

Physics 240A: Homework Problem Set 3

Due 10/24/07.

1. Tight Binding s Band on a Diamond Lattice. 50 points.

Consider a diamond structure lattice with an atom with one s state (spherically symmetric) on each site, with energy ϵ_s . Nearest neighbors (only) are coupled with a hopping parameter t .

(i) Assuming an orthogonal basis (we always assume normalization to unity), construct the tight binding Hamiltonian, solve for the eigenvalues, and plot them along the (100), (110), and (111) directions. In each case, plot only to the zone boundary along that direction; state explicitly where the zone boundary is in each direction. It will be very helpful for you, and the grader, if you are very systematic in your work. (40 points)

(ii) Now suppose the basis functions are not orthogonal, but have an overlap s between nearest neighbors (only). Construct the secular equation that gives the band eigenvalues. (10 points)