Long problem assignment

Consider electrons in a two-dimensional square lattice of identical ions. For simplicity, use units so that $\hbar^2/2m = 1$ and $2\pi/a=1$.

A. Weak periodic potential

(a) Assuming zero lattice potential ($U_K=0$ for all K), make a plot of the 4 lowest energy bands in the [10] direction (i.e. for $k_y = 0$, $-1/2 \le k_x \le 1/2$). Give the degeneracy for each band.

(b) Same as (a) in the [11] direction.

(c) Find expressions for the four lowest energies at k=0 for a weak periodic potential in terms of U_K's. How many different U_K's are involved? What are the $\vec{K}$ values?

(d) Same as (b) for the two lowest energy levels at $\vec{k} = (1/2,0)$.

(e) Assume for the numerical values of the U_K's that enter the energies found in (c) and (d) the following: 0.1, 0.2, 0.3,... so that the smallest K has largest U_K and the smallest U_K involved has value 0.1.

Assuming only those U_K's are nonzero, find and make a plot of the 4 lowest energy bands versus k along the [10] direction using the fact that the potential is weak.

B. Tight binding bands

Consider four atomic orbitals: s, p_x, p_y, p_z.

(f) List all the non-vanishing independent matrix elements of the Hamiltonian up to next nearest neighbors. How many different matrix elements are there? Explain why some are equal to others and why some are zero.

(g) Construct the Hamiltonian matrix $H_{mn}(\vec{k})$ in terms of the matrix elements found in (f).

(h) Find expressions for the energies at $\vec{k} = 0$ and $\vec{k} = (1/2,0)$ in terms of the matrix elements found in (f).

(i) Assume now for simplicity that next-nearest neighbor matrix elements can be neglected. Find numerical values for the other matrix elements that will reproduce as closely as possible the energies of the four lowest bands found in (c) and (d) at the points $\vec{k} = 0$ and $\vec{k} = (1/2,0)$.

(j) Plot the 4 resulting tight binding energy bands in the [10] direction. How do they compare with the weak coupling results found in (e)?

(k) Plot and compare the results of the tight binding and the weak coupling calculation in the [11] direction.

Useful reference for tight binding: Slater and Koster, Phys. Rev. 94, 1498 (1954).