group theory - week 5

It takes class

Georgia Tech PHYS-7143

Homework HW5 due Tuesday 2021-06-15

== 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 *, parts (a) (b) (c) i*	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

2021-06-03 Predrag Lecture 9 It takes class

Section playlist

- Sect. 5.1 It's all about class

Dresselhaus *et al.* [6] Sect. 3.6 *Second Orthogonality Relation for Characters*.

6.1 A character table is a unitary matrix from classes to irreps (9:12 min)

6.2 Projection operator perspective (11:35 min)

Harter's Sect. *3.2 First stage of non-Abelian symmetry analysis*
group multiplication table (3.1.1); class operators; class multiplication table (3.2.1b); all-commuting or central operators;

6.3 Example: the projection operator reduction of D_3 (23:00 min)

Harter's Sect. *3.3 Second stage of non-Abelian symmetry analysis*
projection operators (3.2.15); 1-dimensional irreps (3.3.6); 2-dimensional irrep (3.3.7); Lagrange irreps dimensionality relation (3.3.17)

6.4 Example: A reduction by two commuting operators (Harter problem 1.2.6). What comes next: a nonlinear symmetry reduction; translations; Fourier series. (35:14 min)

2021-06-08 Predrag Lecture 10 It takes grit

Gutkin notes, Lect. 5 *Applications I. Vibration modes*: Example 5.1. C_n symmetry completed.

5.1 It's all about class

In week 1 we introduced projection operators (1.27). 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. You can learn a set of rules that 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 of continuous groups: all semisimple Lie groups will be 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 [4] 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 [8] best. Harter constructs 'class operators', shows that they form a basis for the algebra of 'central' or 'all-commuting' operators, and uses their characteristic equations to construct the projection operators (1.27) 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 [9] *Double group theory on the half-shell* (click here). 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.

There is more detail than what we have time to cover here, but 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.

5.1.1 Dirac characters, Burnside's method (optional)

I told you that everybody who understands anything about group theory, writes a book. This weeks winner is Daniel Arovas, who is writing up his *Lecture Notes on Group Theory in Physics*. Check them out - they are cute, and even contain !jokes!.

For example, here I learn for the first time that Harter's central operators (Harter's Sect. *3.2 First stage of non-Abelian symmetry analysis*) are in condensed matter physics known as 'Dirac characters'.

Dirac characters were introduced by Dirac [5] in *The Principles of Quantum Mechanics* (1930) (click here). He refers to them as "[...] what is called in group theory a character of the group of permutations." Corson [3] *Note on the Dirac character operators* (1948) writes:

> [...] the evaluation of Dirac and similar character operators is all that is required for the solution of the standard molecular problems in the spirit of Dirac's original program which avoids appeal to formal group theory.

Dirac characters use not only the abstract group information, but also account for the symmetry information contained in the basis set used. The diagonalization of Dirac characters has three main advantages:

1. It can be realized by means of a quite simple and general algorithm.
2. The projective irreps obtained are just the ones that are needed to reduce the starting basis set into irreducible sets.
3. No tabulated quantities are required to construct the projective irreps.

The scheme is completely general, in the sense that it applies to all space groups.

Ananda Dasgupta had 1.68K followers on YouTube, now he has one more:

- playlist for his *Symmetries in Physics* course:
- *Lecture 15* (start at about 35 min into the lecture) has a nice discussion of Dirac characters, their relation to characters, and motivates the algorithmic Burnside's method for computing characters via class multiplication tables $(H_i)_{jk}$.
- *PH4213 Discussion Class 8* applies Burnside's method to D_4.

More generally, the whole course is of interest, if covers most topics of our course in greater depth:

- *PH4213 Discussion Class 9* gets projection operators out of characters.
- *Lecture 16 Projection operators* attempts to give you an appreciation of the power of the Wigner Eckart theorem (what in my book is described as all calculations being 'vacuum bubbles', maybe not precisely in these words).

A few textbooks that use Dirac characters:

- Cini [2] *Topics and Methods in Condensed Matter Theory* (2007) (click here)
- Jacobs [10] *Group Theory with Applications in Chemical Physics*, (click here) (2005)
- El-Batanouny and Wooten [1] *Symmetry and Condensed Matter Physics: A Computational Approach* (2008) (click here). In sect. 4.3 they describe the Burnside's method. They give an example of Mathematica code that constructs the character table. If needed, on might use Dixon's method, which is more clever for numerical computations.
- Big Chemical Encyclopedia: Dirac character.
- The *CRYSTAL* package performs ab initio calculations of the ground state energy, energy gradient, electronic wave function and properties of periodic systems. Uses Dirac characters.
- For a bit of history, see J. E. Humphreys review of Pioneers of representation theory.

