group theory - week 4

Hard work builds character

Georgia Tech PHYS-7143

Homework HW4 due Tuesday 2021-06-08

== show all your work for maximum credit,
== put labels, title, legends on any graphs
== acknowledge study group member, if collective effort
== if you are LaTeXing, here is the source code

Exercise 4.3 *All irreducible representations of D_4* 10 points

Bonus points
Exercise 4.4 *Irreducible representations of dihedral group D_n* 2 points
Exercise 4.5 *Perturbation of T_d symmetry* 6 points
Exercise 4.7 *Two particles in a potential* 4 points

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

Table 4.1: The D_3=C_{3v} group multiplication table. The same as table 2.1, but written as a class operator multiplication table.

D_3	1	r	r^2	σ_1	σ_2	σ_3
1	1	r	r^2	σ_1	σ_2	σ_3
r	r	r^2	1	σ_3	σ_1	σ_2
r^2	r^2	1	r	σ_2	σ_3	σ_1
σ_1	σ_1	σ_2	σ_3	1	r	r^2
σ_2	σ_2	σ_3	σ_1	r^2	1	r
σ_3	σ_3	σ_1	σ_2	r	r^2	1

D_3	$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$
$\mathcal{C}_1$	$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$
$\mathcal{C}_2$	$\mathcal{C}_2$	$2\mathcal{C}_1+\mathcal{C}_2$	$2\mathcal{C}_3$
$\mathcal{C}_3$	$\mathcal{C}_3$	$2\mathcal{C}_3$	$3\mathcal{C}_1+3\mathcal{C}_2$

2021-06-01 Lecture 5

Character orthogonality theorem

Character orthogonality relations. (10:53 min)
Character defined. Character of identity = dimension of the representation. Character orthogonality stated as an average of the group over irrep characters (but not derived). Special cases checked. Completeness verified. Example: Reflection group in 1 dimension. Characters and their orthogonality checked.

A summary: it is all about class and character (18:50 min)
Presumes knowledge of C_N irreps, argues that a reflection (D_N) mixes them up, thus reducing the number of irreps. 3-disk classes. Character is labelled by the class and the irrep label. Example: discrete Fourier transform is an $[N \times N]$ unitary matrix. D_4 character table.

(extra) *Discussion: class and character* (7:01 min)

2021-06-01 Predrag Lecture 6

Hard work builds character

Complete Dresselhaus *et al.* [1] sects. 3.3 "Wonderful Orthogonality Theorem for Characters" to 3.8 "Setting up Character Tables" (click here). This material is also covered in Tinkham [7] Chapter 3 *Theory of Group Representations*.

1. theory of finite groups are a natural generalization of discrete Fourier representations

2. it is all about class and character. "Character", in particular, I find very surprising - one complex number suffices to characterize a matrix!

4.1 Other sources (optional)

Group theory? It is all about class & character.
— Predrag Cvitanović, *One minute elevator pitch*

For a continuous group version of the character orthogonality theorem, see sect. 9.4. In particular, the replacement of an irrep matrix representation $D^{(\mu)}(g)_a{}^b$ by its character $\chi^{(\mu)}(g)$ (a single scalar quantity) leads to no loss of any of the matrix indices structure.

I enjoyed reading Mathews and Walker [6] Chap. 16 *Introduction to groups*. You can download it from here. Goldbart writes that the book is "based on lectures by Richard Feynman at Cornell University." Very clever. Try working through the example of fig. 16.2: deadly cute, you get explicit eigenmodes from group theory alone. The main message is that if you think things through first, you never have to construct the representation matrices in explicit form - recasting the calculation in terms of invariants, such characters, will get you there much faster.

You might find Gutkin notes useful:

Lect. 4 *Representation Theory II*, up to Sect. 4.5 *Three types of representations*: Character tables. Dual character orthogonality. Regular representation. Indicators for real, pseudo-real and complex representations. See example 4.3 "Irreps for quaternion multiplication table."

