MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Physics Department

8.231: Physics of Solids I

Due in Ses #28

Problem Set #6

Problem 1: s Bands in a bcc Lattice

Derive the formula for the tight binding s bands through nearest neighbor overlap for a primitive bcc lattice. Sketch the dispersion curve along the 100, 110, and 111 directions and carefully label the results. Draw a contour map of the energy band on the plane in k space for which $k_z = 0$. On a sketch of the first Brillouin zone, indicate the extrema of the band.

Problem 2: p Bands

When dealing with p bands there are three different atomic orbitals involved, each having the same energy: $p_x = x\,f(r)$, $p_y = y\,f(r)$, and $p_z = z\,f(r)$. These states are orthogonal when they sit on the same site, but they may not be orthogonal when centered on different sites. Thus, a given band may involve contributions from all three orbitals, requiring the solution of a 3x3 eigenvalue problem.

a) Show that if one uses nearest neighbors only to form a p band in a simple cubic lattice, the three different p states do not mix. Proceed as in Problem 1 for one of these bands.

b) Show that even if one uses only nearest neighbors to form a p band in an fcc lattice, the bands will have mixed character. That is, the Hamiltonian will couple a tight binding wavefunction made up of the p_x states to ones similarly constructed of p_y or p_z states. Find the matrix element of the Hamiltonian between the p_x and the p_y tight binding wavefunctions and show that it is proportional to $\sin\frac{1}{2}k_x a \sin\frac{1}{2}k_y a$. Do not try to find the entire matrix.

Problem 3: Second Nearest Neighbors

Find an expression for the tight binding s band through second nearest neighbors for a primitive simple cubic lattice.

Problem 4: Overlap Integral

Evaluate the overlap integral $\int \psi^*(\vec{r})\,\psi(\vec{r}-\vec{R})\,dx\,dy\,dz$ between two 1s wavefunctions:

$$\psi_{1s}(\vec{r}) = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-Z\,|\vec{r}|/a_0}.$$

To carry this out use the spheroidal coordinate system

$\lambda = \dfrac{|\vec{r}_a| + |\vec{r}_a|}{R}$, $\mu = \dfrac{|\vec{r}_a| - |\vec{r}_a|}{R}$, and Φ = the angle of rotation about a line joining the centers. For this coordinate system a volume integral transforms as follows:

$$\int\int\int f(x,y,z)\,dx\,dy\,dz = \frac{R^3}{8}\int_0^{2\pi} d\Phi \int_{-1}^{1} d\mu \int_1^{\infty} f(\lambda,\mu,\Phi)\,(\lambda^2-\mu^2)\,d\lambda.$$