

group theory - week 2

Finite groups - definitions

Georgia Tech PHYS-7143

Homework HW2

due Tuesday 2021-05-25

== 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 2.1 $G_x \subset G$	1 point
Exercise 2.2 <i>Transitivity of conjugation</i>	1 point
Exercise 2.3 <i>Isotropy subgroup of gx</i>	1 points
Exercise 2.4 D_3 : <i>symmetries of an equilateral triangle</i>	5 points
Exercise 2.5 C_4 - <i>invariant potential</i>	7 (+2) points

Bonus points

Exercise 2.7 <i>Three masses on a loop</i>	6 points
Exercise 2.6 (a), (b) and (c) <i>Permutation of three objects</i>	2 points

Total of 15 points = 100 % score.

Extra points accumulate, can help you later if you miss a few problems.


2.1 Week's videos, reading

If I had had more time, I would have written less
— Blaise Pascal, a remark made to a correspondent


Please do not get intimidated by the length of this week's notes - they are here more for me than for you, as notes on these topics for future reference. If you understand the main sequence of video clips, and recommended reading, that should suffice to do the problems. The rest is optional, you can quickly skim over...

2.1.1 Don't wanna know group theory

The fastest way to watch any week's lecture videos is by letting YouTube run the

 *Section playlist*


- Sect. 2.4 *Using symmetries*
- Sect. 2.5 *Normal modes*: The free vibrations of systems, for undamped systems with total energy conserved for which the frequencies of oscillation are real.


 *Normal modes* (9:06 min)


- example 2.5 *Vibrational spectra of molecules* is taken from Gutkin lecture notes [example 5.1](#) *C_n symmetry*. The corresponding projection operators (1.25) are worked out in example 2.6.
- Example 2.4 *Vibrations of a classical CO₂ molecule*

 *A Hamiltonian with a symmetry* (4:46 min)

 *CO₂ molecule* (4:07 min)


 *Projection operators* (5:33 min)

 *(Anti)symmetric subspaces* (3:04 min)

 *Zero mode* (5:19 min)









2.1.2 Finite groups

Groups, permutations, rearrangement theorem, subgroups, cosets, classes, all exemplified by the $D_3 \cong C_{3v} \cong S_3$ symmetries of an equilateral triangle.


 *Section playlist*









 Dresselhaus *et al.* [4] [Chapter 1 Basic Mathematical Background: Introduction](#). The MIT course 6.734 [online version](#) contains much of the same material.

 ChaosBook [Chapter 10. Flips, slides and turns](#)

-  *Discrete symmetry, an example: 3-disk pinball (4:03 min)*
-  *What is a group? (10:56 min)*
 -  (extra) *Discussion: There might be many examples of it, but a 'group' itself is an abstract notion. (3 min)*
 -  (extra) *Discussion: permutations, symmetric group, simple groups, Italian renaissance, French revolution, Galois (5:23 min)*
-  *by **Socratica**: (cannot add it to the section YouTube playlist) a delightful introduction to group multiplication (or Cayley) tables. (7:32)*
-  *Active, passive coordinate transformations (3:08 min)*
-  *Following Mefisto: symmetry defined three (3) times (7:01 min)*
-  *Subgroups, classes, group orbits, reduced state space (7:57 min)*

2.2 Other sources (optional)


-  *Group theory and why I love 808,017, ···,000 (cannot add it to the section YouTube playlist)*

is a great video on group theory from 3Blue1Brown, writes Andrew Wu. I agree: Well worth of your time, more motivational than my lectures. What it actually focuses on - the monster group - is totally useless to us.
-  AWH Example 6.2.3 *Degenerate eigenproblem*
-  AWH Example 6.5.2 *Normal modes*
-  For a deep dive into this material, here is your **rabbit hole**.
-  For deeper insights, read Roger Penrose [7] (**click here**).
-  AWH Chapter 17 *Group Theory* (**click here**).
-  For a typical (but for this course advanced) application see, for example, Stone and Goldbart [10], *Mathematics for Physics: A Guided Tour for Graduate Students*, Section 14.3.2 *Vibrational spectrum of H₂O* (**click here**).
- Glance through sect. 2.6 *Group presentations* and sect. 2.8 *Literature*, but I do not expect you to understand this material.
-  *Discussion 4 - Homework. (3 min)*
 -  There is no need to learn all these “Greek” words.
 - If instead, bedside crocheting is your thing, **click here**.

2.3 Using group theory without knowing any

It's a matter of no small pride for a card-carrying dirt physics theorist to claim **full and total ignorance** of group theory (read ChaosBook [Appendix A.6 Gruppenpest](#)). So what we will do first is work out a few examples of physical applications of group theory that you already know without knowing that you have been using "Group Theory."

2.4 Using symmetries

Tyger Tyger burning bright,
In the forests of the night:
What immortal hand or eye,
Dare frame thy fearful symmetry?
—William Blake,  *The Tyger*

The big idea #1 of this is week is *symmetry*.

If our physical problem is defined by a (perhaps complicated) Hamiltonian \mathbf{H} , another matrix \mathbf{M} (hopefully a very simple matrix) is a symmetry if it commutes with the Hamiltonian

$$[\mathbf{M}, \mathbf{H}] = 0. \quad (2.1)$$

Then we can use the spectral decomposition (1.30) of \mathbf{M} to block-diagonalize \mathbf{H} into a sum of lower-dimensional sub-matrices,

$$\mathbf{H} = \sum_i \mathbf{H}_i, \quad \mathbf{H}_i = \mathbf{P}_i \mathbf{H} \mathbf{P}_i, \quad (2.2)$$

and thus significantly simplify the computation of eigenvalues and eigenvectors of \mathbf{H} , the matrix of physical interest.

