Phys 507B - Solid State Physics II

Assignment 2: Applications of group theory. Due Feb. 8th

1. Valence band of a group III-V semiconductor.

Group III-V semiconductors such as GaAs, GaSb, InAs, InSb, etc play an important role in semiconductor physics and technology (e.g. solid-state lasers used in CD players, high frequency electronics in cell phones). They have the zincblende crystal structure with point group T_d .

- (a) Using $\mathbf{k} \cdot \mathbf{p}$ theory, derive the effective 4×4 Hamiltonian for the valence band of a group III-V semiconductor [i.e., derive Eq. (6.15) of Snoke]. You will need to use the Wigner-Eckart theorem and the coupling coefficient table 6.9 from Snoke.
- (b) Use a computer program such as Mathematica to diagonalize this Hamiltonian analytically and sketch the bands along a general direction in k-space. Label the bands by their irreps.
- 2. Effective Hamiltonian for the spin-orbit interaction in an assymmetric quantum well (Rashba effect).

Spintronics or spin electronics is an active field of research in semiconductor physics. One of the goals of spintronics is to control the electron spin state using external electric fields; this is possible in III-V semiconductors because there is strong spinorbit coupling in the conduction band.

Consider an asymmetric quantum well made from a III-V material grown in the [001] direction. In this case we can show that the T_d symmetry gets reduced to C_{2v} . In this case the 2-fold degenerate conduction band (including spin) can be described by the following 2×2 Hamiltonian:

$$\mathcal{H}_{\rm so} = \mathbf{\Omega}(\mathbf{k}) \cdot \boldsymbol{\sigma},\tag{1}$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of Pauli matrices, and $\boldsymbol{k} = (k_x, k_y, k_z)$ is the electron's crystal momentum.

Find the most general form of $\Omega(\mathbf{k})$ that is linear in k_i .

Hint: Which irrep. transforms like σ ? For \mathcal{H}_{so} to be invariant under symmetry operations, Ω has to transform like this same irrep.

3. Rhombohedral distortion of a III-V semiconductor.

Suppose we apply uniaxial stress along the [111] direction of a III-V semiconductor.

- (a) Which point group do we get?
- (b) Explain how the original Γ_6 conduction band, together with the Γ_8 and Γ_7 valence bands are split by this stress. Sketch the level splitting, labeling them by their corresponding irreps. and listing their remaining degeneracies.
 - 4. Normal modes of vibration of the CH_4 molecule.

The CH₄ molecule (methane) is tetrahedron with the carbon atom in the centre and hydrogen atoms at the vertices; hence it belongs to the T_d point group.

- (a) Find the number of normal modes, their symmetry and degeneracy.
- (b) Which modes are IR active?
- (c) Which modes are Raman active?



Figure 1: Unit cell of the antiferromagnet MnO.

5. Symmetry of an antiferromagnet.

In the paramagnetic state, the crystals of MnO, FeO, CoO, NiO, MnO, and MnSe have the fcc "NaCl" structure shown in the figure below. (Point group is $O_h \times T$). In the antiferromagnetic state, all Mn ions in a given (111) plane have their spins parallel; the spin directions in the planes immediately above and below this plane is opposite, i.e., the spins alternate from one (111) plane to the other in an antiferro fashion (this is called "A-type order", as opposed to the more conventional "G-type order" where each spin is antiparallel to its nearest neighbor).

The magnetic symmetry group depends on the particular axis of orientation of the spins. For each of the following spin orientations given below, find: (1) the magnetic point group, specifying any special directions of group operations with respect to the original cube directions; (2) Find the crystal system of the ordered structure; and (3) Find the number of types of domains which will be formed.

- (a) Spins point along the [111] direction (perpendicular to the planes of parallel spins).
- (b) Spins point along [001] direction.
- (c) Spins point along $[01 \ \overline{1}]$ direction that lies in the (111) plane.
- (d) Spins point along a general direction with no special symmetry.