Oliver Pierson *ChaosBook.org chapter Discrete factorization - Character tables* (10:05 min)

Oliver Pierson *ChaosBook.org chapter Discrete factorization - Projection into invariant subspaces* (5:31 min)

Lect. 5 *Applications I. Vibration modes* go through Wigner's theorem, C_n symmetry and D_3 symmetry. Study Example 5.1. C_n symmetry. More quantum mechanics applications follow in

sect. 6.2 *Applications II. Quantum Mechanics*, Sect. 2. *Perturbation theory*.

Does the proof in the Lect. 4 *Representation Theory II Appendix* that the number of irreps equals the number of classes make sense to you? For an easy argument, see Vedensky Theorem 5.2 *The number of irreducible representations of a group is equal to the number of conjugacy classes of that group.* For a proof, work though Murnaghan Theorem 7. If you prefer a proof that your professor cannot understand, click here.

For the record (I retract the heady claim I made in class):
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)." exercise 4.3

Fun read along these lines: Hart and Segerman [2] discuss the distinction between abstract groups and symmetry groups of objects. They exhibit two very different objects with

$$D_4 = \langle r, \sigma \,|\, \sigma r \sigma = r^{-1}, r^4 = \sigma^2 = e \rangle \tag{4.1}$$

symmetry (describing the group this way is called a *presentation* of D_4), and explain the Cayley graph for D_4 (its edges with arrows correspond to rotations, the other edges correspond to reflections). For quaternions they discuss a 1-dimensional space group built of "monkey blocks" (but do not identify its crystallographic name). Q_8 is a subgroup of the symmetries of the 3-dimensional sphere S^3 , the unit sphere in $\mathbb{R}^4$. They offer a visualisation of the action of Q_8 on a hypercube and construct a sculpture whose symmetry group is Q_8, using stereographic projection from the unit sphere in 4-dimensional space. Q_8 is discussed here in example 4.3.

Simon Berman You would think that the analysis of three masses connected by harmonic strings, see figure 4.1, is a simple exercise finding irreps of D_3 symmetry, but no, it merits a 2019 Phys. Rev. Lett., see Katz and Efrati [3] *Self-driven fractional rotational diffusion of the harmonic three-mass system*. The article even starts with our figure 4.1. We continue the discussion in sect. 6.4.

Example 4.1. ***D_3* symmetry:** *Reflections and rotations of a triangle, figure 2.5 (c)*

$$D(T) = \begin{pmatrix} 0&0&0&0&1&0\\ 0&0&0&0&0&1\\ 1&0&0&0&0&0\\ 0&1&0&0&0&0\\ 0&0&1&0&0&0\\ 0&0&0&1&0&0 \end{pmatrix}, \qquad D(\sigma_1) = \begin{pmatrix} -1&0&0&0&0&0\\ 0&1&0&0&0&0\\ 0&0&0&0&-1&0\\ 0&0&0&0&0&1\\ 0&0&-1&0&0&0\\ 0&0&0&1&0&0 \end{pmatrix} \tag{4.2}$$

$$D(\sigma_2) = \begin{pmatrix} 0&0&0&0&-1&0\\ 0&0&0&0&0&1\\ 0&0&-1&0&0&0\\ 0&0&0&1&0&0\\ -1&0&0&0&0&0\\ 0&1&0&0&0&0 \end{pmatrix}, \qquad D(\sigma_3) = \begin{pmatrix} 0&0&-1&0&0&0\\ 0&0&0&1&0&0\\ -1&0&0&0&0&0\\ 0&1&0&0&0&0\\ 0&0&0&0&-1&0\\ 0&0&0&0&0&1 \end{pmatrix} \tag{4.3}$$

$$G = \{[e];[g,g^2];[\sigma_1,\sigma_2,\sigma_3]\}, \qquad \chi^{(1)} = \{1,1,1\}, \chi^{(2)} = \{1,1,-1\}, \chi^{(3)} = \{2,-1,0\}$$