2.5 Normal modes

The big idea #2 of this is week is: *many body systems* (molecules, neuronal networks, ...) are ruled by *collective modes*, not individual particles (atoms, neurons, ...).

In the linear, harmonic oscillator approximation, the classical dynamics of a molecule is governed by the Hamiltonian

$$H = \sum_{i=1}^N \frac{m_i}{2} \dot{x}_i^2 + \frac{1}{2} \sum_{i,j=1}^N x_i^\top V_{ij} x_j,$$

where $\{x_i\}$ are small deviations from the equilibrium, resting points of the molecules labelled i . V_{ij} is a symmetric matrix, so it can be brought to a diagonal form by an

D_3	e	C	C^2	$\sigma^{(1)}$	$\sigma^{(2)}$	$\sigma^{(3)}$
e	e	C	C^2	$\sigma^{(1)}$	$\sigma^{(2)}$	$\sigma^{(3)}$
C	C	C^2	e	$\sigma^{(3)}$	$\sigma^{(1)}$	$\sigma^{(2)}$
C^2	C^2	e	C	$\sigma^{(2)}$	$\sigma^{(3)}$	$\sigma^{(1)}$
$\sigma^{(1)}$	$\sigma^{(1)}$	$\sigma^{(2)}$	$\sigma^{(3)}$	e	C	C^2
$\sigma^{(2)}$	$\sigma^{(2)}$	$\sigma^{(3)}$	$\sigma^{(1)}$	C^2	e	C
$\sigma^{(3)}$	$\sigma^{(3)}$	$\sigma^{(1)}$	$\sigma^{(2)}$	C	C^2	e

Table 2.1: The dihedral group D_3 group multiplication table. Actually, we prefer cyclic and dihedral groups notation ‘rotations’ r^ℓ and ‘flips’ σ_m , as in table 4.1.

orthogonal transformation, to a set of N uncoupled harmonic oscillators or *normal modes* of frequencies $\{\omega_i\}$.

$$x \rightarrow y = Ux, \quad H = \sum_{i=1}^N \frac{m_i}{2} (\dot{y}_i^2 + \omega_i^2 y_i^2) . \quad (2.3)$$

2.6 Group presentations

Group theory? It is all about class & character.

— Predrag Cvitanović, *One minute elevator pitch*

Group multiplication (or Cayley) tables, such as Table 2.1, *define* each distinct discrete group, but they can be hard to digest. A Cayley graph, with links labeled by generators, and the vertices corresponding to the group elements, has the same information as the group multiplication table, but is often a more insightful presentation of the group.

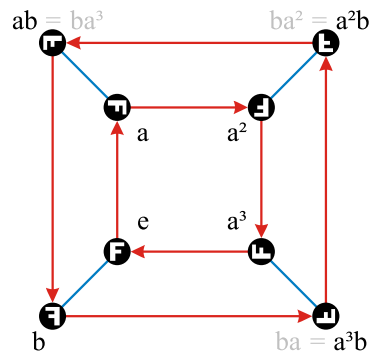


Figure 2.1: A Cayley graph presentation of the dihedral group D_4 . The ‘root vertex’ of the graph, marked e , is here indicated by the letter \mathbb{F} , the links are multiplications by two generators: a cyclic rotation by left-multiplication by element a (directed red link), and the flip by b (undirected blue link). The vertices are the 8 possible orientations of the transformed letter \mathbb{F} .

For example, the Cayley graph figure 2.1 is a clear presentation of the dihedral group D_4 of order 8,

$$D_4 = (e, a, a^2, a^3, b, ba, ba^2, ba^3), \quad \text{generators } a^4 = e, b^2 = e. \quad (2.4)$$

Quaternion group is also of order 8, but with a distinct multiplication table / Cayley graph, see figure 2.2. For more of such, see, for example, [mathoverflow](#) Cayley graph discussion.

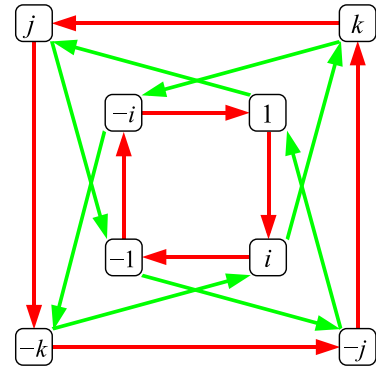
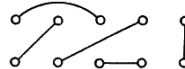


Figure 2.2: A Cayley graph presentation of the quaternion group Q_8 . It is also of order 8, but distinct from D_4 .

2.7 Permutations in birdtracks

The text that follows is a very condensed extract of birdtracks.eu [chapter 6 Permutations](#), from *Group Theory - Birdtracks, Lie's, and Exceptional Groups* [3]. I am usually reluctant to use birdtrack notations in front of graduate students indoctrinated by their professors in the 1890's tensor notation, but I'm emboldened by the very enjoyable article on *The new language of mathematics* by Dan Silver [9]. Your professor's notation is as convenient for actual calculations as -let's say- long division using roman numerals. So leave them wallowing in their early progressive rock of 1968, King Crimson's of their youth. You chill to beats younger than Windows 98, to [grime](#), to [trap](#), to [hardvapour](#), to [birdtracks](#).

