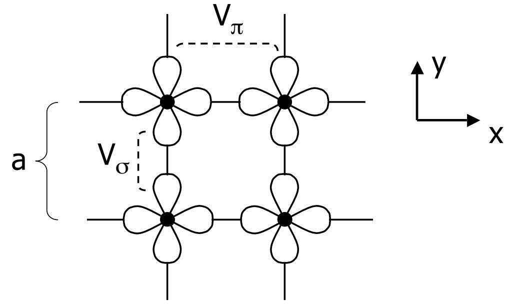
Physics 601 **Homework Set 4** **Fall, 2007**

Due date: Wednesday, Oct. 24.

1) (30 points)
Consider the 2-D square lattice in a tight-binding approximation with two p-orbitals per site (with energy ϵ_p) and hopping matrix elements V_σ and V_π as shown. The tight-binding basis is assumed to be orthonormal.



a) Find the real-space tight-binding matrices $\widetilde{H}_{ij}(\mathbf{R})$, construct the $\mathbf{k}$-space matrices $\widetilde{H}^{\mathbf{k}}_{ij}$, and find the band dispersions $E_{n\mathbf{k}}$.

b) One of the symmetries of this crystal is a reflection across the line $x = y$. What property should your dispersion relation $E_{n\mathbf{k}}$ have, as a consequence of this particular symmetry? Check that your result in part (a) satisfies this property.

c) Sketch the band structure along the (10) and (11) directions, taking $\epsilon_p = -2$ eV, $V_\sigma = 4$ eV, and $V_\pi = -2$ eV in your sketch.

2) (30 points)
The graphite crystal is composed of stacked sheets of carbon planes illustrated below. Recently it has been possible to isolate *individual* sheets of the graphite structure; the single sheet is called *graphene.* The valence π-bands of graphene can be modeled by a single 2-dimensional honeycomb lattice in the xy-plane, with one p_z-orbital per site with energy ϵ_p, and nearest-neighber hopping matrix elements V_π. Calculate and sketch the bands along the $M\Gamma$, ΓK, and KM lines in the Brillouin zone. Where do you think the Fermi level will lie, given that these π-bands are half-occupied in graphite?