

Physics 617 Problem Set 4 Due Monday, Feb. 20

(1) 2D rectangular lattice in tight binding: Consider a set of identical localized states $|m, n\rangle$ on a 2D simple rectangular lattice, where the integers m, n index the positions of these states on 2D lattice sites in x and y directions. Suppose that the Hamiltonian can be expressed as,

$$H = \sum_{m,n} \left[\varepsilon_0 |m, n\rangle \langle m, n| - t_1 (|m, n\rangle \langle m, n+1| + |m, n\rangle \langle m, n-1|) - t_2 (|m, n\rangle \langle m+1, n| + |m, n\rangle \langle m-1, n|) \right],$$

where ε_0 , t_1 , and t_2 are constants. This Hamiltonian couples only the nearest neighbors, along y direction (t_1 term) and x (t_2 term). Assume lattice constants are a (along x) and b (along y).

- (a) Write down a single-particle Bloch wave function composed of the localized states $|m, n\rangle$.
- (b) Plug your wave-function into the Schrodinger equation, show that it is an eigenstate, and solve for the energy vs. k for the resulting band. Find the lowest and highest energies for the band, and identify the k -space coordinates of four saddle points in $\varepsilon(k)$. Sketch the positions of the extrema and saddle points in the first Brillouin zone for this lattice.