In 1937 R. Brauer [2] introduced diagrammatic notation for the Kronecker δ_{ij} operation, in order to represent "Brauer algebra" permutations, index contractions, and matrix multiplication diagrammatically. His equation (39)



(send index 1 to 2, 2 to 4, contract ingoing (3·4), outgoing (1·3)) is the earliest published diagrammatic notation I know about. While in kindergarten (disclosure: we were too poor to afford kindergarten) I sat out to revolutionize modern group theory [3]. But I suffered a terrible setback; in early 1970's Roger Penrose pre-invented my "birdtracks," or diagrammatic notation, for symmetrization operators [6], Levi-Civita tensors [8], and "strand networks" [5]. Here is a little flavor of how one birdtracks:

We can represent the operation of permuting indices (d "billiard ball labels," tensors with d indices) by a matrix with indices bunched together:

$$\sigma_{\alpha}^{\beta} = \sigma_{b_1 \dots b_p}^{a_1 a_2 \dots a_q} \delta_{c_q \dots c_2 c_1}^{d_p \dots d_1} \quad (2.5)$$

To draw this, Brauer style, it is convenient to turn his drawing on a side. For 2-index tensors, there are two permutations:

$$\begin{aligned}
 \text{identity: } \mathbf{1}_{ab, cd} = \delta_a^d \delta_b^c &= \begin{array}{c} \leftarrow \\ \leftarrow \\ \leftarrow \end{array} \\
 \text{flip: } \sigma_{(12)ab, cd} = \delta_a^c \delta_b^d &= \begin{array}{c} \leftarrow \\ \leftarrow \\ \leftarrow \end{array} \cdot \quad (2.6)
 \end{aligned}$$

For 3-index tensors, there are six permutations:

$$\begin{aligned}
 \mathbf{1}_{a_1 a_2 a_3, b_3 b_2 b_1} &= \delta_{a_1}^{b_1} \delta_{a_2}^{b_2} \delta_{a_3}^{b_3} = \begin{array}{c} \leftarrow \\ \leftarrow \\ \leftarrow \end{array} \\
 \sigma_{(12)a_1 a_2 a_3, b_3 b_2 b_1} &= \delta_{a_1}^{b_2} \delta_{a_2}^{b_1} \delta_{a_3}^{b_3} = \begin{array}{c} \leftarrow \\ \leftarrow \\ \leftarrow \end{array} \\
 \sigma_{(23)} &= \begin{array}{c} \leftarrow \\ \leftarrow \\ \leftarrow \end{array}, \quad \sigma_{(13)} = \begin{array}{c} \leftarrow \\ \leftarrow \\ \leftarrow \end{array} \\
 \sigma_{(123)} &= \begin{array}{c} \leftarrow \\ \leftarrow \\ \leftarrow \end{array}, \quad \sigma_{(132)} = \begin{array}{c} \leftarrow \\ \leftarrow \\ \leftarrow \end{array}. \quad (2.7)
 \end{aligned}$$

Here group element labels refer to the standard permutation cycles notation. There is really no need to indicate the “time direction” by arrows, so we omit them from now on.

The symmetric sum of all permutations,

$$\begin{aligned}
 S_{a_1 a_2 \dots a_p, b_p \dots b_2 b_1} &= \frac{1}{p!} \left\{ \delta_{a_1}^{b_1} \delta_{a_2}^{b_2} \dots \delta_{a_p}^{b_p} + \delta_{a_2}^{b_1} \delta_{a_1}^{b_2} \dots \delta_{a_p}^{b_p} + \dots \right\} \\
 S &= \begin{array}{c} \leftarrow \\ \leftarrow \\ \leftarrow \\ \vdots \\ \leftarrow \\ \leftarrow \\ \leftarrow \end{array} = \frac{1}{p!} \left\{ \begin{array}{c} \leftarrow \\ \leftarrow \\ \leftarrow \\ \vdots \\ \leftarrow \\ \leftarrow \\ \leftarrow \end{array} + \begin{array}{c} \leftarrow \\ \leftarrow \\ \leftarrow \\ \vdots \\ \leftarrow \\ \leftarrow \\ \leftarrow \end{array} + \begin{array}{c} \leftarrow \\ \leftarrow \\ \leftarrow \\ \vdots \\ \leftarrow \\ \leftarrow \\ \leftarrow \end{array} + \dots \right\}, \quad (2.8)
 \end{aligned}$$

yields the symmetrization operator S . In birdtrack notation, a white bar drawn across p lines [6] will always denote symmetrization of the lines crossed. A factor of $1/p!$ has been introduced in order for S to satisfy the projection operator normalization

$$\begin{array}{c} S^2 \\ \leftarrow \\ \leftarrow \\ \leftarrow \\ \vdots \\ \leftarrow \\ \leftarrow \\ \leftarrow \end{array} = S \begin{array}{c} \leftarrow \\ \leftarrow \\ \leftarrow \\ \vdots \\ \leftarrow \\ \leftarrow \\ \leftarrow \end{array}. \quad (2.9)$$

You have already seen such “fully-symmetric representation,” in the discussion of discrete Fourier transforms, ChaosBook Example A24.3 ‘Configuration-momentum’ Fourier space duality, but you are not likely to recognize it. There the average was not over all permutations, but the zero-th Fourier mode ϕ_0 was the average over only cyclic permutations. Every finite discrete group has such fully-symmetric representation, and in statistical mechanics and quantum mechanics this is often the most important state (the ‘ground’ state).

