

group theory - week 5

It takes class

Georgia Tech PHYS-7143

Homework HW5

due Tuesday, September 26, 2017

== show all your work for maximum credit,
== put labels, title, legends on any graphs
== acknowledge study group member, if collective effort

Exercise 5.1 *Vibration modes of CH_4* 8 points
Exercise 5.2 *Keep it classy (a)* 2 points

Bonus points

Exercise 5.1 *Vibration modes of CH_4 , part (c) ii* 2 points
Exercise 5.2 *Keep it classy (b)* 2 points
Exercise 5.2 *Keep it classy (c)* 4 points

Total of 10 points = 100 % score. Extra points accumulate, can help you later if you miss a few problems.

Show class, have pride, and display character. If you do, winning takes care of itself.

— Paul Bryant

2017-09-19 Predrag Lecture 9 Irreducible reps decomposition

Gutkin notes, [Lect. 5 Applications I. Vibration modes](#): Example 5.1. C_n symmetry completed.

For the record (I retract the heady claim I made in the lecture 8):

mathworld.wolfram.com: “A character table often contains enough information to identify a given abstract group and distinguish it from others. However, there exist nonisomorphic groups which nevertheless have the same character table, for example D_4 (the symmetry group of the square) and Q_8 (the quaternion group).” We discuss Q_8 in example [4.1](#).

2017-09-21 Predrag Lecture 10 It takes class

In week [1](#) we introduced projection operators ([1.33](#)). How are they related to the character projection operators constructed in the previous lecture? While the character orthogonality might be wonderful, it is not very intuitive - it's a set of solutions to a set of symmetry-consistent orthogonality relations. It is a set of rules then enables you to construct a character table, but it does not tell you what it means. Similar thing will happen again when we turn to the study continuous groups: all semisimple Lie groups are likewise classified by Killing and Cartan by a more complex set of orthogonality and integer-dimensionality (Diophantine) constraints. You obtain all possible Lie algebras, but have no idea what their geometrical significance is.

In my own Group Theory book [\[1\]](#) I (almost) get all simple Lie algebras using projection operators constructed from invariant tensors. What that means is easier to understand for finite groups, and here I like the [Harter's](#) exposition [\[3\]](#) best. Harter constructs ‘class operators’, shows that they form the basis for the algebra of ‘central’ or ‘all-commuting’ operators, and uses their characteristic equations to construct the projection operators ([1.33](#)) from the ‘structure constants’ of the finite group, i.e., its class multiplication tables. Expanded, these projection operators are indeed the same as the ones obtained from character orthogonality.

I find [Harter's Sect. 3.3 Second stage of non-Abelian symmetry analysis](#) particularly illuminating. It shows how physically different (but mathematically isomorphic) higher-dimensional irreps are constructed corresponding to different subgroup embeddings. One chooses the irrep that corresponds to a particular sequence of physical symmetry breakings

You might want to have a look at [Harter \[4\] Double group theory on the half-shell](#). Read appendices B and C on spectral decomposition and class algebras. Article works out some interesting examples.

See also remark [1.1 Projection operators](#) and perhaps watch Harter's [online lecture](#) from Harter's [online course](#).

5.1 Literature

Continuing reading Mathews and Walker [5], now Chap. 14. Porter works out nicely the normal modes of the D_3 springs and masses (again!).

Not all finite groups are as simple or easy to figure out as D_3 . For example, the order of the Ree group ${}^2F_4(2)'$ is $212(26 + 1)(24 - 1)(23 + 1)(2 - 1)/2 = 17\,971\,200$.