$$r_i = \chi(e)\chi^{(i)}(e)/6; \qquad r_i = \{1,1,2\} \quad \Longrightarrow \quad D = 2E \oplus A_1 \oplus A_2 .$$

$$P_i = \frac{1}{3}\sum_{g\in G} \chi^{(i)}(g) D(g)$$

$$P_1 = \frac{1}{3}\begin{pmatrix} 0&0&0&0&0&0\\ 0&1&0&1&0&1\\ 0&0&0&0&0&0\\ 0&1&0&1&0&1\\ 0&0&0&0&0&0\\ 0&1&0&1&0&1 \end{pmatrix}, \qquad P_2 = \frac{1}{3}\begin{pmatrix} 1&0&1&0&1&0\\ 0&0&0&0&0&0\\ 1&0&1&0&1&0\\ 0&0&0&0&0&0\\ 1&0&1&0&1&0\\ 0&0&0&0&0&0 \end{pmatrix} \tag{4.4}$$

The 3 equal masses connected by harmonic springs system of figure 4.1 is a textbook example of such system, see for example problems 6.37 and 9.16 in Kotkin and Serbo [4] Collection of Problems in Classical Mechanics.

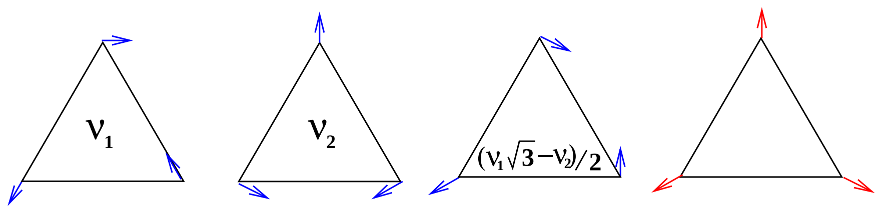

Figure 4.1: Modes of a molecule with D_3 symmetry. (B. Gutkin)

The vibrational modes associated with the two 1-dimensional representations are given by

$$P_{1V} = \alpha \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} \qquad \textit{and} \qquad P_{2V} = \beta \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} ,$$

respectively. Here P_{1V} represents symmetric mode shown in figure 4.1 (red). The second mode P_{2V} corresponds to the rotations of the whole system. The projection operator for the two-dimensional representation is

$$P_3 = \frac{2}{6}(2D(I) - D(T) - D(T^2)) = \frac{1}{3} \begin{pmatrix} 2 & 0 & -1 & 0 & -1 & 0 \\ 0 & 2 & 0 & -1 & 0 & -1 \\ -1 & 0 & 2 & 0 & -1 & 0 \\ 0 & -1 & 0 & 2 & 0 & -1 \\ -1 & 0 & -1 & 0 & 2 & 0 \\ 0 & -1 & 0 & -1 & 0 & 2 \end{pmatrix} \tag{4.5}$$

From this we have to separate two vectors corresponding to shift in x and y directions.

$$\eta_x = \begin{pmatrix} 1 \\ 0 \\ -1/2 \\ \sqrt{3}/2 \\ -1/2 \\ -\sqrt{3}/2 \end{pmatrix} , \qquad \eta_y = \begin{pmatrix} 0 \\ 1 \\ -\sqrt{3}/2 \\ -1/2 \\ \sqrt{3}/2 \\ -1/2 \end{pmatrix}$$

$$P_{3V} = \left\{ \underbrace{\alpha \frac{1}{\sqrt{6}} \begin{pmatrix} 2 \\ 0 \\ -1 \\ 0 \\ -1 \\ 0 \end{pmatrix}}_{\xi_1} \underbrace{+\beta \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ -1 \\ 0 \end{pmatrix}}_{\xi_2} \underbrace{+\gamma \frac{1}{\sqrt{6}} \begin{pmatrix} 0 \\ 2 \\ 0 \\ -1 \\ 0 \\ -1 \end{pmatrix}}_{\xi_3} \underbrace{+\delta \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}}_{\xi_4} \right\} ,$$