5.1.2 William G. Harter (optional)

Who is Bill Harter? He is a prodigy who at age 16 taught himself group theory by reading Hamermesh [7]. 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, C60, or "buckyball." C60 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 C60 since the early 1970s. In 1992 Science named C60 "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 Other sources (optional)

Continuing reading Mathews and Walker [11], 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 $212(26+1)(24-1)(23+1)(2-1)/2 = 17\,971\,200$.

5.3 Discussion

Henriette Roux 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.

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 $g \in \mathrm{SO}(3)$ is a rotation, and $D(i)\boldsymbol{r} = -\boldsymbol{r}$ is the inversion transformation, then rotation combined with the inversion $g\,i$ is an improper rotation $g\,i \in \mathrm{O}(3)$. If $g \in T$ (a discrete tetrahedron rotation) then $g\,i$ 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 $g_i\,ig_j\,i$ is a proper rotation.

References

[1] M. El-Batanouny and F. Wooten, *Symmetry and Condensed Matter Physics: A Computational Approach* (Cambridge Univ. Press, Cambridge UK, 2008).

[2] M. Cini, *Topics and Methods in Condensed Matter Theory - From Basic Quantum Mechanics to the Frontiers of Research* (Springer, Berlin, 2007).

[3] E. M. Corson, "Note on the Dirac character operators", Phys. Rev. **73**, 57–60 (1948).

[4] P. Cvitanović, *Group Theory: Birdtracks, Lie's and Exceptional Groups* (Princeton Univ. Press, Princeton NJ, 2008).

[5] P. A. M. Dirac, *The Principles of Quantum Mechanics* (Oxford Univ. Press, 1930).

[6] M. S. Dresselhaus, G. Dresselhaus, and A. Jorio, *Group Theory: Application to the Physics of Condensed Matter* (Springer, New York, 2007).

[7] M. Hamermesh, *Group Theory and Its Application to Physical Problems* (Dover, New York, 1962).

[8] W. G. Harter, *Principles of Symmetry, Dynamics, and Spectroscopy* (Wiley, New York, 1993).

[9] W. G. Harter and N. dos 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).

[10] P. Jacobs, *Group Theory with Applications in Chemical Physics* (Cambridge Univ. Press, 2005).

[11] J. Mathews and R. L. Walker, *Mathematical Methods of Physics* (W. A. Benjamin, Reading, MA, 1970).

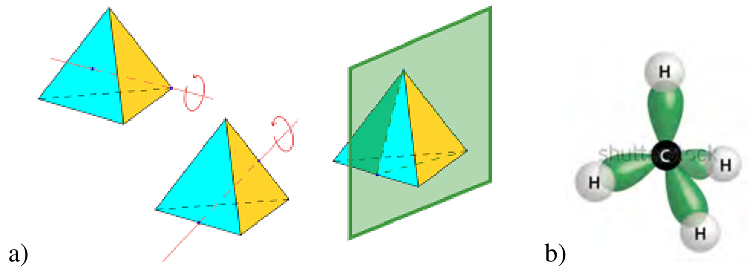

Figure 5.1: a) Two classes of rotational symmetries, and a class of reflection symmetries of a tetrahedron. (left) Hold the Tetra Pak by a tip, turn it by a third. (middle) Hold the Tetra Pak by the midpoints of a pair of opposing edges, make a half-turn. (right) Exchange the vertices outside the reflection 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 $|\mathrm{T}| = 12$, 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).

(a) 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.

(b) 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.

(c) i) 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.
ii) 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.

(d) Find all modes of the methane molecule. Which of them correspond to vibrations, translations and rotations? What are the degeneracies?

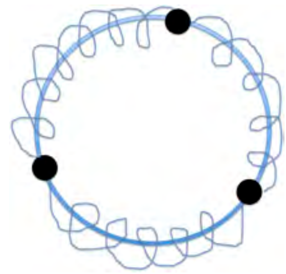

Figure 5.2: Three identical masses are constrained to move on a hoop, connected by three identical springs such that the system wraps completely around the hoop. Find all symmetries of the equations of motion.

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

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

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 "breathing" mode and why? Is it infrared active, i.e., can this mode can be excited by electromagnetic field?

(B. Gutkin)

5.2. **Keep it classy.** Check out Harter's PowerPoint presentation :)

(a) Go through the derivation of the three projection operators for $D_3 = C_{3v}$.

(b) Decompose $P^3 = P^3_1 + P^3_2$. Construct P^3_{ij}. Verify that they are idempotent.

(d) Compute the [2×2] irreducible matrix representation $D^3_{ij}(g)$ 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 2.7 revisited.) Three identical masses, connected by three identical springs, are constrained to move on a circle hoop as shown in figure 5.2.

(a) Find all symmetries of the equations of motion.

(b) Find the normal modes using group-theoretic decompositions to irreps and character orthonormality.

(c) How many eigenvalues are there in all?

(d) Interpret the eigenvalues and eigenvectors from a group-theoretic, symmetry point of view.