Who is Harter? He was a prodigy who at age 16 taught himself group theory by reading Hamermesh [2]. He was a graduate student at Caltech (1964-65), together with Ron Fox. They hated the atmosphere there and the teaching was terrible (Feynman did not teach that year but Harter and Feynman were good friends). Harter and Fox shared an interest in group theory and discovered that most of the group theory books in the physics library had been checked out in 1960-62 by Gell-Mann, Zweig and Glashow. That only half of the entering students were meant to complete their PhD's there led to lots of ugly competition. Harter transferred to UC Irvine, and, upon graduation, got a job at USC in LA. After a few years he suggested in a faculty meeting that the way they could improve their quality as a department was "to get rid of all the old farts." These same "old farts" soon voted to deny him tenure. He ended up in Campinas, Brazil. Fox rescued him from there by bringing him for an interview at Georgia Tech, where he was hired in late 1970's. He was brilliant, an asset for teaching, making all sorts of demonstration devices. He built a giant rotating table upon which he placed billiard balls, a wonderful demonstration of mechanical analogues for charged particle motion in crossed E and B fields. Everyone (except for one nefarious character) liked him, his work, and especially his devices. The faculty unanimously supported his promotion to tenure. He did not, however, think much of the Director of School of Physics, and made that clear. After an argument with the Director, he stormed out, offended. So, he was denied tenure and moved in 1985 to University of Arkansas where he is a professor today.

In 1987 Harter and Weeks used Harter's theory of the rotational dynamics of molecules to calculate the rotational-vibrational spectra of the soccer ball-shaped molecule Buckminsterfullerene, C_{60} , or "buckyball." C_{60} had been proposed in 1985 by chemists, who had seen a mass-spectra peak of atomic mass 720. By 1989 the Harter theory calculations led to a realization that chemists had been making C_{60} since the early 1970s. In 1992 Science named C_{60} "Molecule of the Year," and in 1996 Curl, Kroto and Smalley were awarded the Nobel Prize in Chemistry for their discovery of fullerenes.

You can find here many [Soft Elegant Educational tools](#) developed by Harter, and follow his lectures [on line](#). He is a great teacher. Georgia Tech's loss.

5.2 Discussion

2017-09-25 Lin Xin <lxin9@gatech.edu> I have a few questions about the exercise 5.1 part (d) *Vibration modes of CH_4 : Find all modes of the methane molecule.*

1. When we use the angle of improper rotation, is it true that reflection equals to the π improper rotation?

2. I assume it is π and it gives me other characters are zero. In the case of all symmetry, this will give the , which we usually get non-negative integer. As a result, I'm not perfectly sure that the character formulas you give are correct.
3. Moreover seems it's in the representation of $[12 \times 12]$ matrices instead of $[24 \times 24]$ matrices.

2017-09-25 Predrag The solution set is very detailed, so how about waiting Tuesday afternoon, when it gets posted on T-square? Then –if it is still unclear– we continue the discussion.

1. If $g \in \text{SO}(3)$ is a rotation, and $D(i)\mathbf{r} = -\mathbf{r}$ is the inversion transformation, then rotation combined with the inversion gi is an improper rotation $gi \in \text{O}(3)$. If $g \in T$ (a discrete tetrahedron rotation) then gi is an improper element of T_d .
2. ? (check the solution set).
3. The proper rotations group T of order 12 is a normal subgroup. However, I do not think you can have an improper rotations subgroup of T_d , as $g_i i g_j i$ is a proper rotation.

References

- [1] P. Cvitanović, *Group Theory - Birdtracks, Lie's, and Exceptional Groups* (Princeton Univ. Press, Princeton, NJ, 2008).
- [2] M. Hamermesh, *Group Theory and Its Application to Physical Problems* (Dover, New York, 1962).
- [3] W. G. Harter, *Principles of Symmetry, Dynamics, and Spectroscopy* (Wiley, New York, 1993).
- [4] W. G. Harter and N. D. Santos, "Double-group theory on the half-shell and the two-level system. I. Rotation and half-integral spin states", *Amer. J. Phys.* **46**, 251–263 (1978).
- [5] J. Mathews and R. L. Walker, *Mathematical Methods of Physics* (W. A. Benjamin, Reading, MA, 1970).