where $\eta_x = \sqrt{3/2}(\xi_4 + \xi_1)$, $\eta_y = \sqrt{3/2}(\xi_3 - \xi_2)$. Vectors ξ_i are columns of P_3 and their *linear combinations. The orthogonal vectors are given by*

$$\nu_1 = \sqrt{3/2}(\xi_1 - \xi_4) = \begin{pmatrix} 1 \\ 0 \\ -1/2 \\ -\sqrt{3}/2 \\ -1/2 \\ \sqrt{3}/2 \end{pmatrix}, \qquad \nu_2 = \sqrt{3/2}(\xi_2 + \xi_3) = \begin{pmatrix} 0 \\ 1 \\ \sqrt{3}/2 \\ -1/2 \\ -\sqrt{3}/2 \\ -1/2 \end{pmatrix}.$$

(B. Gutkin)

Example 4.2. ***(Pseudo)real and complex representations.*** *There are three types of representation: real, pseudo-real and complex (see Montaldi for details). For real representations matrices $D(g)$ can be brought into real form such that $D_{ij}(g) = \bar{D}_{ij}(g)$. This implies in particular that all the characters are real. For pseudo-real representation the characters are also real but matrices $D(g)$ cannot be brought into real form. Finally, for complex representations the characters are complex. In the last case $D(g)$ and the conjugate $\bar{D}(g)$ constitute two different representation (since they characters are different), while in the real and pseudo-real case both representations are equivalent, i.e., $\bar{D}(g) = UD(g)U^\dagger$.*

Indicator. *To distinguish between three types of representations one looks at the indicator:*

$$\text{Ind}(\alpha) = \frac{1}{|G|}\sum_{g\in G}\chi^{(\alpha)}(g^2) \in \{1, 0, -1\}\,, \tag{4.6}$$

where 1, -1, 0 are obtained for real, complex and pseudo-real representations, respectively.

Proof: For a general irreducible representation we have

$$D^{(\alpha)}(g) = U\bar{D}^{(\beta)}(g)U^\dagger, \tag{4.7}$$

where $\alpha \neq \beta$ for a complex representation (since $\chi^{(\alpha)}(g) \neq \bar{\chi}^{(\alpha)}(g)$) and $\alpha = \beta$ for real and pseudo-real representations. From $D^{(\alpha)}(g^2) = D^{(\alpha)}(g)D^{(\alpha)}(g)$ follows

$$\text{Ind}(\alpha) = \sum_{i,j=1}^{m_\alpha}\sum_{k,n=1}^{m_\alpha}\sum_{g\in G}\frac{1}{|G|}\sum_{g\in G}U_{k,j}D^{(\alpha)}_{i,k}(g)\bar{D}^{(\beta)}_{j,n}(g)U^\dagger_{ni},$$

with m_α being dimension of α. By the orthogonality theorem this expression is zero for $\alpha \neq \beta$ which is the case of complex α. For real and pseudo-real representations we have

$$\text{Ind}(\alpha) = \frac{1}{m_\alpha}\text{tr}\,\left(U\bar{U}\right).$$

Now note, that for $\alpha = \beta$ eq. (4.7) yields

$$D^{(\alpha)}(g)U\bar{U} = U\bar{U}D^{(\alpha)}(g).$$

By the first Schur's lemma it follows then that $U\bar{U} = \gamma I$, or $U = \gamma U^\top$ which also implies $\gamma^2 = 1$. This leaves only two possibilities $\gamma = 1$ for real and $\gamma = -1$ for pseudo-real representations. In the first case we have $UU^\top = I$ and Ind$(\alpha) = 1$, while in the second one $UU^\top = -I$ and Ind$(\alpha) = -1$. Note finally, that $1 = \det\left(U\bar{U}\right) = \gamma^{m_\alpha}$. So $\gamma = -1$ might appear only if m_α is even. In other words, a pseudo-real irreducible representation must be of even dimension.

