Phys 7143 zipped!

World Wide Quest to Tame Group Theory

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group theory - week 1

Linear algebra

Georgia Tech PHYS-7143

Homework HW1

due Tuesday, August 29, 2017

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

Exercise 1.1 Trace-log of a matrix	4 points
Exercise 1.2 Stability, diagonal case	2 points
Exercise 1.3 Time-ordered exponentials	4 points

Bonus points

Exercise 1.4 Real representation of complex eigenvalues

4 points

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

2017-08-29 Predrag Lecture 1 Linear algebra - a brief recap

Course start: If I am allowed to teach group theory video (click here), then

read Predrag notes - derivation of $e^{(1)}$ eigenvector; sketch eigenvectors.

Sect. 1.3 Matrix-valued functions

Sect. 1.4 A linear diversion

Sect. 1.5 Eigenvalues and eigenvectors

2017-08-31 Predrag Lecture 2 (with spill over into lecture 3)

Recap from Lecture 1: state Hamilton-Cayley equation, projection operators (1.33), any matrix function is evaluated by spectral decomposition (1.36). Work through example 1.6

Predrag notes: Right (column) and left (row) eigenvectors

Predrag notes on moment of inertia tensor,

Predrag handwritten notes are not on the web, for those stretches you might want to take your own notes in the lecture.

1.1 Special projects

Several people have been interested in taking a **special project**, instead of the final in the course. If you propose to work out in detail some group-theory needed for your own research (but you have not taken the time to master the theory), that would be ideal.

- 1. Here is an example of what an interesting topic would be (i.e., something that Predrag would like to learn from you:) the talk by David Weitz on melting of crystal lattices. Can you do a calculation on a Wigner lattice or a graphene, or a silicon carbide polytype used as a substrate in our graphene lab (ask Claire Berger about it), using our group theory methods as applied to space groups (2-or 3-D lattices)?
- 2. If you are really wild about string theory, then you can read Giles and Thorn [5] Lattice approach to string theory, and write up what you have learned as the project report. The Giles-Thorn (GT) discretization of the worldsheet begins with a representation of the free closed or open string propagator as a light-cone worldsheet path integral defined on a lattice. The sequel Papathanasiou and Thorn [11] Worldsheet propagator on the lightcone worldsheet lattice gives in Appendix B 2D lattice Neumann open string, Dirichlet open string, and closed string propagators. Discrete Green's functions are explained, for example, by Chung and Yau [2] who give explicitly, in their Theorem 6, a 2-dimensional lattice Green's function for a rectangular region R^[\ell_1 × \ell_2]. The paper is cited over 100 times, maybe there is a better, more up-to-date one to read in that list.

I recommend that you take a final, as these are hard and time-consuming projects, and the faculty does not want to overburden you with course work. However, if a project dovetails with your research interests, it might be worth it. Fly it by me.

1.2 Literature

Mopping up operations are the activities that engage most scientists throughout their careers.

- Thomas Kuhn, The Structure of Scientific Revolutions

The subject of linear algebra generates innumerable tomes of its own, and is way beyond what we can exhaustively cover. We have added to the course homepage some linear operators and matrices reading: Stone and P. Goldbart [12], *Mathematics for Physics: A Guided Tour for Graduate Students*, Appendix A. This is an advanced summary where you will find almost everything one needs to know. More pedestrian and perhaps easier to read is Arfken and Weber [1] *Mathematical Methods for Physicists: A Comprehensive Guide*, Chapter 3.

1.3 Matrix-valued functions

What is a matrix? —Werner Heisenberg (1925) What is the matrix? —-Keanu Reeves (1999)

Why should a working physicist care about linear algebra? Physicists were blissfully ignorant of group theory until 1920's, but with Heisenberg's sojourn in Helgoland, everything changed. Quantum Mechanics was formulated as

$$\phi(t) = \hat{U}^t \phi(0), \qquad \hat{U}^t = e^{-\frac{i}{\hbar}tH}, \qquad (1.1)$$

where $\phi(t)$ is the quantum wave function t, \hat{U}^t is the unitary quantum evolution operator, and \hat{H} is the Hamiltonian operator. Fine, but what does this equation *mean*? In the first lecture we deconstruct it, make \hat{U}^t computationally explicit as a the time-ordered product (1.25).

The matrices that have to be evaluated are very high-dimensional, in principle infinite dimensional, and the numerical challenges can quickly get out of hand. What made it possible to solve these equations analytically in 1920's for a few iconic problems, such as the hydrogen atom, are the symmetries, or in other words group theory, which start sketching out in the second lecture (and fill in the details in the next 27 lectures).

Whenever you are confused about an "operator", think "matrix". Here we recapitulate a few matrix algebra concepts that we found essential. The punch line is (1.44): Hamilton-Cayley equation $\prod (\mathbf{M} - \lambda_i \mathbf{1}) = 0$ associates with each distinct root λ_i of a matrix \mathbf{M} a projection onto *i*th vector subspace

$$\mathbf{P}_i = \prod_{j \neq i} \frac{\mathbf{M} - \lambda_j \mathbf{1}}{\lambda_i - \lambda_j}$$

What follows - for this week - is a jumble of Predrag's notes. If you understand the examples, we are on the roll. If not, ask :)

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How are we to think of the quantum operator

$$\hat{H} = \hat{T} + \hat{V}, \qquad \hat{T} = \hat{p}^2/2m, \qquad \hat{V} = V(\hat{q}), \qquad (1.2)$$

corresponding to a classical Hamiltonian H = T + V, where T is kinetic energy, and V is the potential?

Expressed in terms of basis functions, the quantum evolution operator is an infinitedimensional matrix; if we happen to know the eigenbasis of the Hamiltonian, the problem is solved already. In real life we have to guess that some complete basis set is good starting point for solving the problem, and go from there. In practice we truncate such operator representations to finite-dimensional matrices, so it pays to recapitulate a few relevant facts about matrix algebra and some of the properties of functions of finite-dimensional matrices.

Matrix derivatives. The derivative of a matrix is a matrix with elements

$$\mathbf{A}'(x) = \frac{d\mathbf{A}(x)}{dx}, \qquad A'_{ij}(x) = \frac{d}{dx}A_{ij}(x). \tag{1.3}$$

Derivatives of products of matrices are evaluated by the chain rule

$$\frac{d}{dx}(\mathbf{AB}) = \frac{d\mathbf{A}}{dx}\mathbf{B} + \mathbf{A}\frac{d\mathbf{B}}{dx}.$$
(1.4)

A matrix and its derivative matrix in general do not commute

$$\frac{d}{dx}\mathbf{A}^2 = \frac{d\mathbf{A}}{dx}\mathbf{A} + \mathbf{A}\frac{d\mathbf{A}}{dx}.$$
(1.5)

The derivative of the inverse of a matrix, if the inverse exists, follows from $\frac{d}{dx}(\mathbf{A}\mathbf{A}^{-1}) = 0$:

$$\frac{d}{dx}\mathbf{A}^{-1} = -\frac{1}{\mathbf{A}}\frac{d\mathbf{A}}{dx}\frac{1}{\mathbf{A}}.$$
(1.6)

Matrix functions. A function of a single variable that can be expressed in terms of additions and multiplications generalizes to a matrix-valued function by replacing the variable by a matrix.

In particular, the exponential of a constant matrix can be defined either by its series expansion, or as a limit of an infinite product:

$$e^{\mathbf{A}} = \sum_{k=0}^{\infty} \frac{1}{k!} \mathbf{A}^k, \qquad \mathbf{A}^0 = \mathbf{1}$$
(1.7)

$$= \lim_{N \to \infty} \left(\mathbf{1} + \frac{1}{N} \mathbf{A} \right)^N \tag{1.8}$$

The first equation follows from the second one by the binomial theorem, so these indeed are equivalent definitions. That the terms of order $O(N^{-2})$ or smaller do not matter for a function of a single variable follows from the bound

$$\left(1+\frac{x-\epsilon}{N}\right)^N < \left(1+\frac{x+\delta x_N}{N}\right)^N < \left(1+\frac{x+\epsilon}{N}\right)^N,$$

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where $|\delta x_N| < \epsilon$. If $\lim \delta x_N \to 0$ as $N \to \infty$, the extra terms do not contribute. A proof for matrices would probably require defining the norm of a matrix (and, more generally, a norm of an operator acting on a Banach space) first. If you know an easy proof, let us know.

