Homework Set 2.

Problem 1. Consider a *tight-binding* Hamiltonian that acts upon a single band of localized orbitals in *one* dimension

$$\hat{H} = \sum_m \cos(2\pi m\alpha)|m\rangle\langle m| + t\sum_m \frac{1}{2}\left(|m\rangle\langle m+1| + |m\rangle\langle m-1|\right),$$

where $\alpha = 5/3$. The integer m should be thought of as indexing sites along the chain of atoms. The ket $|m\rangle$ locates an electron on atom m (e.g., $\langle x|m\rangle = \psi(x-m)$ is the wave function, or "orbital", which decays fast away from the position of an atom m).

(a) What is the periodicity of the Hamiltonian?

(b) Use Bloch theorem to reduct the eigenvalue problem of an infinite matrix $\hat{H}$ (obtained by representing the Hamiltonian in the basis of orbitals $|m\rangle$) to the solution of a small *finite* matrix equation [note that the size of this matrix will be equal to the periodicity of the Hamiltonian found in (a)].

(c) Compute and plot the bands as a function of Bloch wave vector k throughout the first Brillouin zone (this task will have to be carried our numerically).

Extra credit (20 points):

Problem 2. Consider a one-dimensional solid of length $L = Na$ made up of N diatomic molecules, where the interatomic spacing within a molecule is b ($b < a/2$). The centers of adjacent molecules are a distance a apart. We represent the potential energy as a sum of delta functions on each atom:

$$V = -A\sum_{n=0}^{N-1}\left[\delta\left(x - na + \frac{b}{2}\right) + \delta\left(x - na - \frac{b}{2}\right)\right]$$

with A being the positive quantity and $n = 0, 1, 2, \ldots, N-1$. The potential is "shown" in the Figure 1.

(a) Consider free electrons in this solid (i.e., neglect V for the moment) with periodic boundary conditions. Derive the allowed values of the electron wave vector k and normalize the wave functions.

(b) Expressing the potential as a Fourier series $V = \sum V_q e^{iqx}$, find the allowed values of q and the coefficients V_q.

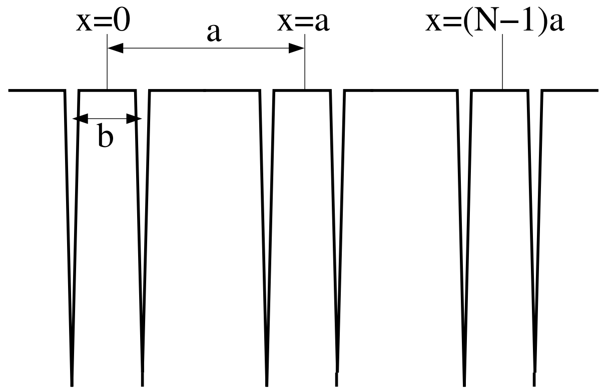

Figure 1: Sketch of the potential V (of course, delta "functions" extend all the way to $-\infty$).

(c) Assuming A to be small, show that for certain values of k there are energy gaps. Derive a general formula for the gaps and show in particular that the gap in energy at the top of the first zone is proportional to $\cos(\pi b/a)$. [Hint: Plug your result from (b) into the Schrödinger equation for eigenstates, where the eigenstates can be expressed as a series $\Psi = \sum_k C_k \phi_k$ with $\phi_k = e^{ikx}/\sqrt{L}$ being the wave functions you have found in (a).]

(d) Derive an expression for the number of state in the first zone. If each atom has one electron, will the substance be a conductor or an insulator?

(e) Suppose $b = a/2$. Show what happens to the results of the previous sections and give a brief qualitative explanation.

HINT: Check the exact solution of the Kronig-Penney model in, e.g., C. Kittel, Introduction to Solid State Physics, 8th edition, page 174.