoms, for example.  And $V_B$ is always associated with the repulsive potential of an electron approaching an atomic core where tightly bound electrons exist and invoke Pauli exclusion.  The principle result of the model is the connection equation between the energy level and the crystal wave vector k:

$$\frac{Q^2 - K^2}{2QK} \sinh Qb \sin Ka + \cosh Qb \cos Ka = \cos k(a+b) \qquad (1)$$

where $K = (2mU)^{1/2}/\hbar$ and $Q = [2m(V_B - U)]^{1/2}/\hbar \, K = (2mU)^{1/2}$ .  This can be solved for k as a function of U easily on a computer (Microsoft Excel is very good for this because of its ability to display the formula, show an embedded plot, and do graphic analysis all in the same Worksheet)
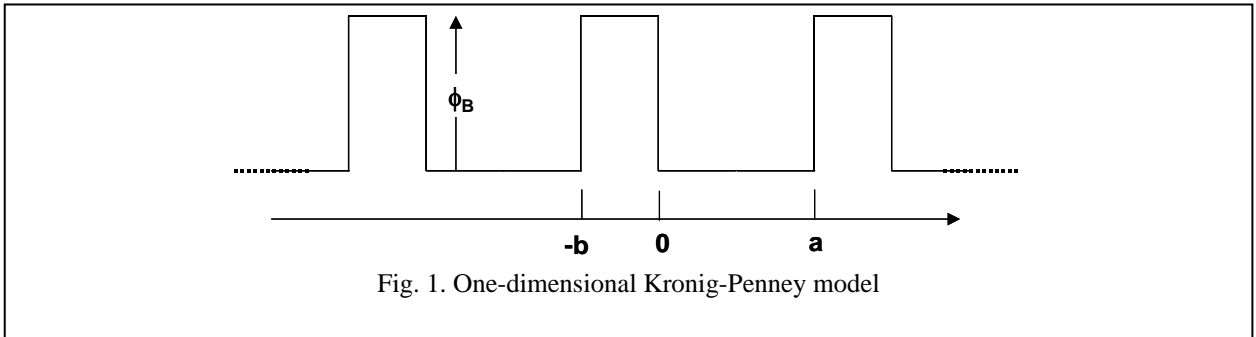


Fig. 1. One-dimensional Kronig-Penney model

(a) Find the "band structure" of U vs k following parameters: $V_B$ = 10 eV, a = 4.0 Ang, and b = 1.0 Ang.   Plot out the result using your favorite computational tool from k = 0 to k = $k_N$.  What is expression for $k_N$ and its numerical value in this case ?  [Clue: if you use Excel and solve (1) with the $\cos^{-1}$ function, the algorithm automatically limits $k_N$ to the correct domain]

(b) What is the energy of the lowest allowed electron state in (a) ?  What is the "bandwidth" of the first energy band associated with this state (in units of eV) ?    What is the effective mass associated with the lowest energy state ?  What is the effective mass associated with the highest energy state in this band ? (clue consider numerical differentiation).

(c)  How many allowed bands are there between U = 0 and 10 eV ?  What is the "bandwidth" of any higher-energy band (in units of eV) ?  Compare the bandwidth of any higher bands to the first band.  Which is wider and why ?

(d) What is the size of the energy gap between the top of the 1st band and the bottom of the 2nd band (in units of eV) ?

(e) What is the effective mass at the lowest and highest energies of the 2nd band ?  What is the highest group velocity in the first and second bands ?

2.  Perhaps the greatest utility of the Kronig-Penney model is in understanding physical trends.

(a)    Suppose $V_B$ in problem 1 is raised 10 times to 100 eV with a and b kept the same.  Use your numerical simulator to determine what happens to the bandwidth of the first two few bands and what energy levels do they tend towards ?  What problem in elementary quantum mechanics can be used to evaluate these levels ?  Carry out this evaluation for the first two levels.

   (b) Now suppose $V_B$ is kept at 10 eV but b is increased 10 times to 10 Ang.  What energy value does the first band tend towards ?  What problem in elementary quantum mechanics (and what structure in modern crystal epitaxial technology) does this case represent ?  Referring to your favorite quantum mechanics textbook, solve for this level and compare with the numerical Kronig-Penney solution.

   (c) Now suppose $V_B$ is kept at 10 eV, b at 1 Ang, but a is reduced 10 times to 0.4 Ang.  What is the lowest allowed energy level, how many bands, and what is the bandwidth ?   Now strictly for academic reasons, reduce a 1000 times to 0.004 Ang.  Where is the lowest energy level ?  What fundamental principle of quantum mechanics does this represent, as generalized to Bloch states ?

3.  The density-of-states D(U), first derived for the Fermi gas of free electrons, can be generalized to a Bloch electron in the form:

$$g_n(U) = \int_{S_n(U)} \frac{dS}{4\pi^3} \frac{1}{\vec{\nabla} U_n(\vec{k})}$$

   where $S_n(U)$ is a surface of constant energy U within band n. This is such an elegant expression of vector calculus that it deserves to be exercised, at least in special cases.

  (a)  Evaluate this integral for the very special case of a Fermi gas for which
$$U_n(\vec{k}) = (\hbar^2/2m)|\vec{k}|^2$$

  (b)   Now evalute the general $g_n(U)$ for ellipsoidal constant energy surface expressed as
$$U_n(\vec{k}) = U_0 + (\hbar^2/2)(k_x^2/m_x + k_y^2/m_y + k_z^2/m_z)$$
  and the show the answer can be written as $g_n(U) \propto (U-U_0)^{1/2}$. Then show that if the Fermi surface lies entirely within the nth band, that $g_n(U_F) = (3/2) n/(U_F - U_0)$ where n is the number of electrons populating this band.  This is a very useful form for a variety of different crystal structures, including those of cubic and orthorhombic symmetry.