Logarithm of a matrix. The logarithm of a matrix is defined by the power series

$$\ln(\mathbf{1} - \mathbf{A}) = -\sum_{k=1}^{\infty} \frac{\mathbf{A}^k}{k} \,. \tag{1.9}$$

log det = tr log matrix identity. Consider now the determinant

$$\det\left(e^{\mathbf{A}}\right) = \lim_{N \to \infty} \left(\det\left(\mathbf{1} + \mathbf{A}/N\right)\right)^{N} \,.$$

To the leading order in 1/N

det
$$(\mathbf{1} + \mathbf{A}/N) = 1 + \frac{1}{N} \operatorname{tr} \mathbf{A} + O(N^{-2})$$
.

hence

$$\det e^{\mathbf{A}} = \lim_{N \to \infty} \left(1 + \frac{1}{N} \operatorname{tr} \mathbf{A} + O(N^{-2}) \right)^N = \lim_{N \to \infty} \left(1 + \frac{\operatorname{tr} \mathbf{A}}{N} \right)^N = e^{\operatorname{tr} \mathbf{A}} \quad (1.10)$$

Defining $M = e^A$ we can write this as

$$\ln \det M = \operatorname{tr} \ln M \,. \tag{1.11}$$

Functions of several matrices. Due to non-commutativity of matrices, generalization of a function of several variables to a function of several matrices is not as straightforward. Expression involving several matrices depend on their commutation relations. For example, the Baker-Campbell-Hausdorff commutator expansion

$$e^{t\mathbf{A}}\mathbf{B}e^{-t\mathbf{A}} = \mathbf{B} + t[\mathbf{A}, \mathbf{B}] + \frac{t^2}{2}[\mathbf{A}, [\mathbf{A}, \mathbf{B}]] + \frac{t^3}{3!}[\mathbf{A}, [\mathbf{A}, [\mathbf{A}, \mathbf{B}]]] + \cdots$$
 (1.12)

sometimes used to establish the equivalence of the Heisenberg and Schrödinger pictures of quantum mechanics, follows by recursive evaluation of t derivatives

$$\frac{d}{dt} \left(e^{t\mathbf{A}} \mathbf{B} e^{-t\mathbf{A}} \right) = e^{t\mathbf{A}} [\mathbf{A}, \mathbf{B}] e^{-t\mathbf{A}} \,.$$

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Expanding $\exp(A + B)$, $\exp A$, $\exp B$ to first few orders using (1.7) yields

$$e^{(A+B)/N} = e^{A/N} e^{B/N} - \frac{1}{2N^2} [A, B] + O(N^{-3}), \qquad (1.13)$$

and the Trotter product formula: if \mathbf{B} , \mathbf{C} and $\mathbf{A} = \mathbf{B} + \mathbf{C}$ are matrices, then

$$e^{\mathbf{A}} = \lim_{N \to \infty} \left(e^{\mathbf{B}/N} e^{\mathbf{C}/N} \right)^N \tag{1.14}$$

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In particular, we can now make sense of the quantum evolution operator (1.1) as a succession of short free flights (kinetic term) interspersed by small acceleration kicks (potential term),

$$e^{-it\hat{H}} = \lim_{N \to \infty} \left(e^{-i\Delta t \,\hat{T}} e^{-i\Delta t \,\hat{V}} \right)^N \,, \qquad \Delta t = t/N \,, \tag{1.15}$$

where we have set $\hbar = 1$.

1.4 A linear diversion

Linear is good, nonlinear is bad. —Jean Bellissard

(Notes based of ChaosBook.org/chapters/stability.pdf)

Linear fields are the simplest vector fields, described by linear differential equations which can be solved explicitly, with solutions that are good for all times. The state space for linear differential equations is $\mathcal{M} = \mathbb{R}^d$, and the equations of motion are written in terms of a vector x and a constant stability matrix A as

$$\dot{x} = v(x) = Ax. \tag{1.16}$$

Solving this equation means finding the state space trajectory

$$x(t) = (x_1(t), x_2(t), \dots, x_d(t))$$

passing through a given initial point x_0 . If x(t) is a solution with $x(0) = x_0$ and y(t) another solution with $y(0) = y_0$, then the linear combination ax(t) + by(t) with $a, b \in \mathbb{R}$ is also a solution, but now starting at the point $ax_0 + by_0$. At any instant in time, the space of solutions is a *d*-dimensional vector space, spanned by a basis of *d* linearly independent solutions.

How do we solve the linear differential equation (1.16)? If instead of a matrix equation we have a scalar one, $\dot{x} = \lambda x$, the solution is $x(t) = e^{t\lambda}x_0$. In order to solve the *d*-dimensional matrix case, it is helpful to rederive this solution by studying what happens for a short time step Δt . If time t = 0 coincides with position x(0), then

$$\frac{x(\Delta t) - x(0)}{\Delta t} = \lambda x(0), \qquad (1.17)$$

which we iterate m times to obtain Euler's formula for compounding interest

$$x(t) \approx \left(1 + \frac{t}{m}\lambda\right)^m x(0) \approx e^{t\lambda}x(0)$$
. (1.18)

The term in parentheses acts on the initial condition x(0) and evolves it to x(t) by taking m small time steps $\Delta t = t/m$. As $m \to \infty$, the term in parentheses converges to $e^{t\lambda}$. Consider now the matrix version of equation (1.17):

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$$\frac{x(\Delta t) - x(0)}{\Delta t} = Ax(0).$$
(1.19)

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A representative point x is now a vector in \mathbb{R}^d acted on by the matrix A, as in (1.16). Denoting by 1 the identity matrix, and repeating the steps (1.17) and (1.18) we obtain Euler's formula (1.8) for the exponential of a matrix:

$$x(t) = J^{t}x(0), \qquad J^{t} = e^{tA} = \lim_{m \to \infty} \left(\mathbf{1} + \frac{t}{m}A \right)^{m},$$
 (1.20)

where $J^t = J(t)$ is a short hand for $\exp(tA)$. We will find this definition for the exponential of a matrix helpful in the general case, where the matrix A = A(x(t)) varies along a trajectory.

Now that we have some feeling for the qualitative behavior of linear flows, we are ready to return to the nonlinear case. How do we compute the exponential (1.20)?

$$x(t) = f^{t}(x_{0}), \quad \delta x(x_{0}, t) = J^{t}(x_{0}) \,\delta x(x_{0}, 0). \tag{1.21}$$

The equations are linear, so we should be able to integrate them–but in order to make sense of the answer, we derive this integral step by step. The Jacobian matrix is computed by integrating the equations of variations

$$\dot{x}_i = v_i(x), \quad \dot{\delta x}_i = \sum_j A_{ij}(x)\delta x_j$$
(1.22)

Consider the case of a general, non-stationary trajectory x(t). The exponential of a constant matrix can be defined either by its Taylor series expansion or in terms of the Euler limit (1.20):

$$e^{tA} = \sum_{k=0}^{\infty} \frac{t^k}{k!} A^k = \lim_{m \to \infty} \left(1 + \frac{t}{m} A \right)^m.$$
 (1.23)

Taylor expanding is fine if A is a constant matrix. However, only the second, taxaccountant's discrete step definition of an exponential is appropriate for the task at hand. For dynamical systems, the local rate of neighborhood distortion A(x) depends on where we are along the trajectory. The linearized neighborhood is deformed along the flow, and the m discrete time-step approximation to J^t is therefore given by a generalization of the Euler product (1.23):

$$J^{t} = \lim_{m \to \infty} \prod_{n=m}^{1} (1 + \delta t A(x_{n})) = \lim_{m \to \infty} \prod_{n=m}^{1} e^{\delta t A(x_{n})}$$
(1.24)
=
$$\lim_{m \to \infty} e^{\delta t A(x_{m})} e^{\delta t A(x_{m-1})} \cdots e^{\delta t A(x_{2})} e^{\delta t A(x_{1})},$$

where $\delta t = (t - t_0)/m$, and $x_n = x(t_0 + n\delta t)$. Indexing of the products indicates that the successive infinitesimal deformation are applied by multiplying from the left. The $m \to \infty$ limit of this procedure is the formal integral

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$$J_{ij}^t(x_0) = \left[\mathbf{T} e^{\int_0^t d\tau A(x(\tau))} \right]_{ij}, \qquad (1.25)$$

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where **T** stands for time-ordered integration, *defined* as the continuum limit of the successive multiplications (1.24). This integral formula for J^t is the finite time companion of the differential definition. The definition makes evident important properties of Jacobian matrices, such as their being multiplicative along the flow,

$$J^{t+t'}(x) = J^{t'}(x') J^{t}(x), \quad \text{where } x' = f^{t}(x_0), \quad (1.26)$$

which is an immediate consequence of the time-ordered product structure of (1.24). However, in practice J is evaluated by integrating differential equation along with the ODEs that define a particular flow.

1.5 Eigenvalues and eigenvectors

10. Try to leave out the part that readers tend to skip.
 — Elmore Leonard's Ten Rules of Writing.

Eigenvalues of a $[d \times d]$ matrix **M** are the roots of its characteristic polynomial

$$\det \left(\mathbf{M} - \lambda \mathbf{1}\right) = \prod (\lambda_i - \lambda) = 0.$$
(1.27)

Given a nonsingular matrix \mathbf{M} , with all $\lambda_i \neq 0$, acting on *d*-dimensional vectors \mathbf{x} , we would like to determine *eigenvectors* $\mathbf{e}^{(i)}$ of \mathbf{M} on which \mathbf{M} acts by scalar multiplication by eigenvalue λ_i

$$\mathbf{M} \mathbf{e}^{(i)} = \lambda_i \mathbf{e}^{(i)} \,. \tag{1.28}$$

If $\lambda_i \neq \lambda_j$, $\mathbf{e}^{(i)}$ and $\mathbf{e}^{(j)}$ are linearly independent. There are at most *d* distinct eigenvalues and eigenspaces, which we assume have been computed by some method, and ordered by their real parts, $\operatorname{Re} \lambda_i \geq \operatorname{Re} \lambda_{i+1}$.