A subset of indices $a_1, a_2, \dots, a_q, q < p$ can be symmetrized by symmetrization

matrix $S_{12\dots q}$

$$\begin{aligned}
 (S_{12\dots q})_{a_1 a_2 \dots a_q \dots a_p, b_p \dots b_q \dots b_2 b_1} &= \\
 \frac{1}{q!} \left\{ \delta_{a_1}^{b_1} \delta_{a_2}^{b_2} \dots \delta_{a_q}^{b_q} + \delta_{a_2}^{b_1} \delta_{a_1}^{b_2} \dots \delta_{a_q}^{b_q} + \dots \right\} \delta_{a_q+1}^{b_q+1} \dots \delta_{a_p}^{b_p} \\
 S_{12\dots q} &= \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \vdots \\ \text{---} \\ \text{---} \\ \text{---} \\ \vdots \\ \text{---} \\ \text{---} \end{array} \frac{1}{q} \cdot \quad (2.10)
 \end{aligned}$$

Overall symmetrization also symmetrizes any subset of indices:

$$\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \vdots \\ \text{---} \\ \text{---} \\ \text{---} \\ \vdots \\ \text{---} \\ \text{---} \end{array} S_{12\dots q} = S = \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \vdots \\ \text{---} \\ \text{---} \\ \text{---} \\ \vdots \\ \text{---} \\ \text{---} \end{array} \cdot \quad (2.11)$$

Any permutation has eigenvalue 1 on the symmetric tensor space:

$$\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \vdots \\ \text{---} \\ \text{---} \end{array} \sigma S = S = \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \vdots \\ \text{---} \\ \text{---} \end{array} \cdot \quad (2.12)$$

Diagrammatically this means that legs can be crossed and uncrossed at will.

One can construct a projection operator onto the fully antisymmetric space in a similar manner [3]. Other representations are trickier - that's precisely what the theory of finite groups is about.

2.8 Other sources (optional)

The exposition (or the corresponding chapter in Tinkham [11]) that we follow here largely comes from Wigner's classic *Group Theory and Its Application to the Quantum Mechanics of Atomic Spectra* [12], which is a harder going, but the more group theory you learn the more you'll appreciate it.

The structure of finite groups was understood by late 19th century. A full list of finite groups was another matter. The complete proof of the classification of all finite groups takes about 3 000 pages, a collective 40-years undertaking by over 100 mathematicians, read the [wiki](#). 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 $212(26 + 1)(24 - 1)(23 + 1)(2 - 1)/2 = 17\,971\,200$.

From Emory Math Department: **A pariah is real!** The simple finite groups fit into 18 families, except for the 26 sporadic groups. 20 sporadic groups AKA the Happy Family are parts of the Monster group. The remaining six loners are known as the pariahs.

Hang in there! And relax. None of this will be on the test. As a matter of fact, there will be no test.

Question 2.1. Henriette Roux asks

Q What did you do this weekend?

A The same as every other weekend - prepared week's lecture, with my helpers Avi the Little, Edvard the Nordman, and Malbec el Argentino, under Master Roger's watchful eye, [see here](#).

2.9 Examples

Example 2.1. Discrete symmetries in physics:

- Point groups i.e., subgroups of $O(3)$.
- Point groups + discrete translations e.g., symmetry groups of crystals.
- Permutation groups

$$S\Psi(x_1, x_2, \dots, x_n) = \Psi(x_2, x_1, \dots, x_n).$$

- Boson wave functions are symmetric while fermion wave functions are anti-symmetric under exchange of variables.

(B. Gutkin)

Example 2.2. The group multiplication table for D_3 : See table 4.1.

Example 2.3. Reflection and discrete rotation symmetries:

(a) Reflection symmetry $V(x) = PV(x) = V(-x)$:

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi(x) = E_n \psi(x) \quad (2.13)$$

(see figure 2.3). If $\psi(x)$ is solution then $P\psi(x)$ is also solution. From this and non-degeneracy of the spectrum follows that either $P\psi(x) = \psi(x)$ or $P\psi(x) = -\psi(x)$. The first case corresponds to symmetric functions while the second one to anti-symmetric one. Thus the whole spectrum can be decomposed in accordance to a symmetry of the Hamiltonian (equations of motion).

(b) Rotation symmetry $V(x) = gV(x)$, $G = \{e, g, g^2\}$: By the same argument we have three possibilities:

$$g\psi(x) = \psi(x); \quad g\psi(x) = e^{i2\pi/3}\psi(x); \quad g^{-1}\psi(x) = e^{-i2\pi/3}\psi(x).$$

In addition, by the time reversal symmetry if $\psi(x)$ is solution then $\psi^*(x)$ is solution with the same eigenvalue as well. From this follows that the spectrum must be degenerate. The spectrum is split into a real eigenfunction $\{\psi_1(x)\}$, and a degenerate pair of real eigenfunctions

$$\psi_2(x) = \psi(x) + \psi^*(x); \quad \psi_3(x) = i(\psi(x) - \psi^*(x)), \quad \text{where } g\psi(x) = e^{i2\pi/3}\psi(x)$$

invariant under rotations by 1/3-rd of a circle.

(B. Gutkin)

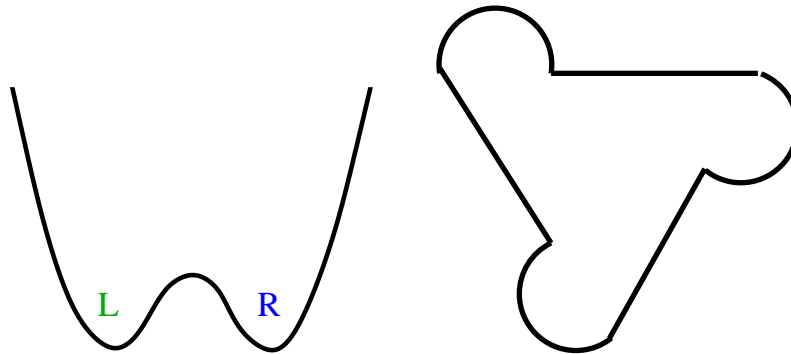


Figure 2.3: (left) A reflection-symmetric double-well potential. (right) A 1/3rd-circle rotation-symmetric plane billiard (infinite wall potential in 2D). (B. Gutkin)

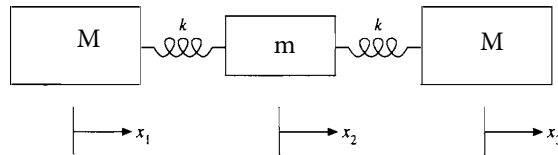


Figure 2.4: A classical colinear CO₂ molecule [1].

