

PHYSICS 220 : GROUP THEORY
FINAL EXAMINATION

This exam is due in my office, 5438 Mayer Hall, at 9 am, Monday, June 6. You are allowed to use the course lecture notes, the Lax text, and the character tables (link from lecture notes web page), but no other sources, and please do not discuss the exam with anyone other than me, other than to reassure your classmates that indeed this is a most fair and excellent exam.

[1] C_{20} is the smallest fullerene. It has the structure of a dodecahedron, *i.e.* a threefold coordinated cage with 20 sites arranged in 12 pentagonal faces and 30 edges. Its symmetry group is I_h .

- (a) Similar story to C_{60} : The sp^2 hybridized orbitals account for three of the four electrons in the 2s and 2p shells. (The 1s shell is completely inert.) The remaining orbital is the π orbital, oriented along a line from each carbon atom to the center of the molecule. Such orbitals transform trivially under I_h . Consider a tight-binding Hamiltonian

$$\hat{H} = -t \sum_{\langle ij \rangle} \left(|i\rangle\langle j| + |j\rangle\langle i| \right) \quad , \quad (1)$$

where $|i\rangle$ and $|j\rangle$ are π -orbitals for neighboring carbon atoms i and j . Classify the multiplets in the tight binding eigenspectrum according to IRREPS of I_h . For extra credit, write a computer program which diagonalizes \hat{H} for $t = 1$ and plot the spectrum, labeling each multiplet accordingly.

- (b) If pressure is applied to opposite pentagonal faces, the symmetry is broken from I_h down to D_{5d} . Find how the tight-binding multiplets from part (a) split into D_{5d} IRREPS.
- (c) Classify all vibrational modes of C_{20} according to IRREPS of I_h . Indicate whether each multiplet is IR active, Raman active, or Raman silent. If you really want to impress me, find the normal modes numerically for a ball and spring model, where all masses and spring constants are the same.

[2] Consider the structure in Fig. 2, which is the Shastry-Sutherland lattice with nonsymmorphic wallpaper group $p4g$ (from Fig. 5.11 of the notes).

- (a) Let the length of each bond be a . Choose as the origin the center of the figure, and find expressions for the four basis vectors $\delta_{1,2,3,4}$ corresponding to the red, yellow, grey, and blue sites in the first Wigner-Seitz cell (counterclockwise starting from the right, for the color blind among you). You may assume that the smaller of the two internal angles of each rhombus is α .
- (b) Find two elementary direct lattice vectors $\mathbf{a}_{1,2}$. Find the corresponding reciprocal lattice vectors $\mathbf{b}_{1,2}$.

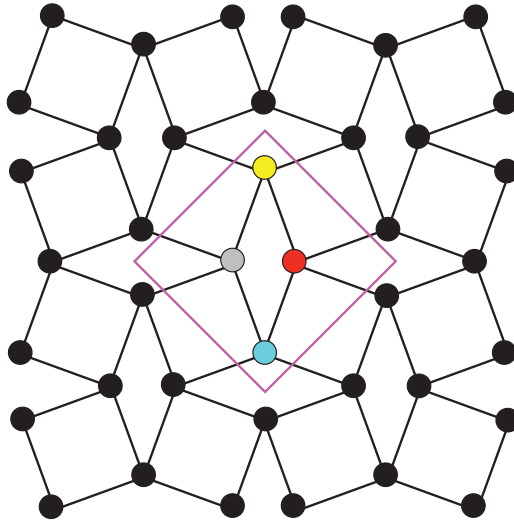


Figure 1: A lattice with $p4g$ symmetry.

- (c) Find the scattering form factor $F(\mathbf{K})$ defined in Eqn. 5.16 of the notes and show there are extinctions in the Bragg pattern.
- (d) When $\alpha = \frac{1}{2}\pi$, the lattice becomes square. Explain the Bragg extinctions in this case.
- (e) How do the basis points transform under the glide mirror? *I.e.* what basis color does yellow get mapped to, *etc.*? Also indicate which glide mirror you have chosen.

[3] Consider a V^{2+} ion in a D_4 environment.

- (a) The electronic configuration is $[\text{Ar}]4s^0 3d^3$. Hund's first two rules say $S = \frac{3}{2}$ and $L = 3$ (F). What is the ground state term according to Hund's third rule?
- (b) Using the notation of Atkins, Child, and Phillips (the character tables linked from the lecture notes page), the double group D_4' has two spin representations, $E_{1/2}$ and $E_{3/2}$, both of which are two-dimensional. Ignoring spin-orbit, decompose F into IRREPs of D_4 (the decomposition will be the same in D_4'). You may find some of the results in Tab. 6.5 of the notes useful (*e.g.* for the characters of certain rotations in the $l = 3$ representation of $O(3)$). Then decompose the $\Gamma_{3/2}$ representation for $S = \frac{3}{2}$ in D_4' . (Hint: it can give only some combination of the two spin IRREPs.) Finally, decompose the product $\Gamma_{3/2} \times F = {}^4F$ and find the IRREPs for all crystal field levels. Once again, your answer can only involve the $E_{1/2}$ and $E_{3/2}$ IRREPs, so in the end this isn't so nasty. For a template of how to proceed, see the section "Co⁺⁺ in a cubic environment" in §6.2.6 of the notes. You may find Tab. 6.10 helpful as well.
- (c) Starting on the dominant LS coupling end, decompose 4F into IRREPs of $O(3)$, *i.e.* by good old addition of angular momentum. Then decompose into D_4' IRREPs and check that you get the same answer as in part (b).