If all eigenvalues are distinct, $e^{(j)}$ are d linearly independent vectors which can be used as a (non-orthogonal) basis for any d-dimensional vector $\mathbf{x} \in \mathbb{R}^d$

$$\mathbf{x} = x_1 \,\mathbf{e}^{(1)} + x_2 \,\mathbf{e}^{(2)} + \dots + x_d \,\mathbf{e}^{(d)} \,. \tag{1.29}$$

However, r, the number of distinct eigenvalues, is in general smaller than the dimension of the matrix, $r \leq d$ (see example 1.4).

From (1.28) it follows that

$$(\mathbf{M} - \lambda_i \mathbf{1}) \mathbf{e}^{(j)} = (\lambda_j - \lambda_i) \mathbf{e}^{(j)},$$

matrix $(\mathbf{M} - \lambda_i \mathbf{1})$ annihilates $\mathbf{e}^{(i)}$, the product of all such factors annihilates any vector, and the matrix \mathbf{M} satisfies its characteristic equation

$$\prod_{i=1}^{d} (\mathbf{M} - \lambda_i \mathbf{1}) = 0.$$
(1.30)

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This humble fact has a name: the Hamilton-Cayley theorem. If we delete one term from this product, we find that the remainder projects x from (1.29) onto the corresponding eigenspace:

$$\prod_{j\neq i} (\mathbf{M} - \lambda_j \mathbf{1}) \mathbf{x} = \prod_{j\neq i} (\lambda_i - \lambda_j) x_i \mathbf{e}^{(i)} \,.$$

Dividing through by the $(\lambda_i - \lambda_j)$ factors yields the *projection operators*

$$\mathbf{P}_{i} = \prod_{j \neq i} \frac{\mathbf{M} - \lambda_{j} \mathbf{1}}{\lambda_{i} - \lambda_{j}}, \qquad (1.31)$$

which are *orthogonal* and *complete*:

$$\mathbf{P}_i \mathbf{P}_j = \delta_{ij} \mathbf{P}_j, \quad (\text{no sum on } j), \qquad \sum_{i=1}^r \mathbf{P}_i = \mathbf{1}, \qquad (1.32)$$

with the dimension of the *i*th subspace given by $d_i = \operatorname{tr} \mathbf{P}_i$. For each distinct eigenvalue λ_i of \mathbf{M} ,

$$(\mathbf{M} - \lambda_j \mathbf{1}) \mathbf{P}_j = \mathbf{P}_j (\mathbf{M} - \lambda_j \mathbf{1}) = 0, \qquad (1.33)$$

the colums/rows of \mathbf{P}_j are the right/left eigenvectors $\mathbf{e}^{(j)}$, $\mathbf{e}_{(j)}$ of \mathbf{M} which (provided \mathbf{M} is not of Jordan type, see example 1.4) span the corresponding linearized subspace. Once the distinct non-zero eigenvalues $\{\lambda_i\}$ are computed, projection operators are polynomials in \mathbf{M} which need no further diagonalizations or orthogonalizations.

It follows from the characteristic equation (1.33) that λ_i is the eigenvalue of M on \mathbf{P}_i subspace:

$$\mathbf{M} \mathbf{P}_i = \lambda_i \mathbf{P}_i \qquad (\text{no sum on } i). \tag{1.34}$$

Using M = M 1 and completeness relation (1.32) we can rewrite M as

$$\mathbf{M} = \lambda_1 \mathbf{P}_1 + \lambda_2 \mathbf{P}_2 + \dots + \lambda_d \mathbf{P}_d \,. \tag{1.35}$$

Any matrix function $f(\mathbf{M})$ takes the scalar value $f(\lambda_i)$ on the \mathbf{P}_i subspace, $f(\mathbf{M}) \mathbf{P}_i = f(\lambda_i) \mathbf{P}_i$, and is thus easily evaluated through its *spectral decomposition*

$$f(\mathbf{M}) = \sum_{i} f(\lambda_i) \mathbf{P}_i \,. \tag{1.36}$$

This, of course, is the reason why anyone but a fool works with irreducible reps: they reduce matrix (AKA "operator") evaluations to manipulations with numbers.

By (1.33) every column of \mathbf{P}_i is proportional to a right eigenvector $\mathbf{e}^{(i)}$, and its every row to a left eigenvector $\mathbf{e}_{(i)}$. In general, neither set is orthogonal, but by the idempotence condition (1.32), they are mutually orthogonal,

$$\mathbf{e}_{(i)} \cdot \mathbf{e}^{(j)} = c_j \,\delta_i^j \,. \tag{1.37}$$

The non-zero constant c is convention dependent and not worth fixing, unless you feel nostalgic about Clebsch-Gordan coefficients. We shall set c = 1. Then it is convenient to collect all left and right eigenvectors into a single matrix as follows.

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Example 1.1. *Fundamental matrix.* If *A* is constant in time, the system (1.22) is autonomous, and the solution is

$$x(t) = e^{A t} x(0) \,,$$

where $\exp(A t)$ is defined by the Taylor series for $\exp(x)$. As the system is linear, the sum of any two solutions is also a solution. Therefore, given *d* independent initial conditions, $x_1(0), x_2(0), \ldots x_d(0)$ we can write the solution for an arbitrary initial condition based on its projection on to this set,

$$x(t) = \mathbf{F}(t) \mathbf{F}(0)^{-1} x(0) = e^{At} x(0),$$

where $\mathbf{F}(t) = (x_1(t), x_2(t), \dots, x_d(t))$ is a fundamental matrix of the system.

Fundamental matrix (take 1). As the system is a linear, a superposition of any two solutions to $x(t) = J^t x(0)$ is also a solution. One can take any *d* independent initial states, $x^{(1)}(0), x^{(2)}(0), \ldots, x^{(d)}(0)$, assemble them as columns of a matrix $\Phi(0)$, and formally write the solution for an arbitrary initial condition projected onto this basis,

$$x(t) = \Phi(t)\Phi(0)^{-1}x(0)$$
(1.38)

where $\Phi(t) = [x^{(1)}(t), x^{(2)}(t), \dots, x^{(d)}(t)]$. $\Phi(t)$ is called the fundamental matrix of the system, and the Jacobian matrix $J^t = \Phi(t)\Phi(0)^{-1}$ can thus be fashioned out of d trajectories $\{x^{(j)}(t)\}$. Numerically this works for sufficiently short times.

Fundamental matrix (take 2). The set of solutions $x(t) = J^t(x_0)x_0$ for a system of homogeneous linear differential equations $\dot{x}(t) = A(t)x(t)$ of order 1 and dimension d forms a d-dimensional vector space. A basis $\{e^{(1)}(t), \ldots, e^{(d)}(t)\}$ for this vector space is called a fundamental system. Every solution x(t) can be written as

$$x(t) = \sum_{i=1}^{d} c_i \mathbf{e}^{(i)}(t).$$

The $[d \times d]$ matrix $\mathbf{F}_{ii}^{-1} = \mathbf{e}_i^{(j)}$ whose columns are the right eigenvectors of J^t

$$\mathbf{F}(t)^{-1} = (\mathbf{e}^{(1)}(t), \dots, \mathbf{e}^{(d)}(t)), \qquad \mathbf{F}(t)^{T} = (\mathbf{e}_{(1)}(t), \dots, \mathbf{e}_{(d)}(t))$$
(1.39)

is the inverse of a fundamental matrix.

Jacobian matrix. The Jacobian matrix $J^t(x_0)$ is the linear approximation to a differentiable function $f^t(x_0)$, describing the orientation of a tangent plane to the function at a given point and the amount of local rotation and shearing caused by the transformation. The inverse of the Jacobian matrix of a function is the Jacobian matrix of the inverse function. If *f* is a map from *d*-dimensional space to itself, the Jacobian matrix is a square matrix, whose determinant we refer to as the 'Jacobian.'

The Jacobian matrix can be written as transformation from basis at time t_0 to the basis at time t_1 ,

$$J^{t_1-t_0}(x_0) = \mathbf{F}(t_1)\mathbf{F}(t_0)^{-1}.$$
 (1.40)

Then the matrix form of (1.37) is $\mathbf{F}(t)\mathbf{F}(t)^{-1} = \mathbf{1}$, i.e., for zero time the Jacobian matrix is the identity. (J. Halcrow)

exercise 1.4

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Example 1.2. Linear stability of 2-dimensional flows: For a 2-dimensional flow the eigenvalues λ_1, λ_2 of A are either real, leading to a linear motion along their eigenvectors, $x_j(t) = x_j(0) \exp(t\lambda_j)$, or form a complex conjugate pair $\lambda_1 = \mu + i\omega$, $\lambda_2 = \mu - i\omega$, leading to a circular or spiral motion in the $[x_1, x_2]$ plane, see example 1.3.