Example 2.4. Vibrations of a classical CO₂ molecule: Consider one carbon and two oxygens constrained to the x -axis [1] and joined by springs of stiffness k , as shown in figure 2.4. Newton's second law says

$$\begin{aligned} \ddot{x}_1 &= -\frac{k}{M}(x_1 - x_2) \\ \ddot{x}_2 &= -\frac{k}{m}(x_2 - x_3) - \frac{k}{m}(x_2 - x_1) \\ \ddot{x}_3 &= -\frac{k}{M}(x_3 - x_2). \end{aligned} \tag{2.14}$$

The normal modes, with time dependence $x_j(t) = x_j \exp(it\omega)$, are the common frequency ω vibrations that satisfy (2.14),

$$\mathbf{H}\mathbf{x} = \begin{pmatrix} A & -A & 0 \\ -a & 2a & -a \\ 0 & -A & A \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \omega^2 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}, \tag{2.15}$$

where $a = k/m$, $A = k/M$. Secular determinant $\det(\mathbf{H} - \omega^2\mathbf{1}) = 0$ now yields a cubic equation for ω^2 .

You might be tempted to stick this 3×3 matrix into *Mathematica* or whatever, but please do that in some other course. What would understood by staring at the output? In this course we think.

First thing to always ask yourself is: does the system have a symmetry? Yes! Note that the CO₂ molecule (2.14) of figure 2.4 is invariant under $x_1 \leftrightarrow x_3$ interchange, i.e.,

coordinate relabeling by matrix σ that commutes with our law of motion \mathbf{H} ,

$$\sigma = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \sigma \mathbf{H} = \mathbf{H} \sigma = \begin{pmatrix} 0 & -A & A \\ -a & 2a & -a \\ A & -A & 0 \end{pmatrix}. \quad (2.16)$$

We can now use the symmetry operator σ to simplify the calculation. As $\sigma^2 = \mathbf{1}$, its eigenvalues are ± 1 , and the corresponding symmetrization, anti-symmetrization projection operators (1.38) are

$$\mathbf{P}_+ = \frac{1}{2}(\mathbf{1} + \sigma), \quad \mathbf{P}_- = \frac{1}{2}(\mathbf{1} - \sigma). \quad (2.17)$$

The dimensions $d_i = \text{tr } \mathbf{P}_i$ of the two subspaces are

$$d_+ = 2, \quad d_- = 1. \quad (2.18)$$

As σ and \mathbf{H} commute, we can now use spectral decomposition (1.30) to block-diagonalize \mathbf{H} to a 1-dimensional and a 2-dimensional matrix.

On the 1-dimensional antisymmetric subspace, the trace of a $[1 \times 1]$ matrix equals its sole matrix element equals its eigenvalue

$$\lambda_- = \text{tr } \mathbf{H} \mathbf{P}_- = \frac{1}{2}(\text{tr } \mathbf{H} - \text{tr } \mathbf{H} \sigma) = (a + A) - a = \frac{k}{M},$$

so the corresponding eigenfrequency is $\omega_-^2 = k/M$. To understand its physical meaning, write out the antisymmetric subspace projection operator (2.18) explicitly. Its non-vanishing columns are proportional to the sole eigenvector

$$\mathbf{P}_- = \frac{1}{2} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} \Rightarrow \mathbf{e}^{(-)} = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}. \quad (2.19)$$

In this subspace the outer oxygens are moving in opposite directions, with the carbon stationary.

On the 2-dimensional symmetric subspace, the trace yields the sum of the remaining two eigenvalues

$$\lambda_+ + \lambda_0 = \text{tr } \mathbf{H} \mathbf{P}_+ = \frac{1}{2}(\text{tr } \mathbf{H} + \text{tr } \mathbf{H} \sigma) = (a + A) + a = \frac{k}{M} + 2 \frac{k}{m}.$$

We could disentangle the two eigenfrequencies by evaluating $\text{tr } \mathbf{H}^2 \mathbf{P}_+$, for example, but thinking helps again.

There is still another, translational symmetry, so obvious that we forgot it; if we change the origin of the x -axis, the three coordinates $x_j \rightarrow x_j - \delta x$ change, for any continuous translation δx , but the equations of motion (2.14) do not change their form,

$$\mathbf{H} \mathbf{x} = \mathbf{H} \mathbf{x} + \mathbf{H} \delta \mathbf{x} = \omega^2 \mathbf{x} \Rightarrow \mathbf{H} \delta \mathbf{x} = 0. \quad (2.20)$$

So any translation $\mathbf{e}^{(0)} = \delta \mathbf{x} = (\delta x, \delta x, \delta x)$ is a nul, 'zero mode' eigenvector of \mathbf{H} in (2.16), with eigenvalue $\lambda_0 = \omega_0^2 = 0$, and thus the remaining eigenfrequency is $\omega_+^2 = k/M + 2k/m$. As we can add any nul eigenvector $\mathbf{e}^{(0)}$ to the corresponding $\mathbf{e}^{(+)}$ eigenvector, there is some freedom in choosing $\mathbf{e}^{(+)}$. One visualization of the corresponding eigenvector is the carbon moving opposite to the two oxygens, with total momentum set to zero.

