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

$$H = \frac{p^2}{2m} + V(\vec{r}) + V_{scr}(\vec{r})$$

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 $k_x, k_y, k_z$ 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 Schrödinger 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.
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, where \( \varepsilon_i = -\varepsilon_0/2 \) 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 caused by a Peierls or an Overhauser mechanism.