Figure 1.1: Streamlines for several typical 2dimensional flows: saddle (hyperbolic), in node (attracting), center (elliptic), in spiral.

These two possibilities are refined further into sub-cases depending on the signs of the real part. In the case of real $\lambda_1 > 0$, $\lambda_2 < 0$, x_1 grows exponentially with time, and x_2 contracts exponentially. This behavior, called a saddle, is sketched in figure 1.1, as are the remaining possibilities: in/out nodes, inward/outward spirals, and the center. The magnitude of out-spiral |x(t)| diverges exponentially when $\mu > 0$, and in-spiral contracts into (0,0) when $\mu < 0$; whereas, the phase velocity ω controls its oscillations.

If eigenvalues $\lambda_1 = \lambda_2 = \lambda$ are degenerate, the matrix might have two linearly independent eigenvectors, or only one eigenvector, see example 1.4. We distinguish two cases: (a) *A* can be brought to diagonal form and (b) *A* can be brought to Jordan form, which (in dimension 2 or higher) has zeros everywhere except for the repeating eigenvalues on the diagonal and some 1's directly above it. For every such Jordan $[d_{\alpha} \times d_{\alpha}]$ block there is only one eigenvector per block.

We sketch the full set of possibilities in figures 1.1 and 1.2.

Example 1.3. *Complex eigenvalues: in-out spirals.* As M has only real entries, it will in general have either real eigenvalues, or complex conjugate pairs of eigenvalues. Also the corresponding eigenvectors can be either real or complex. All coordinates used in defining a dynamical flow are real numbers, so what is the meaning of a complex eigenvector?

If λ_k, λ_{k+1} eigenvalues that lie within a diagonal $[2 \times 2]$ sub-block $\mathbf{M}' \subset \mathbf{M}$ form a complex conjugate pair, $\{\lambda_k, \lambda_{k+1}\} = \{\mu + i\omega, \mu - i\omega\}$, the corresponding complex eigenvectors can be replaced by their real and imaginary parts, $\{\mathbf{e}^{(k)}, \mathbf{e}^{(k+1)}\} \rightarrow \{\operatorname{Re} \mathbf{e}^{(k)}, \operatorname{Im} \mathbf{e}^{(k)}\}$. In this 2-dimensional real representation, $\mathbf{M}' \rightarrow A$, the block A is a sum of the rescaling×identity and the generator of SO(2) rotations in the $\{\operatorname{Re} \mathbf{e}^{(1)}, \operatorname{Im} \mathbf{e}^{(1)}\}$ plane.

$$A = \begin{bmatrix} \mu & -\omega \\ \omega & \mu \end{bmatrix} = \mu \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \omega \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

Trajectories of $\dot{\mathbf{x}} = A \mathbf{x}$, given by $\mathbf{x}(t) = J^t \mathbf{x}(0)$, where (omitting $\mathbf{e}^{(3)}, \mathbf{e}^{(4)}, \cdots$ eigendirections)

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$$J^{t} = e^{tA} = e^{t\mu} \begin{bmatrix} \cos \omega t & -\sin \omega t \\ \sin \omega t & \cos \omega t \end{bmatrix},$$
(1.41)

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Figure 1.2: Qualitatively distinct types of exponents $\{\lambda^{(1)}, \lambda^{(2)}\}$ of a $[2 \times 2]$ Jacobian matrix. Here the eigenvalues of the Jacobian matrix are *multipliers* $\Lambda^{(j)}$, and the *exponents* are defined as the deformation rates $\lambda^{(j)} = \log(\Lambda^{(j)})/t$.

spiral in/out around (x, y) = (0, 0), see figure 1.1, with the rotation period T and the radial expansion /contraction multiplier along the $e^{(j)}$ eigen-direction per a turn of the spiral:

$$T = 2\pi/\omega , \qquad \Lambda_{radial} = e^{T\mu} . \tag{1.42}$$

We learn that the typical turnover time scale in the neighborhood of the equilibrium (x, y) = (0, 0) is of order $\approx T$ (and not, let us say, 1000 T, or $10^{-2}T$).

Example 1.4. Degenerate eigenvalues. While for a matrix with generic real elements all eigenvalues are distinct with probability 1, that is not true in presence of symmetries, or spacial parameter values (bifurcation points). What can one say about situation where d_{α} eigenvalues are degenerate, $\lambda_{\alpha} = \lambda_i = \lambda_{i+1} = \cdots = \lambda_{i+d_{\alpha}-1}$? Hamilton-Cayley (1.30) now takes form

$$\prod_{\alpha=1}^{\prime} (\mathbf{M} - \lambda_{\alpha} \mathbf{1})^{d_{\alpha}} = 0, \qquad \sum_{\alpha} d_{\alpha} = d.$$
(1.43)

We distinguish two cases:

M can be brought to diagonal form. The characteristic equation (1.43) can be replaced by the minimal polynomial,

$$\prod_{\alpha=1}^{\prime} (\mathbf{M} - \lambda_{\alpha} \mathbf{1}) = 0, \qquad (1.44)$$

where the product includes each distinct eigenvalue only once. Matrix ${\bf M}$ acts multiplicatively

$$\mathbf{M}\,\mathbf{e}^{(\alpha,k)} = \lambda_i \mathbf{e}^{(\alpha,k)}\,,\tag{1.45}$$

on a d_{α} -dimensional subspace spanned by a linearly independent set of basis eigenvectors $\{e^{(\alpha,1)}, e^{(\alpha,2)}, \cdots, e^{(\alpha,d_{\alpha})}\}$. This is the easy case. Luckily, if the degeneracy is due to a finite or compact symmetry group, relevant \mathbf{M} matrices can always be brought to such Hermitian, diagonalizable form.

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M can only be brought to upper-triangular, Jordan form. This is the messy case, so we only illustrate the key idea in example 1.5.

Example 1.5. Decomposition of 2-dimensional vector spaces: Enumeration of every possible kind of linear algebra eigenvalue / eigenvector combination is beyond what we can reasonably undertake here. However, enumerating solutions for the simplest case, a general $[2 \times 2]$ non-singular matrix

$$\mathbf{M} = \left[\begin{array}{cc} M_{11} & M_{12} \\ M_{21} & M_{22} \end{array} \right]$$

takes us a long way toward developing intuition about arbitrary finite-dimensional matrices. The eigenvalues

$$\lambda_{1,2} = \frac{1}{2} \operatorname{tr} \mathbf{M} \pm \frac{1}{2} \sqrt{(\operatorname{tr} \mathbf{M})^2 - 4 \det \mathbf{M}}$$
(1.46)

are the roots of the characteristic (secular) equation (1.27):

$$\det (\mathbf{M} - \lambda \mathbf{1}) = (\lambda_1 - \lambda)(\lambda_2 - \lambda)$$
$$= \lambda^2 - \operatorname{tr} \mathbf{M} \lambda + \det \mathbf{M} = 0.$$

Distinct eigenvalues case has already been described in full generality. The left/right eigenvectors are the rows/columns of projection operators (see example 1.6)

$$P_1 = \frac{\mathbf{M} - \lambda_2 \mathbf{1}}{\lambda_1 - \lambda_2}, \qquad P_2 = \frac{\mathbf{M} - \lambda_1 \mathbf{1}}{\lambda_2 - \lambda_1}, \qquad \lambda_1 \neq \lambda_2.$$
(1.47)

Degenerate eigenvalues. If $\lambda_1 = \lambda_2 = \lambda$, we distinguish two cases: (a) M can be brought to diagonal form. This is the easy case. (b) M can be brought to Jordan form, with zeros everywhere except for the diagonal, and some 1's directly above it; for a [2×2] matrix the Jordan form is

$$\mathbf{M} = \begin{bmatrix} \lambda & 1\\ 0 & \lambda \end{bmatrix}, \qquad \mathbf{e}^{(1)} = \begin{bmatrix} 1\\ 0 \end{bmatrix}, \quad \mathbf{v}^{(2)} = \begin{bmatrix} 0\\ 1 \end{bmatrix}$$

 $\mathbf{v}^{(2)}$ helps span the 2-dimensional space, $(\mathbf{M} - \lambda)^2 \mathbf{v}^{(2)} = 0$, but is not an eigenvector, as $\mathbf{M}\mathbf{v}^{(2)} = \lambda \mathbf{v}^{(2)} + \mathbf{e}^{(1)}$. For every such Jordan $[d_{\alpha} \times d_{\alpha}]$ block there is only one eigenvector per block. Noting that

$$\mathbf{M}^{m} = \left[\begin{array}{cc} \lambda^{m} & m\lambda^{m-1} \\ 0 & \lambda^{m} \end{array} \right] \,,$$

we see that instead of acting multiplicatively on \mathbb{R}^2 , Jacobian matrix $J^t = \exp(t\mathbf{M})$

$$e^{t\mathbf{M}} \begin{pmatrix} u \\ v \end{pmatrix} = e^{t\lambda} \begin{pmatrix} u + tv \\ v \end{pmatrix}$$
(1.48)

picks up a power-low correction. That spells trouble (logarithmic term $\ln t$ if we bring the extra term into the exponent).