(Taken from AWH Example 6.2.3 Degenerate eigenproblem, but done here using symmetries.)

Example 2.5. Vibrational spectra of molecules: In the linear, harmonic oscillator approximation the classical dynamics of the molecule is governed by the Hamiltonian

$$H = \sum_{i=1}^N \frac{m_i}{2} \dot{x}_i^2 + \frac{1}{2} \sum_{i,j=1}^N x_i^\top V_{ij} x_j,$$

where $\{x_i\}$ are small deviations from the resting the equilibrium, resting points of the molecules labelled i . V_{ij} is a symmetric matrix, so it can be brought to a diagonal form by an orthogonal transformation, a set of N uncoupled harmonic oscillators or normal modes of frequencies $\{\omega_i\}$.

$$x \rightarrow y = Ux, \quad H = \sum_{i=1}^N \frac{m_i}{2} (y_i^2 + \omega_i^2 y_i^2). \quad (2.21)$$

Consider now the ring of pair-wise interactions of two kinds of molecules sketched in figure 2.5 (a), given by the potential

$$V(z) = \frac{1}{2} \sum_{i=1}^N (k_1(x_i - y_i)^2 + k_2(x_{i+1} - y_i)^2), \quad z_i = \begin{pmatrix} x_i \\ y_i \end{pmatrix}, \quad (2.22)$$

whose $[2N \times 2N]$ matrix form is (aside to the cognoscenti: this is a Toeplitz matrix):

$$V_{ij} = \frac{1}{2} \begin{pmatrix} k_1 + k_2 & -k_1 & 0 & 0 & 0 & \dots & 0 & 0 & -k_2 \\ -k_1 & k_1 + k_2 & -k_2 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & -k_2 & k_1 + k_2 & -k_1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & -k_1 & k_1 + k_2 & -k_2 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \dots & -k_2 & k_1 + k_2 & -k_1 \\ -k_2 & 0 & 0 & 0 & 0 & \dots & 0 & -k_1 & k_1 + k_2 \end{pmatrix}$$

This potential matrix is a holy mess. How do we find an orthogonal transformation (2.21) that diagonalizes it? Look at figure 2.5 (a). Molecules lie on a circle, so that suggests we should use a Fourier representation. As the $i = 1$ labelling of the starting molecule on a ring is arbitrary, we are free to relabel them, for example use the next molecule pair as the starting one. This relabelling is accomplished by the $[2N \times 2N]$ permutation matrix (or 'one-step shift', 'stepping' or 'translation' matrix) M of form

$$\underbrace{\begin{pmatrix} 0 & 0 & \dots & 0 & I \\ I & 0 & \dots & 0 & 0 \\ 0 & I & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & I & 0 \end{pmatrix}}_M \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ \vdots \\ z_n \end{pmatrix} = \begin{pmatrix} z_n \\ z_1 \\ z_2 \\ \vdots \\ z_{n-1} \end{pmatrix}, \quad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad z_i = \begin{pmatrix} x_i \\ y_i \end{pmatrix} \quad (2.23)$$

Projection operators corresponding to M are worked out in example 2.6. They are N

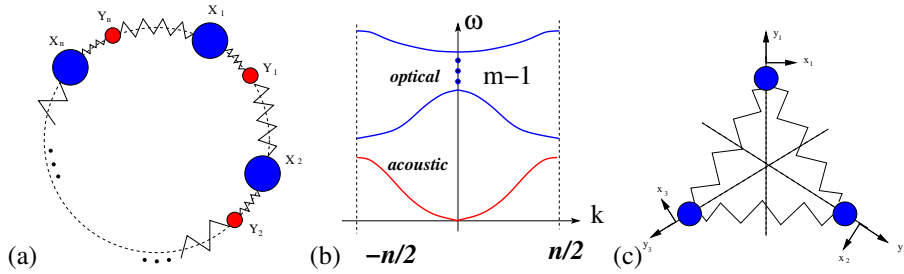


Figure 2.5: (a) Chain with circular symmetry. (b) Dependence of frequency on the representation wavenumber k . (c) Molecule with D_3 symmetry. (B. Gutkin)

distinct $[2N \times 2N]$ matrices,

$$\mathbf{P}_k = \begin{pmatrix} I & \bar{\lambda}I & \bar{\lambda}^2I & \dots & \bar{\lambda}^{N-2}I & \bar{\lambda}^{N-1}I \\ \lambda I & I & \bar{\lambda}I & \dots & \bar{\lambda}^{N-3}I & \bar{\lambda}^{N-2}I \\ \lambda^2I & \lambda I & I & \dots & \bar{\lambda}^{N-4}I & \bar{\lambda}^{N-3}I \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \lambda^{N-2}I & \lambda^{N-3}I & \lambda^{N-4}I & \dots & I & \bar{\lambda}I \\ \lambda^{N-1}I & \lambda^{N-2}I & \lambda^{N-2}I & \dots & \lambda I & I \end{pmatrix}, \quad \lambda = \exp\left(\frac{2\pi i}{N}k\right) \quad (2.24)$$

which decompose the $2N$ -dimensional configuration space of the molecule ring into a direct sum of N 2-dimensional spaces, one for each discrete Fourier mode $k = 0, 1, 2, \dots, N-1$.