Example 4.3. ***Quaternions:*** *Quaternion multiplication table is*

$$\{\pm 1, \pm i, \pm j, \pm k\} \qquad i^2 = j^2 = k^2; \quad ij = k.$$

This group has five conjugate classes:

$$\{1\}, \{-1\}, \{\pm i\}, \{\pm j\}, \{\pm k\}.$$

The only possible solution for the equation $\sum_{i=1}^{5} m_i^2 = 8$ *is* $m_i = 1, i = 1, \dots 4, m_5 = 2$. *In addition to fully symmetric representation, the other three one-dimensional representations are easy to find:* $\chi(1) = 1, \chi(-1) = 1$*, while* $\chi(i) = -1, \chi(j) = -1, \chi(k) = 1$*;* $\chi(i) = -1, \chi(k) = -1, \chi(j) = 1$ *or* $\chi(k) = -1, \chi(j) = -1, \chi(i) = 1$. *The two-dimensional representation can be find by the orthogonality relation:*

$$2 + \chi(-1) \pm \chi(k) \pm \chi(i) \pm \chi(j) = 0, \Longrightarrow \chi(-1) = -2, \chi(k) = \chi(i) = \chi(j) = 0\,.$$

Since the indicator equals

$$Ind = (2\chi(1) + 6\chi(-1))/8 = -1,$$

the last representation is pseudo-real. Note that this representation can be realized using Pauli matrices:

$$\{\pm I, \pm\sigma_x, \pm\sigma_y, \pm\sigma_z\}.$$

(B. Gutkin)

References

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

[2] V. Hart and H. Segerman, The quaternion group as a symmetry group, in Proc. Bridges 2014: Mathematics, Music, Art, Architecture, Culture, edited by G. H. G. Greenfield and R. Sarhangi (2014), pp. 143–150.

[3] O. Katz-Saporta and E. Efrati, "Self-driven fractional rotational diffusion of the harmonic three-mass system", Phys. Rev. Lett. **122**, 024102 (2019).

[4] G. L. Kotkin and V. G. Serbo, *Collection of Problems in Classical Mechanics* (Elsevier, 2013).

[5] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory* (Pergamon Press, Oxford, 1959).

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

[7] M. Tinkham, *Group Theory and Quantum Mechanics* (Dover, New York, 2003).

Exercises

4.1. **Characters of D_3.** (continued from exercise 2.4) $\mathrm{D}_3 \cong \mathrm{C}_{3v}$, the group of symmetries of an equilateral triangle: has three irreducible representations, two one-dimensional and the other one of multiplicity 2.

(a) All finite discrete groups are isomorphic to a permutation group or one of its subgroups, and elements of the permutation group can be expressed as cycles. Express the elements of the group D_3 as cycles. For example, one of the rotations is (123), meaning that vertex 1 maps to 2, $2 \to 3$, and $3 \to 1$.

(b) Use your representation from exercise 2.4 to compute the D_3 character table.

(c) Use a more elegant method from the group-theory literature to verify your D_3 character table.

(d) Two D_3 irreducible representations are one dimensional and the third one of multiplicity 2 is formed by $[2\times2]$ matrices. Find the matrices for all six group elements in this representation.

4.2. **Decompose a representation of S_3.** As an illustration of the utility of the character orthonormality relations (3.1), let's work out the reduction of the matrix representation of S_3 permutations. The identity element acting on three objects $[a\ b\ c]$ is a 3×3 identity matrix,

$$D(E) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Transposing the first and second object yields $[b\ a\ c]$, represented by the matrix

$$D(A) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

since

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} b \\ a \\ c \end{pmatrix}$$

1. Find all six matrices for this representation.
2. Split this representation into its conjugacy classes.
3. Evaluate the characters $\chi(\mathcal{C}_j)$ for this representation.
4. Determine multiplicities c_a of irreps contained in this representation.
5. (bonus) Construct explicitly all irreps.
6. (bonus) Explain whether any irreps are missing in this decomposition, and why.