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Example 1.6. *Projection operator decomposition in 2 dimensions:* Let's illustrate how the distinct eigenvalues case works with the $[2 \times 2]$ matrix [8]

$$\mathbf{M} = \left[\begin{array}{cc} 4 & 1 \\ 3 & 2 \end{array} \right] \,.$$

Its eigenvalues $\{\lambda_1, \lambda_2\} = \{5, 1\}$ are the roots of (1.46):

$$\det (\mathbf{M} - \lambda \mathbf{1}) = \lambda^2 - 6\lambda + 5 = (5 - \lambda)(1 - \lambda) = 0$$

That M satisfies its secular equation (Hamilton-Cayley theorem) can be verified by explicit calculation:

4	1]	$^{2}-6$	4	1	15	1	0		0	0]
3	2		3	2 _	+ ³ [0	1	_ [0	0

Associated with each root λ_i is the projection operator (1.47)

$$P_{1} = \frac{1}{4}(\mathbf{M} - \mathbf{1}) = \frac{1}{4} \begin{bmatrix} 3 & 1 \\ 3 & 1 \end{bmatrix}$$
(1.49)

$$P_2 = -\frac{1}{4}(\mathbf{M} - 5 \cdot \mathbf{1}) = \frac{1}{4} \begin{bmatrix} 1 & -1 \\ -3 & 3 \end{bmatrix}.$$
 (1.50)

Matrices \mathbf{P}_i are orthonormal and complete. The dimension of the *i*th subspace is given by $d_i = \operatorname{tr} \mathbf{P}_i$; in case at hand both subspaces are 1-dimensional. From the characteristic equation it follows that \mathbf{P}_i satisfies the eigenvalue equation $\mathbf{M} \mathbf{P}_i = \lambda_i \mathbf{P}_i$. Two consequences are immediate. First, we can easily evaluate any function of \mathbf{M} by spectral decomposition, for example

$$\mathbf{M}^{7} - 3 \cdot \mathbf{1} = (5^{7} - 3)\mathbf{P}_{1} + (1 - 3)\mathbf{P}_{2} = \begin{bmatrix} 58591 & 19531\\ 58593 & 19529 \end{bmatrix}$$

Second, as P_i satisfies the eigenvalue equation, its every column is a right eigenvector, and every row a left eigenvector. Picking first row/column we get the eigenvectors:

- -

$\{\mathbf{e}^{(1)}, \mathbf{e}^{(2)}\}$	=	$\left\{ \begin{bmatrix} 1\\1 \end{bmatrix}, \begin{bmatrix} 1\\-3 \end{bmatrix} \right\}$
$\{{\bf e}_{(1)},{\bf e}_{(2)}\}$	=	$\left\{ \begin{bmatrix} 3\\1 \end{bmatrix}, \begin{bmatrix} 1\\-1 \end{bmatrix} \right\}$

with overall scale arbitrary. The matrix is not symmetric, so $\{e^{(j)}\}\$ do not form an orthogonal basis. The left-right eigenvector dot products $e_{(j)} \cdot e^{(k)}$, however, are orthogonal as in (1.37), by inspection. (Continued in example 1.8.)

Example 1.7. Computing matrix exponentials. If A is diagonal (the system is uncoupled), then e^{tA} is given by



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If A is diagonalizable, $A = FDF^{-1}$, where D is the diagonal matrix of the eigenvalues of A and F is the matrix of corresponding eigenvectors, the result is simple: $A^n = (FDF^{-1})(FDF^{-1}) \dots (FDF^{-1}) = FD^nF^{-1}$. Inserting this into the Taylor series for e^x gives $e^{At} = Fe^{Dt}F^{-1}$.

But *A* may not have *d* linearly independent eigenvectors, making *F* singular and forcing us to take a different route. To illustrate this, consider $[2 \times 2]$ matrices. For any linear system in \mathbb{R}^2 , there is a similarity transformation

$$B = U^{-1}AU.$$

where the columns of U consist of the generalized eigenvectors of A such that B has one of the following forms:

$$B = \begin{bmatrix} \lambda & 0 \\ 0 & \mu \end{bmatrix}, \qquad B = \begin{bmatrix} \lambda & 1 \\ 0 & \lambda \end{bmatrix}, \qquad B = \begin{bmatrix} \mu & -\omega \\ \omega & \mu \end{bmatrix}.$$

These three cases, called normal forms, correspond to *A* having (1) distinct real eigenvalues, (2) degenerate real eigenvalues, or (3) a complex pair of eigenvalues. It follows that

$$e^{Bt} = \begin{bmatrix} e^{\lambda t} & 0\\ 0 & e^{\mu t} \end{bmatrix}, \qquad e^{Bt} = e^{\lambda t} \begin{bmatrix} 1 & t\\ 0 & 1 \end{bmatrix}, \qquad e^{Bt} = e^{at} \begin{bmatrix} \cos bt & -\sin bt\\ \sin bt & \cos bt \end{bmatrix},$$

and $e^{At} = Ue^{Bt}U^{-1}$. What we have done is classify all $[2 \times 2]$ matrices as belonging to one of three classes of geometrical transformations. The first case is scaling, the second is a shear, and the third is a combination of rotation and scaling. The generalization of these normal forms to \mathbb{R}^d is called the Jordan normal form. (J. Halcrow)

Figure 1.3: The stable/unstable manifolds of the equilibrium $(x_q, x_q) = (0, 0)$ of 2-dimensional flow (1.51).



Example 1.8. A simple stable/unstable manifolds pair: Consider the 2-dimensional ODE system

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$$\frac{dx}{dt} = -x, \quad \frac{dy}{dt} = y + x^2, \tag{1.51}$$

The flow through a point $x(0) = x_0, y(0) = y_0$ can be integrated

$$x(t) = x_0 e^{-t}, \quad y(t) = (y_0 + x_0^2/3) e^t - x_0^2 e^{-2t}/3.$$
 (1.52)

Linear stability of the flow is described by the stability matrix

$$\mathbf{A} = \left(\begin{array}{cc} -1 & 0\\ 2x & 1 \end{array}\right) \,. \tag{1.53}$$

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The flow is hyperbolic, with a real expanding/contracting eigenvalue pair $\lambda_1 = 1$, $\lambda_2 = -1$, and area preserving. The right eigenvectors at the point (x, y),

$$\mathbf{e}^{(1)} = \begin{pmatrix} 0\\1 \end{pmatrix}, \quad \mathbf{e}^{(2)} = \begin{pmatrix} 1\\-x \end{pmatrix},$$
 (1.54)

can be obtained by acting with the projection operators (see example 1.5 Decomposition of 2-dimensional vector spaces)

$$\mathbf{P}_{i} = \frac{\mathbf{A} - \lambda_{j} \mathbf{1}}{\lambda_{i} - \lambda_{j}} : \qquad \mathbf{P}_{1} = \begin{bmatrix} 0 & 0\\ x & 1 \end{bmatrix}, \quad \mathbf{P}_{2} = \begin{bmatrix} 1 & 0\\ -x & 0 \end{bmatrix}$$
(1.55)

on an arbitrary vector. Matrices \mathbf{P}_i are orthonormal and complete. The left eigenvectors are

$$\mathbf{e}_{(1)} = (x, 1), \qquad \mathbf{e}_{(2)} = (1, 0), \qquad (1.56)$$

and $\mathbf{e}_{(i)}\mathbf{e}^{(j)} = \delta_i^j$. The flow has a degenerate pair of equilibria at $(x_q, y_q) = (0, 0)$, with eigenvalues (stability exponents), $\lambda_1 = 1$, $\lambda_2 = -1$, eigenvectors $\mathbf{e}^{(1)} = (0, 1)$, $\mathbf{e}^{(2)} = (1, 0)$. The unstable manifold is the *y* axis, and the stable manifold is given by (see figure 1.3)

$$y_0 + \frac{1}{3}x_0^2 = 0 \Rightarrow y(t) + \frac{1}{3}x(t)^2 = 0.$$
 (1.57)

(N. Lebovitz)

1.5.1 Yes, but how do you really do it?

As M has only real entries, it will in general have either real eigenvalues (over-damped oscillator, for example), or complex conjugate pairs of eigenvalues (under-damped oscillator, for example). That is not surprising, but also the corresponding eigenvectors can be either real or complex. All coordinates used in defining the flow are real numbers, so what is the meaning of a *complex* eigenvector?

