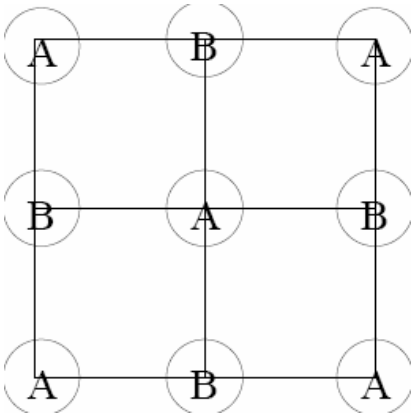
PHY 556 Spring 2007 **Homework #7** due Friday April 20, 2007

1. Lax, p228, problem 7.4.1
2. Lax, p228, problem 7.4.2
3. The conduction band minimum of silicon occurs at 6 $\vec{k}$-points $\vec{k}_i = \frac{2\pi}{a}(\pm 0.85,0,0)$ and permutations. The energy $E(\vec{k}_i)$ can be taken as the zero of energy. If there is a phosphorus impurity at the origin, the one-electron Hamiltonian has the form $H = p^2/2m + V(\vec{r}) + V_{scr}(\vec{r})$ where V is the silicon crystal potential, and V_{scr} is the attractive potential $-Ze^2/r$ of the P impurity with Z=5, but screened by the electrons. At large distances r, the screening is by 4 bound phosphorus electrons plus additional long-range screening accounted for by dividing by the dielectric constant $\varepsilon \approx 16$, ($V = -e^2/\varepsilon r$) but for smaller distances, the potential is screened mainly by 4 phosphorus electrons, and equals $-e^2/r$. To find the new eigenstates near the conduction band minimum, the effective mass Hamiltonian (Lax 7.10.16) works well except for small r (*i.e.*, in the "central cell.") There are 6 such equations, one for each minimum, with 6 degenerate solutions G_i, each of them being a kind of anisotropic hydrogenic *s*-function. The anisotropy comes because the effective mass tensor, although diagonal in the kx, ky, kz basis, has a large value along the direction of the $\vec{k}$-vector, and smaller values perpendicular. The "central-cell correction" will couple these 6 states, leading to a 6 x 6 matrix Schroedinger equation for the donor levels. With this background, do problem 7.10.1 in Lax p262.
4. The figure to the left is a partition of a square lattice into two sublattices, A and B. Each A site has all first neighbors on the B lattice and vice-versa. When this happens, the underlying lattice is called "bi-partite." The electron problem on this lattice is discussed by Lax, for example, Fig.



7.9.1 on page 222. The electron energy (of the 3-d version) is solved in "single-orbital nearest-neighbor tight-binding approximation" in Eq. 7.9.13. The Hamiltonian matrix is completely diagonalized by forming Bloch states from the single orbital. Now suppose that there is an on-site energy $H' = \sum_i \varepsilon_i c_i^+ c_i$, where ε_i is $-\varepsilon_0/2$ on the A sites and $+\varepsilon_0/2$ on the B sites. Write the Hamiltonian matrix and find the energies *E(k)*. Find wavevectors $\vec{K}$ such that $\exp(i\vec{K}\cdot\vec{r})$ is +1 on A sites and -1 on B sites. Show that because the coupling is to nearest neighbors and the lattice is bipartite, the energy obeys $E(\vec{k}) = -E(\vec{k}+\vec{K})$. You can do all of this for the 2-d square lattice, although it also works in 3-d. Use this relation to explain why the *E=0* contour on the plot 7.9.1 (interpreted for the 2-d rather than the more complicated 3-d case) is rather peculiar, and why, after adding the on-site energies, a gap opens up at *E=0*. This happens to be the Fermi level when there is one electron per atom, and the gap can be causes by a Peierls or an Overhauser mechanism.