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PROBLEM SET 6

**Reading:** Ashcroft and Mermin (AM) Chapters 9 and 10

1. AM Problem 9.1
2. Consider a bcc crystal with one atom per primitive unit cell. Apply the tight-binding (LCAO) approximation to the band derived from atomic s-state, assuming that the overlap integral  $\gamma(R)$  (defined, e.g., in AM eqn. (10.18)) is zero except for nearest neighbors, when it is  $\gamma_o$ .
  - (a) Find the form of  $E(\vec{k})$  as a function of  $\vec{k}$ .
  - (b) Sketch the approximate form of the energy contours in the cross section of the first Brillouin zone corresponding to  $k_z = 0$ . Indicate the maxima, minima and saddle points, if any, of  $E(\vec{k})$ .
  - (c) Find the density of states  $g(E)$  and effective mass for  $\vec{k}$  near zero. (Note: for an isotropic spectrum the effective mass  $m^*$  is defined by the relation  $E(\vec{k}) \equiv \text{const} + \hbar^2 k^2 / 2m^*$ ).
  - (d) If there is one free electron per atom, find the approximate or, if you can, the exact shape of the Fermi surface. Does it intersect the zone edge? (Hint: What is the volume of the cube of side  $2\pi/a$  as a fraction of the volume of the first Brillouin zone?)
  - (e) Qualitatively, what would you expect to be the effect of taking higher neighbor interactions into account?