If two eigenvalues form a complex conjugate pair, $\{\lambda_k, \lambda_{k+1}\} = \{\mu + i\omega, \mu - i\omega\}$, they are in a sense degenerate: while a real λ_k characterizes a motion along a line, a complex λ_k characterizes a spiralling motion in a plane. We determine this plane by replacing the corresponding complex eigenvectors by their real and imaginary parts, $\{\mathbf{e}^{(k)}, \mathbf{e}^{(k+1)}\} \rightarrow \{\operatorname{Re} \mathbf{e}^{(k)}, \operatorname{Im} \mathbf{e}^{(k)}\}$, or, in terms of projection operators:

$$\mathbf{P}_k = \frac{1}{2} (\mathbf{R} + i\mathbf{Q}), \qquad \mathbf{P}_{k+1} = \mathbf{P}_k^*,$$

where $\mathbf{R} = \mathbf{P}_k + \mathbf{P}_{k+1}$ is the subspace decomposed by the *k*th complex eigenvalue pair, and $\mathbf{Q} = (\mathbf{P}_k - \mathbf{P}_{k+1})/i$, both matrices with real elements. Substitution

$$\begin{bmatrix} \mathbf{P}_k \\ \mathbf{P}_{k+1} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & i \\ 1 & -i \end{bmatrix} \begin{bmatrix} \mathbf{R} \\ \mathbf{Q} \end{bmatrix} ,$$

brings the $\lambda_k \mathbf{P}_k + \lambda_{k+1} \mathbf{P}_{k+1}$ complex eigenvalue pair in the spectral decomposition into the real form,

$$\begin{bmatrix} \mathbf{P}_{k} \mathbf{P}_{k+1} \end{bmatrix} \begin{bmatrix} \lambda & 0 \\ 0 & \lambda^{*} \end{bmatrix} \begin{bmatrix} \mathbf{P}_{k} \\ \mathbf{P}_{k+1} \end{bmatrix} = \begin{bmatrix} \mathbf{R} \mathbf{Q} \end{bmatrix} \begin{bmatrix} \mu & -\omega \\ \omega & \mu \end{bmatrix} \begin{bmatrix} \mathbf{R} \\ \mathbf{Q} \end{bmatrix}, \quad (1.58)$$

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where we have dropped the superscript $^{(k)}$ for notational brevity.

To summarize, spectrally decomposed matrix \mathbf{M} acts along lines on subspaces corresponding to real eigenvalues, and as a $[2 \times 2]$ rotation in a plane on subspaces corresponding to complex eigenvalue pairs.

Commentary

Remark 1.1. Projection operators. The construction of projection operators given in sect. 1.5.1 is taken from refs. [3, 4]. Who wrote this down first we do not know, lineage certainly goes all the way back to Lagrange polynomials [10], but projection operators tend to get drowned in sea of algebraic details. Arfken and Weber [1] ascribe spectral decomposition (1.36) to Sylvester. Halmos [6] is a good early reference - but we like Harter's exposition [7–9] best, for its multitude of specific examples and physical illustrations. In particular, by the time we get to (1.33) we have tacitly assumed full diagonalizability of matrix **M**. That is the case for the compact groups we will study here (they are all subgroups of U(n)) but not necessarily in other applications. A bit of what happens then (nilpotent blocks) is touched upon in example 1.5. Harter in his lecture Harter's lecture 5 (starts about min. 31 into the lecture) explains this in great detail - its well worth your time.

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Exercises

1.1. Trace-log of a matrix. Prove that

det
$$M = e^{\operatorname{tr} \ln M}$$

for an arbitrary nonsingular finite dimensional matrix M, det $M \neq 0$.

1.2. **Stability, diagonal case.** Verify that for a diagonalizable matrix *A* the exponential is also diagonalizable

$$J^{t} = e^{tA} = \mathbf{U}^{-1} e^{tA_{D}} \mathbf{U}, \quad A_{D} = \mathbf{U} \mathbf{A} \mathbf{U}^{-1}.$$
(1.59)

1.3. Time-ordered exponentials. Given a time dependent matrix A(t), show that the time-ordered exponential

$$J(t) = \mathbf{T}e^{\int_0^t d\tau A(\tau)}$$

may be written as

$$J(t) = \mathbf{1} + \sum_{m=1}^{\infty} \int_{0}^{t} dt_{1} \int_{0}^{t_{1}} dt_{2} \cdots \int_{0}^{t_{m-1}} dt_{m} A(t_{1}) A(t_{2}) \cdots A(t_{m}). \quad (1.60)$$

(Hint: for a warmup, consider summing elements of a finite-dimensional symmetric matrix $S = S^{\top}$. Use the symmetry to sum over each matrix element once; (1.60) is a continuous limit generalization, for an object symmetric in m variables. If you find this hint confusing, ignore it:) Verify, by using this representation, that J(t) satisfies the equation

$$\dot{J}(t) = A(t)J(t),$$

with the initial condition J(0) = 1.

- 1.4. Real representation of complex eigenvalues. (Verification of example 1.3.) λ_k , λ_{k+1} eigenvalues form a complex conjugate pair, $\{\lambda_k, \lambda_{k+1}\} = \{\mu + i\omega, \mu i\omega\}$. Show that
 - (a) corresponding projection operators are complex conjugates of each other,

$$\mathbf{P} = \mathbf{P}_k, \qquad \mathbf{P}^* = \mathbf{P}_{k+1},$$

where we denote \mathbf{P}_k by \mathbf{P} for notational brevity.

(b) **P** can be written as

$$\mathbf{P} = \frac{1}{2} (\mathbf{R} + i\mathbf{Q}) \,,$$

where $\mathbf{R} = \mathbf{P}_k + \mathbf{P}_{k+1}$ and \mathbf{Q} are matrices with real elements.

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(c)

$$\begin{bmatrix} \mathbf{P}_k \\ \mathbf{P}_{k+1} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & i \\ 1 & -i \end{bmatrix} \begin{bmatrix} \mathbf{R} \\ \mathbf{Q} \end{bmatrix} \, .$$

(d) The $\cdots + \lambda_k \mathbf{P}_k + \lambda_k^* \mathbf{P}_{k+1} + \cdots$ complex eigenvalue pair in the spectral decomposition (1.35) is now replaced by a real [2×2] matrix

$$\cdots + \left[\begin{array}{cc} \mu & -\omega \\ \omega & \mu \end{array} \right] \left[\begin{array}{c} \mathbf{R} \\ \mathbf{Q} \end{array} \right] + \cdots$$

or whatever you find the clearest way to write this real representation.

group theory - week 2

Finite groups - definitions

Georgia Tech PHYS-7143

Homework HW2

due Tuesday, September 5, 2017

== 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 Transitivity of conjugation	1 point
Exercise 2.3 Isotropy subgroup of gx	1 points
Exercise 2.5 C ₄ -invariant potential	7 (+2) points

Total of 10 points = 100 % score.

Bonus points

Exercise 2.X: fix the errors in example 2.3 <i>Vibrational spectra of molecules</i> .	
LaTeX source code	3 points
Exercise 2.8 Three masses on a loop	6 points
Exercise 2.7 An arrangement of five particles	4 points

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

2017-08-29 Predrag Lecture 3 Don't wonna know group theory

Today's example 2.3 whiteboard derivation of normal-modes of the ring of N asymmetric pairs of oscillators is taken from Gutkin lecture notes example 5.1 C_n symmetry. The corresponding projection operators (1.31) are worked out in example 2.4.

2017-08-31 Predrag Lecture 4 Finite groups

Groups, permutations, rearrangement theorem, subgroups, cosets, all exemplified by the $S_3 = C_{3v} = D_3$ symmetries of an equilateral triangle. This lecture follows closely Chapter 1 *Basic Mathematical Background: Introduction* of Dresselhaus *et al.* textbook [1] (click here, ask for password if you have forgotten it). This book (or Tinkham [3]) is good on discrete and space groups, but perhaps not so good on continuous groups. The MIT course 6.734 online version contains much of the same material.

If instead, bedside crocheting is your thing, click here.

2.1 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 sect. A.6 *Gruppenpest* of ref. [2]). 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."

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. Reflection and discrete rotation symmetries:

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

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x) = E_n\psi(x)$$
(2.1)

(see figure 2.1). If $\psi(x)$ is solution then $P\psi(x)$ is also solution. From this and nondegeneracy 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 antisymmetric one. Thus the whole spectrum can be decomposed in accordance to a symmetry of the Hamiltonian (equations of motion).

