PHY 241, Quantum Magnetism: Homework Set #6

Due: March 2003

1. **Tight Binding Model on the CsCl Lattice** .

Consider two distinct atoms, each with a single ("s") orbital, on the CsCl lattice (bcc-like, but with two different atoms).

(a) Create the tight binding Hamiltonian for this crystal for near neighbor hopping t and 2nd neighbor hopping t'.

(b) Plot the bands along the lines Γ-X-M-R-Γ. Choose t, t', and the difference $\Delta\epsilon$ of on-site energies to be comparable, but make your own choice. Interpret the results.

2. **Non-collinear Band Structure.**

(a) To the TB Hamiltonian of Problem 1, add an on-site exchange potential $\frac{1}{2}\vec{\Delta} \cdot \vec{\sigma}$, where $\vec{\Delta} = I\vec{m}$ as discussed in class . Write out the explicit form of the Hamiltonian.

(b) Choose $\Delta\epsilon = 1$ eV, $t = 0.5$ eV, $t' = 0$, and $|\Delta| = 0.2$ eV on both atoms. Plot, along the symmetry lines mentioned in Problem 1, the band structure for relative directions of the moments of the two atoms of $0°$, $45°$, $90°$, $180°$. Considering the Hamiltonian, try to interpret the behavior.