PHYS 5040: Algebra and Topology in Physics **Spring 2021**

Homework 5

- **Due:** 11:59 PM, February 22. 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 (Selection rules for BH_3): Consider the molecule BH_3, which we discussed in Lecture 1. In full 3d space, the symmetry group of this molecule is $\mathrm{D}_6 \times \mathbb{Z}_2$, with the extra $\mathbb{Z}_2$ associated to reflections in the z-direction. The character table of $\mathrm{D}_6 = \mathrm{S}_3$ can be found in Zee II.3, and will be needed for this problem. Also needed is the fact that vectors (x, y) of coordinates in the plane transform in the $\mathbf{2}$ of D_6. You can denote r, s as the usual generators of D_6, and let t denote the reflection in the z-direction.

(a) We begin by developing the representation theory for our symmetry group.

i. Follow the example in Lecture 9 to determine the 6 irreps of $\mathrm{D}_6 \times \mathbb{Z}_2$. I'll use the natural generalization of our notation there in what follows.

ii. Write out the full character table for this group.

iii. Explain why the dipole moment (p_x, p_y, p_z) belongs to the representation $\mathbf{1}_- \oplus \mathbf{2}_+$.

(b) The electronic orbitals in BH_3 can be classified according to the 6 irreps found above.

i. Find the selection rules for electromagnetic radiation (in the dipole approximation). Namely, between orbitals in which pairs of irreps are transitions allowed?[1]

ii. Do you think the selection rules are more or less restrictive than they would be for a more symmetric object, like the isotropic hydrogen atom?

Problem 2 ($\mathrm{SL}(2, \mathbb{R})$): Consider the set of all 2×2 real matrices of determinant 1: this is called

$$\mathrm{SL}(2, \mathbb{R}) := \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} : a, b, c, d \in \mathbb{R}, \;\; ad - bc = 1. \right\}. \tag{1}$$

i. Show that $\mathrm{SL}(2, \mathbb{R})$ is a group under matrix multiplication. Argue that it is also a Lie group.

ii. Show that, for infinitesimal ϵ, if

$$M = 1 + \epsilon N + \mathrm{O}(\epsilon^2) \in \mathrm{SL}(2, \mathbb{R}), \tag{2}$$

then $\mathrm{tr}(N) = 0$. Conclude that there are 3 generators of the Lie algebra of $\mathrm{SL}(2, \mathbb{R})$.

iii. Find the Lie algebra $\mathfrak{sl}(2, \mathbb{R})$.

[1] *Hint:* The dipole is in a reducible representation, so you can think of determine the selection rules for dipoles in the $\mathbf{1}_-$ irrep alone, or the $\mathbf{2}_+$ irrep alone, first. Why are the total selection rules the sum of the selection rules for each of the 2 irreps alone?

Problem 3 (Lie groups with one generator): In this problem, we'll study the representation theory of Lie groups with one generator.

15 (a) Consider the additive group $\mathbb{R}$. This is a Lie group, generated by your favorite non-zero real number a. Show that all the irreducible representations R of this Lie group are characterized by an arbitrary complex number $\lambda \neq 0$, with $R(a) = \lambda^a$.

15 (b) Consider the additive group $\mathbb{R}/\mathbb{Z}$, which we discussed on Homework 1.

i. Explain why $\mathbb{R}/\mathbb{Z} = \mathrm{SO}(2)$; you can use results from Lecture 10 if desired.

ii. Find all the irreps of $\mathbb{R}/\mathbb{Z}$.

Problem 4 (Piezoelectricity): Certain crystals can develop electrical polarization when they are strained – this is called **piezoelectricity**, and is responsible for numerous practical technologies, including the timers in "older" wristwatches.

Mechanical strain of a crystal is parameterized by a symmetric tensor s_{ij}; polarizability of a crystal is a two dimensional vector P_i. Hence, in a piezoelectric crystal, we expect to see

$$P_i = A_{i,jk} s_{jk} \tag{3}$$

with the tensor coefficient $A_{i,jk}$ invariant under the symmetry group G of the crystal.

In this problem, we'll consider two dimensional crystals with dihedral symmetry. Let $\mathbf{2}$ denote the "vector" irrep (in which P_i transforms).

15 (a) When is piezoelectricity possible?

i. Explain why piezoelectricity is possible only if $\mathbf{2} \otimes \mathbf{2} \otimes \mathbf{2}$ contains a trivial representation ($\mathbf{1}$).

ii. Show that crystals with D_8 symmetry cannot be piezoelectric.

iii. Show that crystals with D_6 symmetry *can* be piezoelectric.

15 (b) In a crystal with D_6 symmetry, determine the form of the piezoelectric tensor $A_{i,jk}$.[2]

[2] *Hint:* Calculate Clebsch-Gordan coefficients!