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Figure 2.1: (left) A reflection-symmetric double-well potential. (right) A 1/3rd-circle rotation-symmetric plane billiard (infinite wall potential in 2D). (B. Gutkin)

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

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

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

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

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

(B. Gutkin)

Example 2.3. 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 $\{\omega_i\}$.

$$x \to y = Ux, \qquad H = \sum_{i=1}^{N} \frac{m_i}{2} \left(\dot{y}_i^2 + \omega_i^2 y_i^2 \right) \,.$$
 (2.2)

Consider now the ring of pair-wise interactions of two kinds of molecules sketched in figure 2.2 (a), given by the potential

$$V(z) = \frac{1}{2} \sum_{i=1}^{N} \left(k_1 (x_i - y_i)^2 + k_2 (x_{i+1} - y_i)^2 \right), \qquad z_i = \begin{pmatrix} x_i \\ y_i \end{pmatrix}, \qquad (2.3)$$

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whose $[2N \times 2N]$ matrix form is (aside for the cognoscenti: kind of a Toeplitz matrix):

	$(k_1 + k_2)$	$-k_1$	0	0	0		0	0	$-k_2$
	$-k_1$	$k_1 + k_2$	$-k_2$	0	0		0	0	0
	0	$-k_2$	$k_1 + k_2$	$-k_1$	0		0	0	0
$V_{ii} = \frac{1}{-}$	0	0	$-k_1$	$k_1 + k_2$	$-k_2$		0	0	0
2		:	:	:	:	۰.	:	:	:
	l .					•			
	0	0	0	0	0		$-k_2$	$k_1 + k_2$	$-k_1$
	$\langle -k_2$	0	0	0	0		0	$-k_1$	$k_1 + k_2$

This potential matrix is a holy mess. How do we find an orthogonal transformation (2.2) that diagonalizes it? Look at figure 2.2 (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



Figure 2.2: (a) Chain with circular symmetry. (b) Dependence of frequency on the representation wavenumber k. (c) Molecule with D_3 symmetry. (B. Gutkin)

$$\underbrace{\begin{pmatrix} 0 & 0 & \dots & 0 & I \\ I & 0 & \dots & 0 & 0 \\ 0 & I & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & I & 0 \end{pmatrix}}_{M} \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ \vdots \\ z_n \end{pmatrix} = \begin{pmatrix} z_n \\ z_1 \\ z_2 \\ \vdots \\ z_{n-1} \end{pmatrix}, \quad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad z_i = \begin{pmatrix} x_i \\ y_i \end{pmatrix} \quad (2.4)$$

Projection operators corresponding to M are worked out in example 2.4. They are N distinct $[2N \times 2N]$ matrices,

$$P_{k} = \begin{pmatrix} I & \bar{\lambda}I & \bar{\lambda}^{2}I & \dots & \bar{\lambda}^{N-2}I & \bar{\lambda}^{N-1}I \\ \lambda I & I & \bar{\lambda}I & \dots & \bar{\lambda}^{N-3}I & \bar{\lambda}^{N-2}I \\ \lambda^{2}I & \lambda I & I & \dots & \bar{\lambda}^{N-4}I & \bar{\lambda}^{N-3}I \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \lambda^{N-2}I & \lambda^{N-3}I & \lambda^{N-4}I & \dots & I & \bar{\lambda}I \\ \lambda^{N-1}I & \lambda^{N-2}I & \lambda^{N-2}I & \dots & \lambda I & I \end{pmatrix}, \qquad \lambda = \exp\left(\frac{2\pi i}{N}k\right)$$
(2.5)

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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 $k = 0, 1, 2, \cdots, N-1$.

The system (2.3) 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 P_k decompose the the interaction potential V as well, and reduce its action to the kth 2-dimensional subspace. Thus the $[2N \times 2N]$ diagonalization (2.2) is now reduced to a $[2 \times 2]$ diagonalization which one can do by hand. The resulting kth space is spanned by two 2N-dimensional vectors, which we guess to be of form:

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

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

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

The corresponding eigenfrequencies are determined by the equation:

$$0 = \det \left(\begin{pmatrix} k_1 + k_2 & -(k_1 + k_2\lambda) \\ -(k_1 + k_2\bar{\lambda}) & k_1 + k_2 \end{pmatrix} - \frac{\omega^2}{2}I \right) \implies \\ \frac{1}{2}\omega_{\pm}^2(k) = k_1 + k_2 \pm |k_1 + k_2\lambda^k|, \qquad (2.6)$$

one acoustic ($\omega(0) = 0$), one optical, see figure 2.2 (b) and the acoustic and optical phonons wiki. (B. Gutkin)

Example 2.4. 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 (1.31), the N distinct eigenvalues of M, the Nth roots of unity $\lambda_n = \lambda^n$, $\lambda = \exp(i2\pi/N)$, $n = 0, \dots N - 1$, split the 2N-dimensional space into N 2-dimensional subspaces by means of projection operators

$$P_n = \prod_{m \neq n} \frac{M - \lambda_m I}{\lambda_n - \lambda_m} = \prod_{m=1}^{N-1} \frac{\lambda^{-n} M - \lambda^m I}{1 - \lambda^m}, \qquad (2.7)$$

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

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

we obtain the projection operator in form of a discrete Fourier sum (rather than the product (1.31)),

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

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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)

Example 2.5. D₃ symmetry: Reflactions and rotations of a triangle, figure 2.2 (c)

$$D(T) = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}, \qquad D(\sigma_1) = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$
(2.8)
$$\begin{pmatrix} 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

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

$$(2.9)$$

$$G = \{[e]; [g, g^2]; [\sigma_1, \sigma_2, \sigma_3]\}, \qquad \chi^{(1)} = \{1, 1, 1\}, \chi^{(2)} = \{1, 1, -1\}, \chi^{(3)} = \{2, -1, 0\}$$
$$r_i = \chi(e)\chi^{(i)}(e)/6; \qquad r_i = \{1, 1, 2\} \implies D = 2E \oplus A_1 \oplus A_2.$$

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

$$P_{1} = \frac{1}{3} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \end{pmatrix}, \qquad P_{2} = \frac{1}{3} \begin{pmatrix} 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$
(2.10)

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

$$P_1 V = \alpha \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}$$
 and $P_2 V = \beta \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}$,

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respectively. Here P_1V represents symmetric mode shown in figure 2.3 (red). The second mode P_2V corresponds to the rotations of the whole system. Finally the projection operator for the two-dimensional representation is

$$P_{3} = \frac{2}{6}(2D(I) - D(T) - D(T^{2})) = \frac{1}{3} \begin{pmatrix} 2 & 0 & -1 & 0 & -1 & 0 \\ 0 & 2 & 0 & -1 & 0 & -1 \\ -1 & 0 & 2 & 0 & -1 & 0 \\ 0 & -1 & 0 & 2 & 0 & -1 \\ -1 & 0 & -1 & 0 & 2 & 0 \\ 0 & -1 & 0 & -1 & 0 & 2 \end{pmatrix}$$
(2.11)

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

$$\eta_{x} = \begin{pmatrix} 1 \\ 0 \\ -1/2 \\ \sqrt{3}/2 \\ -1/2 \\ -\sqrt{3}/2 \end{pmatrix}, \qquad \eta_{y} = \begin{pmatrix} 0 \\ 1 \\ -\sqrt{3}/2 \\ -1/2 \\ \sqrt{3}/2 \\ -1/2 \end{pmatrix}$$
$$P_{3}V = \begin{cases} \alpha \frac{1}{\sqrt{6}} \begin{pmatrix} 2 \\ 0 \\ -1 \\ 0 \\ -1 \\ 0 \\ -1 \\ 0 \end{pmatrix} + \beta \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ -1 \\ 0 \\ -1 \\ 0 \end{pmatrix} + \gamma \frac{1}{\sqrt{6}} \begin{pmatrix} 0 \\ 2 \\ 0 \\ -1 \\ 0 \\ -1 \\ 0 \\ -1 \end{pmatrix} + \delta \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ -1 \\ 0 \\ -1 \end{pmatrix} \right\},$$

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

$$\nu_{1} = \sqrt{3/2}(\xi_{1} - \xi_{4}) = \begin{pmatrix} 1 \\ 0 \\ -1/2 \\ -\sqrt{3}/2 \\ -1/2 \\ \sqrt{3}/2 \end{pmatrix}, \qquad \nu_{2} = \sqrt{3/2}(\xi_{2} + \xi_{3}) = \begin{pmatrix} 0 \\ 1 \\ \sqrt{3}/2 \\ -1/2 \\ -\sqrt{3}/2 \\ -1/2 \\ -\sqrt{3}/2 \\ -1/2 \end{pmatrix}.$$

Figure 2.3: Modes of a molecule with D_3 symmetry. (B. Gutkin)

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(B. Gutkin)

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2.2 Discussion

- **2017-08-31 Michael Meehan** <xmeehan@gatech.edu>, 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?
- **2017-08-31 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.* [1] 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.
- **2017-08-31 Michael Meehan** You talked about the period of an element *X*, and said that that *period* is the *set*

$$\{E, X, \cdots, X^{n-1}\},$$
 (2.12)

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?

2017-09-04 Predrag To keep things as simple as possible, in Thursday's lecture I followed Sect. 1.3 *Basic Definitions* of Dresselhaus *et al.* textbook [1], 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 (2.12) 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 (2.12) 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).

References

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

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- [2] R. Mainieri and P. Cvitanović, "A brief history of chaos", in *Chaos: Classical and Quantum*, edited by P. Cvitanović, R. Artuso, R. Mainieri, G. Tanner, and G. Vattay (Niels Bohr Inst., Copenhagen, 2017).
- [3] M. Tinkham, Group Theory and Quantum Mechanics (Dover, New York, 2003).