The system (2.22) is clearly invariant under the cyclic permutation relabelling M , $[V, M] = 0$ (though checking this by explicit matrix multiplications might be a bit tedious), so the \mathbf{P}_k decompose the interaction potential V as well, and reduce its action to the k th 2-dimensional subspace. Thus the $[2N \times 2N]$ diagonalization (2.21) is now reduced to a $[2 \times 2]$ diagonalization which one can do by hand. The resulting k th space is spanned by two $2N$ -dimensional vectors, which we guess to be of form:

$$\eta_1 = \frac{1}{\sqrt{n}} \begin{pmatrix} 1 \\ 0 \\ \lambda \\ 0 \\ \vdots \\ \lambda^{n-1} \\ 0 \end{pmatrix}, \quad \eta_2 = \frac{1}{\sqrt{n}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ \lambda \\ \vdots \\ 0 \\ \lambda^{n-1} \end{pmatrix}.$$

In order to find eigenfrequencies we have to consider action of V on these two vectors:

$$V\eta_1 = (k_1 + k_2)\eta_1 - (k_1 + k_2\lambda)\eta_2, \quad V\eta_2 = (k_1 + k_2)\eta_2 - (k_1 + k_2\bar{\lambda})\eta_1.$$

The corresponding eigenfrequencies are determined by the equation:

$$0 = \det \left(\begin{pmatrix} k_1 + k_2 & -(k_1 + k_2\lambda) \\ -(k_1 + k_2\bar{\lambda}) & k_1 + k_2 \end{pmatrix} - \frac{\omega^2}{2}I \right) \implies \frac{1}{2}\omega_{\pm}^2(k) = k_1 + k_2 \pm |k_1 + k_2\lambda^k|, \quad (2.25)$$

one acoustic ($\omega(0) = 0$), one optical, see figure 2.5(b) and the [acoustic and optical phonons](#) wiki. (B. Gutkin)

Example 2.6. Projection operators for cyclic group C_N .

Consider a cyclic group $C_N = \{e, g, g^2, \dots, g^{N-1}\}$, and let $M = D(g)$ be a $[2N \times 2N]$ representation of the one-step shift g . In the projection operator formulation (1.25), the N distinct eigenvalues of M , the N th roots of unity $\lambda_n = \lambda^n$, $\lambda = \exp(i 2\pi/N)$, $n = 0, \dots, N - 1$, split the $2N$ -dimensional space into N 2-dimensional subspaces by means of projection operators

$$P_n = \prod_{m \neq n} \frac{M - \lambda_m I}{\lambda_n - \lambda_m} = \prod_{m=1}^{N-1} \frac{\lambda^{-n} M - \lambda^m I}{1 - \lambda^m}, \quad (2.26)$$

where we have multiplied all denominators and numerators by λ^{-n} . The numerator is now a matrix polynomial of form $(x - \lambda)(x - \lambda^2) \dots (x - \lambda^{N-1})$, with the zeroth root $(x - \lambda^0) = (x - 1)$ quotiented out from the defining matrix equation $M^N - 1 = 0$. Using

$$\frac{1 - x^N}{1 - x} = 1 + x + \dots + x^{N-1} = (x - \lambda)(x - \lambda^2) \dots (x - \lambda^{N-1})$$

we obtain the projection operator in form of a discrete Fourier sum (rather than the product (1.25)),

$$P_n = \frac{1}{N} \sum_{m=0}^{N-1} e^{i \frac{2\pi}{N} nm} M^m.$$

This form of the projection operator is the simplest example of the key group theory tool, projection operator expressed as a sum over characters,

$$P_n = \frac{1}{|G|} \sum_{g \in G} \bar{\chi}(g) D(g),$$

upon which stands all that follows in this course. (B. Gutkin and P. Cvitanović)

2.10 What are cosets good for? (a discussion)

Question 2.2. Henriette Roux asks

Q What are cosets good for?

A Apologies for glossing over their meaning in the lecture. I try to minimize group-theory jargon, but cosets cannot be ignored.

Dresselhaus *et al.* [4] ([click here](#)) Chapter 1 *Basic Mathematical Background: Introduction* needs them to show that the dimension of a subgroup is a divisor of the dimension of the group. For example, C_3 of dimension 3 is a subgroup of D_3 of dimension 6.

In ChaosBook [Chapter 10. Flips, slides and turns](#) cosets are absolutely essential. The significance of the coset is that if a solution has a symmetry, then the elements in a coset act on the solution the same way, and generate all equivalent copies of this solution. Example 10.7. *Subgroups, cosets of D_3* should help you understand that.

Henriette Roux writes: When talking about the cosets of a subgroup we demonstrated multiplication between cosets with a specific example, but this wasn't leading to something along the lines of that the set of all left cosets of a subgroup (or the set of all the right cosets of a subgroup) form a group, correct? It didn't appear so in the example since the "unit" $\{E, A\}$ we looked appears to only have the properties of an identity with multiplication from one direction (the direction depending on if it is the set of left cosets or the set of right cosets). In the context of the lecture I think this point was related to Lagrange's theorem (although we didn't call it that) and I vaguely remember cosets being used in the proof of Lagrange's theorem but I wasn't connecting it today. Are we going to cover that in a future lecture?

Predrag You are right - Lagrange's theorem (see the [wiki](#)) simply says the order of a subgroup has to be a divisor of the order of the group. We used cosets to partition elements of G to prove that. But what we really need cosets for is to define (see Dresselhaus *et al.* [4] Sect. 1.7) *Factor Groups* whose elements are cosets of a self-conjugate subgroup ([click here](#)). I will not cover that in a subsequent lecture, so please read up on it yourself.

Henriette Roux You talked about the period of an element X , and said that that *period* is the *set*

$$\{E, X, \dots, X^{n-1}\}, \quad (2.27)$$

where n is the *order* of the element X . I had thought that set was the subgroup generated by the element X and that the period of the element X was a synonym for the order of the element X ? Is that incorrect?