4.3. **All irreducible representations of D_4.** Dihedral group D_4, the symmetry group of a square, consists of 8 elements: identity, rotations by $\pi/2$, π, $3\pi/2$, and 4 reflections across symmetry axes: $\mathrm{D}_4 = \langle g, \sigma | g^4 = \sigma^2 = e, g\sigma = \sigma g^3 \rangle$

(a) Find all conjugacy classes.

(b) Determine the dimensions of irreducible representations using the relationship

$$\sum_i d_i^2 = |G|, \tag{4.8}$$

where d_i is the dimension of ith irreducible representation.

(c) Determine the remaining items of the character table.

(d) Compare with the character table of quaternions, example 4.3. Are they the same or different?

(e) Determine the indicators for all irreps of D_4. Are they the same as for the irreps of the quaternion group?

If you are at loss how to proceed, take a look at Landau and Lifschitz [5] *Vol.3: Quantum Mechanics*

(Boris Gutkin)

4.4. **Irreducible representations of dihedral group D_n.**

(a) Determine the dimensions of all irreps of dihedral group D_n, n odd.

(b) Determine the dimensions of all irreps of dihedral group D_n, n even.

This exercise is meant to be easy - guess the answer from the irreps dimension sum rule (4.8), and what you already know about D_1, D_3 and D_4. Working out also D_2 case (cut a disk into two equal halves) might be helpful. A more serious attempt would require counting conjugacy classes first. This exercise might help you later, when you are looking at irreps of the orthogonal groups $O(n)$; turns out they are different for n odd or even n, and that has physical consequences: what you learn by working out a problem in 2 dimensions might be misleading for working it out in 3 dimensions.

4.5. **Perturbation of T_d symmetry.**
A non-relativistic charged particle moves in an infinite bound potential $V(x)$ with T_d symmetry. Consult exercise 5.1 *Vibration Modes of CH_4* for the character table and other T_d details.

(a) What are the degeneracies of the quantum energy levels? How often do they appear relative to each other (i.e., what is the level density)?

A weak constant electric field is now added now along one of the $2\pi/3$ rotation axes, splitting energy levels into multiplets.

(b) What is the symmetry group of the system now?

(c) How are the levels of the original system split? What are the new degeneracies?

(Boris Gutkin)

4.6. **Selection rules for T_d symmetry.**
The setup is the same as in exercise 4.5, but now assume that instead of a constant field, a time dependent electric field $\boldsymbol{E}_0 \cos(\omega t)$ is added to the system, with $\boldsymbol{E}_0$ not necessarily directed along any of the symmetry axes. In general, when $|E_n - E_m| = \hbar\omega$, such time-dependent perturbation induces transitions between energy levels E_n and E_m.

(a) What are the selection rules? Between which energy levels of the system are transitions possible?

(b) Would the answer be different if a magnetic field $\boldsymbol{B}_0 \cos(\omega t)$ is added instead? Explain how and why.

4.7. **Two particles in a potential.**

Two distinguishable particles of the same mass move in a 2-dimensional potential $V(r)$ having D_4 symmetry. In addition they interact with each other with the term $\lambda W(|\boldsymbol{r}_1 - \boldsymbol{r}_2|)$.

(a) What is the symmetry group of the Hamiltonian if $\lambda = 0$? If $\lambda \neq 0$?.

(b) What are the degeneracies of the energy levels if $\lambda = 0$?

(c) Assuming that $\lambda \ll 1$ (weak interaction), describe the energy level structure, i.e., degeneracies and quasi-degeneracies of the energy levels. What will be the answer if the interaction is strong?

Hint: when interaction is weak we can think about it as perturbation. (Boris Gutkin)