Physics 556 Spring 2007   homework # 8   (due Wednesday May 9)

Two band triangular lattice

The lattice is shown to the right. Primitive translation vectors are

$\vec{a} = a\left(\sqrt{3}/2, -1/2\right)$

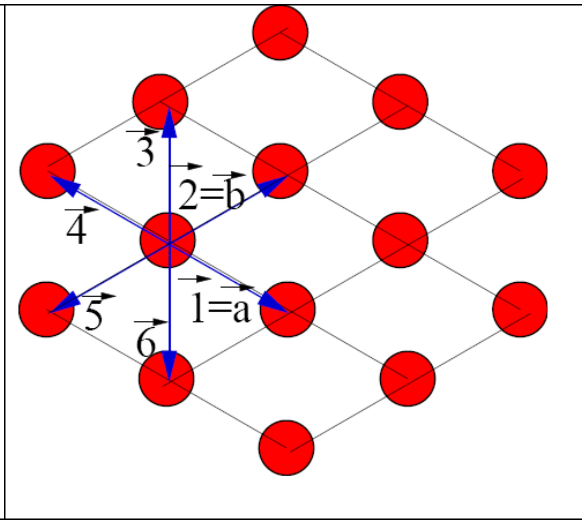
$\vec{b} = a\left(\sqrt{3}/2, +1/2\right)$;

corresponding primitive reciprocal lattice vectors are

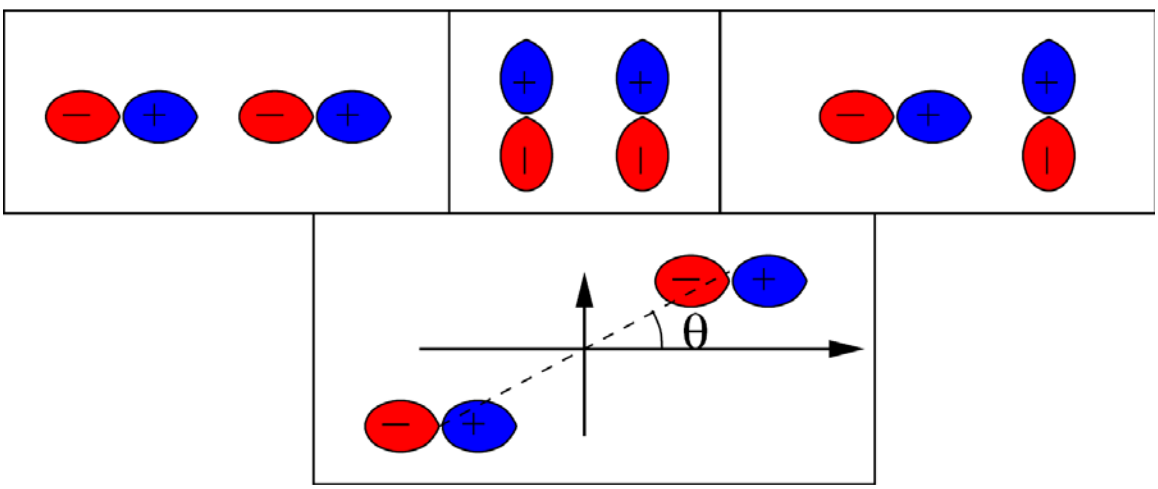
$$\vec{G}_1 = \left(\frac{2\pi}{a}\right)\frac{2}{\sqrt{3}}\left(1/2, -\sqrt{3}/2\right)$$

$$\vec{G}_2 = \left(\frac{2\pi}{a}\right)\frac{2}{\sqrt{3}}\left(1/2, +\sqrt{3}/2\right)$$

The nearest neighbor atoms are labeled with vectors $\vec{1}$, …, $\vec{6}$.



The problem is to study the electronic band structure of electrons on this lattice. As an easy first problem, suppose there is only one orbital per atom, a p_z orbital. As a second, more interesting problem, let there be two orbitals, p_x and p_y, which are degenerate in free space. The p_x and p_y orbitals are shown below. On the left, two orbitals give an energy overlap t_σ (known as ppσ in Slater-Koster notation). In the middle, the two orbitals give an energy overlap $-t_\pi$ (known as ppπ). The minus sign just permits both t_σ and t_π to be taken as positive numbers. On the right, the overlap energy matrix element is 0 by symmetry. On the bottom, after suitable rotation, the overlap matrix element is $\cos\theta\, t_\sigma - \sin\theta\, t_\pi$. You will need to use this result in the problem below. This process is known as Slater-Koster theory to solid state physicists, and as Hückel theory to chemists.



1. Show that these two subspaces (called π and σ subspaces) decouple. To do this, remember that the translation group is two dimensional, and the space group is D_{6h}. Which element(s) of D_{6h} commute with all translations?

2. Sketch the Brillouin zone in the conventional Wigner-Seitz representation. The corner points are called "*K*". What are their wavevectors?
3. Find $E(\vec{k})$ for the π model (p_z orbital.)
4. Find the 2 x 2 matrix $H(\vec{k})$ for the σ model. The two eigenvalues of this matrix are the bands $E_{\pm}(\vec{k})$.
5. Show that the two bands are degenerate both at $\vec{k}$ =0 and at $\vec{k}$ a corner *K* point.
6. Taylor expand (to lowest order in $\delta\vec{k} = \vec{K} - \vec{k}$) the matrix elements of $H(\vec{k})$ for $\vec{k}$ near a corner *K* point. Show that the eigenfunctions acquire a Berry phase of π when they evolve once around a *K* point.
7. Taylor expand (to lowest order in $\vec{k}$) the matrix elements of $H(\vec{k})$ for $\vec{k}$ near 0. Show that the eigenfunctions change by 2π when they evolve once around the $\vec{k}$ =0 point (that is, there is no Berry phase.)