Predrag To keep things as simple as possible, in Thursday's lecture I followed Sect. 1.3 *Basic Definitions* of Dresselhaus *et al.* textbook [4], to the letter. In Def. 3 the *order* of an element X is the smallest n such that $X^n = E$, and they call the set (2.27) the *period* of X . I do not like that usage (and do not remember seeing it anywhere else). As you would do, in ChaosBook.org Chap. *Flips, slides and turns* I also define the smallest n to be the *period* of X and refer to the set (2.27) as the *orbit* generated by X . When we get to compact continuous groups, the orbit will be a (great) circle generated by a given Lie algebra element, and look more like what we usually think of as an orbit.

I am not using my own [ChaosBook.org](#) here, not to confuse things further by discussing both time evolution and its discrete symmetries. Here we focus on the discrete group only (typically spatial reflections and finite angle rotations).

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Exercises

- 2.1. $G_x \subset G$. The maximal set of group actions which maps a state space point x into itself,

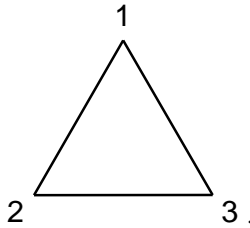
$$G_x = \{g \in G : gx = x\}, \quad (2.28)$$

is called the *isotropy group* (or *stability subgroup* or *little group*) of x . Prove that the set G_x as defined in (2.28) is a subgroup of G .

- 2.2. **Transitivity of conjugation.** Assume that $g_1, g_2, g_3 \in G$ and both g_1 and g_2 are conjugate to g_3 . Prove that g_1 is conjugate to g_2 .
- 2.3. **Isotropy subgroup of gx .** Prove that for $g \in G$, x and gx have conjugate isotropy subgroups:

$$G_{gx} = g G_x g^{-1}$$

- 2.4. **D_3 : symmetries of an equilateral triangle.** Consider group $D_3 \cong C_{3v}$, the symmetry group of an equilateral triangle:



- (a) List the group elements and the corresponding geometric operations
 - (b) Find the subgroups of the group D_3 .
 - (c) Find the classes of D_3 and the number of elements in them, guided by the geometric interpretation of group elements. Verify your answer using the definition of a class.
 - (d) List the conjugacy classes of subgroups of D_3 . (continued as exercise 4.1)
- 2.5. **C_4 invariant potential.** Consider the Schrödinger equation for a particle moving in a two-dimensional bounding potential V , such that the spectrum is discrete. Assume that V is C_N -invariant (in some literature, Z_N -invariant), i.e., V remains invariant under the rotation R by the angle $2\pi/N$. For $N = 3$ case, figure 2.6 (a), the spectrum of the system can be split into two sectors: $\{E_n^0\}$ non-degenerate levels corresponding to symmetric eigenfunctions $\phi_n(Rx) = \phi_n(x)$ and doubly degenerate levels $\{E_n^\pm\}$ corresponding to non-symmetric eigenfunctions $\phi_n(Rx) = e^{\pm 2\pi i/3} \phi_n(x)$.
- (a) What is the spectral structure in the case of $N = 4$, figure 2.6 (b)?
How many sectors appear and what are their degeneracies?
 - (b) What is the spectral structure for general N ?
 - (c) A constant magnetic field normal to the $2D$ plane is added to V .
How will it affect the spectral structure?
 - (d) (bonus question) Figure out the spectral structure if the symmetry group of potential is D_3 (also includes 3 reflections), figure 2.6 (c).

(Boris Gutkin)

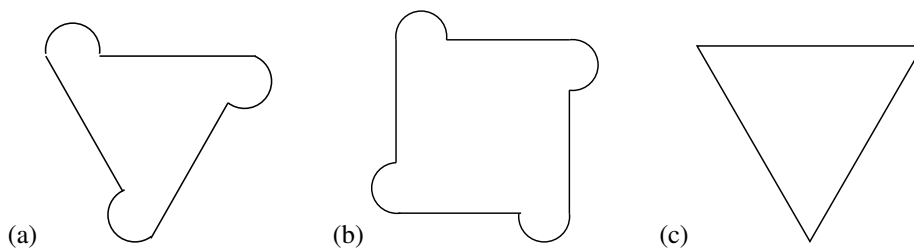


Figure 2.6: Hard wall potential with (a) symmetry C_3 , (b) symmetry C_4 , and (c) symmetry D_3 .

- 2.6. **Permutation of three objects.** Consider S_3 , the group of permutations of 3 objects.
- (a) Show that S_3 is a group.
 - (b) List the conjugacy classes of S_3 .

- (c) Give an interpretation of these classes if the group elements are substitution operations on a set of three objects.
- (c) Give a geometrical interpretation in case of group elements being symmetry operations on equilateral triangle.
- 2.7. **Three masses on a loop.** Three identical masses, connected by three identical springs, are constrained to move on a circle hoop as shown in figure 2.7. Find the normal modes. Hint: write down coupled harmonic oscillator equations, guess the form of oscillatory solutions. Then use basic matrix methods, i.e., find zeros of a characteristic determinant, find the eigenvectors, etc.. (K. Y. Short)

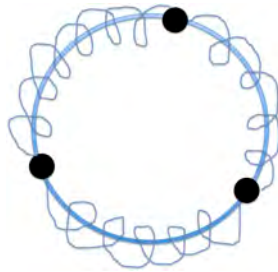


Figure 2.7: Three identical masses are constrained to move on a hoop, connected by three identical springs such that the system wraps completely around the hoop. Find the normal modes.