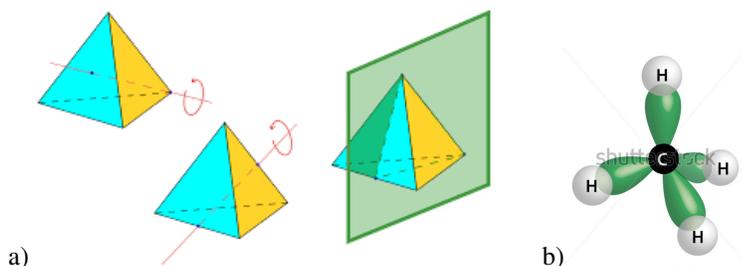


Figure 5.1: a) Two classes of rotational symmetries, and a class of reflection symmetries of a **tetrahedron**. (left) Hold the **Tetra Pak** by a tip, turn it by a third. (middle) Hold the **Tetra Pak** by the midpoints of a pair of opposing edges, make a half-turn. (right) Exchange the vertices outside the reflection plane. b) Methane molecule with the symmetry T_d .

Exercises

5.1. **Vibration modes of CH_4 .** Tetrahedral group T describes rotational symmetries of a **tetrahedron**. The order of the group is $|G| = 12$, and its conjugacy classes are:

- The identity mapping.
- Four rotations by $\varphi = 2\pi/3$, with each of the four rotation axes going through a vertex, and piercing the midpoint of the triangle opposite.
- Four inverse rotations by $\varphi = -2\pi/3$.
- Three rotations by $\varphi = \pi$, one for each of the three rotation axes going through midpoints of opposing edges.

The full group of tetrahedron symmetries T_d includes also reflections. This is the symmetry group of molecules such as methane CH_4 , see figure 5.1).

- What is the order of the group T_d ? Show that the group is isomorphic to i) the group of permutations S_4 ; ii) to the group O of rotational symmetries of the cube. iii) Show that T is normal subgroup of T_d .
- Find all conjugacy classes of the group. Which of these classes correspond to proper ($\det R(\varphi) = +1$), improper ($\det R(\varphi) = -1$) rotations? *Information on T might help. Note that φ might be also 0.*
- Find all irreducible representations of the group & build the character table. *A shortcut: find all one-dimensional representations, assume that characters are integers, then use the orthogonality relationship between characters.*
 - Really compute the character table, without assuming that characters are integers (2 bonus points). *One-dimensional representations + orthogonality of characters is not enough to build the whole character table for T_d . One needs more black magic, such as representation of permutation group by matrices.*
- Find all modes of the methane molecule. Which of them correspond to vibrations, translations and rotations? What are the degeneracies?

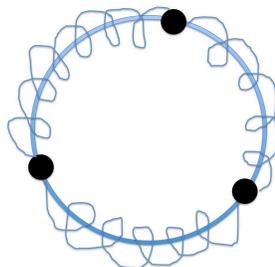


Figure 5.2: Three identical masses are constrained to move on a hoop, connected by three identical springs such that the system wraps completely around the hoop. Find all symmetries of the equations of motion.

Path: Find characters of the full (reducible) representation by using formulas from the lecture:

$$\chi(g) = \begin{cases} n_g(1 + 2 \cos(\varphi)) & \text{rotation,} \\ n_g(-1 + 2 \cos(\varphi)) & \text{improper rotation.} \end{cases}$$

Here n_g is the number of atoms staying at the same place under the action of g , φ is the rotation angle corresponding to $g = R(\varphi)$. Then decompose this representation into irreducible representations. Identify the rotational and translational parts.

- (e) To what representation corresponds the most symmetric "brezing" mode and why? Is it infrared active, i.e., can this mode can be excited by electromagnetic field?

5.2. **Keep it classy.** Check out Harter's [PowerPoint](#) presentation :)

- Go through the derivation of the three projection operators for $D_3 = C_{3v}$.
- Decompose $P^3 = P_1^3 + P_2^3$. Construct P_{ij}^3 . Verify that they are idempotent.
- Compute the $[2 \times 2]$ irreducible matrix representation $D_{ij}^3(g)$ for a few typical group elements g , in the spirit of Harter's slides 13-8 and 13-9.

5.3. **Three masses on a loop.** (Exercise 2.8 revisited.) Three identical masses, connected by three identical springs, are constrained to move on a circle hoop as shown in figure 5.2.

- Find all symmetries of the equations of motion.
- Find the normal modes using group-theoretic decompositions to irreps and character orthonormality.
- How many eigenvalues are there in all?
- Interpret the eigenvalues and eigenvectors from a group-theoretic, symmetry point of view.