Homework 3

- **Due:** 11:59 PM, February 8. Submit electronically on Canvas.
- **Prove/show** means to provide a mathematically rigorous proof. **Argue/describe/explain why** means a non-rigorous (but convincing) argument is acceptable.

Problem 1 (Ethylene): Consider the ethylene molecule C_2H_4, sketched in Figure 1.

10 (a) Assume that the molecule lives in two dimensions only, for simplicity.

i. Argue that the symmetry group of this molecule under spatial transformations is (isomorphic to) $\mathbb{Z}_2 \times \mathbb{Z}_2$. What does this group physically correspond to?

ii. Why do you expect no degeneracy in the electronic Hamiltonian in this system? Do not consider the electronic spin in this problem.

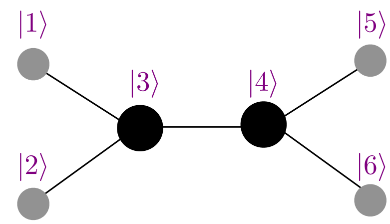

Figure 1: The ethylene molecule, with the 6 electronic wave functions localized on each atom. These orbitals correspond to rows/columns 1-6 of H, as given in (1).

5 (b) In the simplest theories of chemical bonding, we might imagine that there is one accessible low energy orbital on each atom. Using the bra-ket notation suggested in the figure, we might expect that the Hamiltonian describing electrons hopping on this molecule is given by

$$H = \begin{pmatrix} c & 0 & a & 0 & 0 & 0 \\ 0 & c & a & 0 & 0 & 0 \\ a & a & d & b & 0 & 0 \\ 0 & 0 & b & d & a & a \\ 0 & 0 & 0 & a & c & 0 \\ 0 & 0 & 0 & a & 0 & c \end{pmatrix}. \tag{1}$$

Assume that a, b, c, d are real. a describes the tunneling energy of the C-H bond, b the tunneling energy of the C-C bond, c the on-site energy of H, and d the on-site energy of C.

Use software (e.g. `Mathematica`) to find the eigenvalues of H. You should find that H is degenerate.

10 (c) The results from parts (a) and (b) are in tension. What is going on?

i. Show that the actual symmetry group of the Hamiltonian H is non-Abelian.[1]

ii. Resolve the discrepancy between parts (a) and (b).

5 (d) If you looked at the actual spectrum of ethylene, do you expect a degeneracy to exist? If yes, explain why the naive symmetry from part (a) is not the true symmetry group. If no, explain how the effective H above should be modified to lift the degeneracy in a more physically realistic model.

[1] *Hint:* Construct this symmetry group as a subgroup of S_4, taken to act in a straightforward way on the 4 H atoms. Do not worry about trying to find an isomorphism with some other group we have discussed in this class.

15 **Problem 2:** Let G be a group and let R be an n-dimensional representation of G. Let $g \in G$ obey $g^2 = 1$. Find all possible values of the character $\chi^{(R)}(g)$.[2]

Problem 3 (Character table of S_4): In this problem, we will construct the character table of S_4.

10 (a) We begin by counting conjugacy classes of group elements.

i. Let $\tau = (a_1 a_2 \cdots)(b_1 b_2 \cdots)\cdots$. Show that[3]

$$\sigma\tau\sigma^{-1} = (\sigma(a_1)\sigma(a_2)\cdots)\cdots(\sigma(b_1)\sigma(b_2)\cdots). \tag{2}$$

ii. Conclude that there are 5 conjugacy classes in S_4, classified by the structure of the cycles – the number of cycles of various lengths.

10 (b) Next, let's figure out the dimensions of the irreps of S_4. Note that $|\mathrm{S}_4| = 4! = 24$.

i. Show that there must be at least 2 irreps that are 1-dimensional.[4]

ii. Using only this fact, and basic representation theory, show that there must also be 1 irrep of dimension 2, and 2 irreps of dimension 3.

10 (c) One way to construct a 4 dimensional (evidently reducible) representation R of S_4 is to consider S_4's action on the vector space $\mathrm{span}\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}$, with

$$R(\sigma)|i\rangle = |\sigma(i)\rangle. \tag{3}$$

i. Show that

$$R(\sigma)(|1\rangle + |2\rangle + |3\rangle + |4\rangle) = |1\rangle + |2\rangle + |3\rangle + |4\rangle. \tag{4}$$

ii. Evaluate $\chi^{(R)}(c)$ for each conjugacy class c.

iii. Use reducibility test(s) to conclude that $R = \mathbf{1} \oplus \mathbf{3}$. Here $\mathbf{1}$ denotes the trivial representation and $\mathbf{3}$ one of the 3-dimensional ones.

iv. Fill in the $\mathbf{1}$ and $\mathbf{3}$ columns of the character table for S_4.

10 (d) One way to construct a 6 dimensional (evidently reducible) representation Q of S_4 is to consider S_4's action on the vector space $\mathrm{span}\{|12\rangle, |13\rangle, |14\rangle, |23\rangle, |24\rangle, |34\rangle\}$, with $|ij\rangle = |ji\rangle$ identified as the same vector, and with

$$Q(\sigma)|ij\rangle = |\sigma(i)\sigma(j)\rangle. \tag{5}$$

i. Evaluate $\chi^{(Q)}(c)$ for each conjugacy class c.

ii. Show that $Q = \mathbf{1} \oplus \mathbf{2} \oplus \mathbf{3}$.[5]

iii. Fill in the column for $\mathbf{2}$ in the character table.

10 (e) We can now complete the character table.

i. Fill in the column for "$\mathbf{1'}$" (the other 1d irrep).

ii. Complete the character table by filling in the column for "$\mathbf{3'}$".

[2] *Hint:* Think about the eigenvalues of the matrix $R(g)$.

[3] *Hint:* Evaluate $(\sigma\tau\sigma^{-1}) \cdot \sigma(j)$. Here $j \in \{1, 2, 3, 4\}$, but the argument immediately generalizes to any S_n.

[4] *Hint:* Think about the sign homomorphism from Homework 2.

[5] *Hint:* Evaluate $\sum_c n_c \overline{\chi^{(Q)}(c)} \chi^{(r)}(c)$ for $r = \mathbf{1}, \mathbf{3}$, and use reducibility tests.

20 **Problem 4 (Permutation symmetric matrix):** Consider an $n \times n$ real and symmetric matrix H (which might represent a physical Hamiltonian acting on some quantum system). Consider the "canonical" action of the permutation group S_n, which exchanges the basis vectors of $\mathbb{R}^n$:

$$\sigma \cdot (\mathbf{e}_1, \ldots, \mathbf{e}_n) = (\mathbf{e}_{\sigma(1)}, \ldots, \mathbf{e}_{\sigma(n)}). \tag{6}$$

i. Show that

$$H_{ij} = a\delta_{ij} + b \tag{7}$$

for real constants a and b, is the most general possible S_n-invariant Hamiltonian.

ii. What are the eigenvalues and eigenvectors of H?

iii. Show that $\mathbb{R}^n$ is acted on by a reducible representation of S_n.

iv. What do you think are the (vector spaces associated with the) irreducible representations? Explain your answer (but you do not need to prove it).

v. For which values of a, b is the symmetry group of H enhanced to $\mathrm{O}(n)$ (acting on $\mathbb{R}^n$ in the canonical way)? What happens to the spectrum?