Exercises

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

$$G_x = \{g \in G : gx = x\},$$
(2.13)

is called the *isotropy group* (or *stability subgroup* or *little group*) of x. Prove that the set G_x as defined in (2.13) 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. $\underline{\mathbf{D}_3: \text{ symmetries of an equilateral triangle.}}_{\text{group of an equilateral triangle:}}$ Consider group $D_3 \cong C_{3v}$, the symmetry



- (a) List the group elements and the corresponding geometric operations
- (b) Find the subgroups of the group D_3 .
- (c) Find the classes of D₃ 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. C₄-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, i.e., V remains invariant under the rotation R by the angle $2\pi/N$. For N = 3 case, figure 2.4 (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 $\phi_n(Rx) = e^{\pm 2\pi i/3}\phi_n(x)$.

- **Q** 1 What is the spectral structure in the case of N = 4, figure 2.4 (b)? How many sectors appear and what are their degeneracies?
- **Q** 2 What is the spectral structure for general N?
- **Q** 3 A constant magnetic field normal to the 2D plane is added to V. How will it affect the spectral structure?
- ${f Q}$ 4 (bonus question) Figure out the spectral structure if the symmetry group of potential is D₃ (also includes 3 reflections), figure 2.4 (c).

(Boris Gutkin)



Figure 2.4: 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.



Figure 2.5: 4 identical particles of type C lie on the vertices of a square. In the center of the square, but out of the plane, is a particle of type A. (K. Y. Short)

2.7. Arrangement of five particles. Consider the arrangement of particles illustrated in figure 2.5: on each corner (vertex) of a rigid square lies a particle C; in the center of the square, but out of the plane on the z axis, is the particle A.

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- (a) What are the symmetries of this arrangement?
- (b) Find its multiplication table.
- (c) Find its subgroups.
- (d) Determine the corresponding left and right cosets.
- (e) Determine its conjugacy classes.
- (f) Which subgroups are self-conjugate?
- (g) Describe their factor groups.

(K. Y. Short)

2.8. **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 2.6. 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 2.6: 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.
group theory - week 3

Group representations

Georgia Tech PHYS-7143

Exercise 3.3 3-dimensional representations of D_3

Homework HW3

due September 14, 2017

5 points

== 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 3.1 *1-dimensional representation of anything*1 point
Exercise 3.2 2-dimensional representation of S₃

Bonus points

Exercise 3.4 Abelian groups	1 point
Exercise 3.5 Representations of C_N	1 point

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

2017-09-05 Predrag Lecture 5 Representation theory

Irreps, unitary reps and Schur's Lemma.

This lecture covers Chapter 2 *Representation Theory and Basic Theorems* of Dresselhaus *et al.* textbook [1] (click here), up to the proof of Schur's Lemma. The exposition (or the corresponding chapter in Tinkham [2]) comes from Wigner's classic *Group Theory and Its Application to the Quantum Mechanics of Atomic Spectra* [3], which is a harder going, but the more group theory you learn the more you'll appreciate it. Eugene Wigner got the 1963 Nobel Prize in Physics, so by mid 60's gruppenpest was accepted in finer social circles.

2017-09-07 Predrag Lecture 6 Schur's Lemma

This lecture covers Sects. 2.5 and 2.6 *Schur's Lemma* of Dresselhaus *et al.* textbook [1] (click here).

3.1 Literature

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.

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. (Check the previous week notes sect. 5.1 *Literature* for links to the Ree group and the whole classification.)

References

- [1] M. S. Dresselhaus, G. Dresselhaus, and A. Jorio, *Group Theory: Application to the Physics of Condensed Matter* (Springer, New York, 2007).
- [2] M. Tinkham, Group Theory and Quantum Mechanics (Dover, New York, 2003).
- [3] E. P. Wigner, *Group Theory and Its Application to the Quantum Mechanics of Atomic Spectra* (Academic, New York, 1931).

Exercises

3.1. 1-dimensional representation of anything. Let D(g) be a representation of a group G. Show that $d(g) = \det D(g)$ is one-dimensional representation of G as well.

(B. Gutkin)

3.2. **2-dimensional representation of** S_3 **.**

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(i) Show that the group S_3 can be generated by two permutations:

$$a = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix}, \qquad d = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix}$$

(ii) Show that matrices:

$$\rho(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \ \rho(a) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \rho(d) = \begin{pmatrix} z & 0 \\ 0 & z^2 \end{pmatrix},$$

with $z = e^{i2\pi/3}$, provide proper (faithful) representation for these elements and find representation for the remaining elements of the group.

(iii) Is this representation irreducible?

(B. Gutkin)

3.3. **3-dimensional representations of** D_3 . The group D_3 is the symmetry group of the equilateral triangle. It has 6 elements

$$D_3 = \{E, C, C^2, \sigma^{(1)}, \sigma^{(2)}, \sigma^{(3)}\},\$$

where C is rotation by $2\pi/3$ and $\sigma^{(i)}$ is reflection along one of the 3 symmetry axes.

- (i) Prove that this group is isomorphic to S_3
- (ii) Show that matrices

$$\mathcal{D}(E) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \\ \mathcal{D}(C) = \begin{pmatrix} z & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & z^2 \end{pmatrix}, \\ \mathcal{D}(\sigma^{(1)}) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$
(3.1)

generate a 3-dimensional representation \mathcal{D} of D_3 . Hint: Calculate products for representations of group elements and compare with the group table (see lecture).

(iii) Show that this is a reducible representation which can be split into one dimensional A and two-dimensional representation Γ . In other words find a matrix R such that

$$\mathbf{R}\mathcal{D}(g)\mathbf{R}^{-1} = \begin{pmatrix} A(g) & 0\\ 0 & \Gamma(g) \end{pmatrix}$$

for all elements g of D_3 . (Might help: D_3 has only one (non-equivalent) 2-dim irreducible representation).

(B. Gutkin)

3.4. **Abelian groups.** Let *G* be a group with only one-dimensional irreducible representations. Show that *G* is Abelian.

(B. Gutkin)

3.5. Representations of C_N . Find all irreducible representations of C_N .

(B. Gutkin)

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group theory - week 4

Hard work builds character

Georgia Tech PHYS-7143

Homework HW4

due Tuesday, September 19, 2017

== 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.

2017-09-12 Tropic Depression Irma Lecture 7

Character orthogonality theorem

Please study Dresselhaus [1] (click here) sects. 2.7 "Wonderful Orthogonality Theorem," 2.8 "Representations and vector spaces," 3.1 "Definition of Character" and 3.2 "Characters and Class." Tinkham [5] covers the same material in Chapter 3 *Theory of Group Representations*, in a more compact way.

2017-09-14 Predrag Lecture 8

Hard work builds character

Complete Dresselhaus *et al.* [1] (click here) sects. 3.3 "Wonderful Orthogonality Theorem for Characters" to 3.8 "Setting up Character Tables". This material is also covered in Tinkham [5] Chapter 3 *Theory of Group Representations*.

4.1 Literature

I enjoyed reading Mathews and Walker [4] 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 4.1 "Irreps for quaternion multiplication table."

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

Lect. 6 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 ob-

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jects with $D_4 = \langle g, \sigma | g^4 = \sigma^2 = e, g\sigma = \sigma g^3 \rangle$ symmetry, 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 4.1.

Example 4.1. *Quaternions: Quaternion multiplication table is*

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

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 $m_i = 1, i = 1, ...4, m_5 = 2$. 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:

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

References

- 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] L. Landau and E. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory* (Pergamon Press, Oxford, 1959).
- [4] J. Mathews and R. L. Walker, *Mathematical Methods of Physics* (W. A. Benjamin, Reading, MA, 1970).
- [5] M. Tinkham, Group Theory and Quantum Mechanics (Dover, New York, 2003).

Exercises

- 4.1. Characters of D₃. (continued from exercise 2.4) $D_3 \cong C_{3v}$, 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 D₃ as cycles. For example, one of the rotations is (123), meaning that vertex 1 maps to 2, 2 → 3, and 3 → 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 D₃ character table.
 - (d) Two D_3 irreducible representations are one dimensional and the third one of multiplicity 2 is formed by $[2 \times 2]$ matrices. Find the matrices for all six group elements in this representation.
- 4.2. Decompose a representation of S_3 . Consider a reducible representation D(g), i.e., a representation of group element g that after a suitable similarity transformation takes form

$$D(g) = \begin{pmatrix} D^{(a)}(g) & 0 & 0 & 0\\ 0 & D^{(b)}(g) & 0 & 0\\ 0 & 0 & D^{(c)}(g) & 0\\ 0 & 0 & 0 & \ddots \end{pmatrix}$$

with character for class C given by

$$\chi(\mathcal{C}) = c_a \,\chi^{(a)}(\mathcal{C}) + c_b \,\chi^{(b)}(\mathcal{C}) + c_c \,\chi^{(c)}(\mathcal{C}) + \cdots,$$

where c_a , the multiplicity of the *a*th irreducible representation (colloquially called "irrep"), is determined by the character orthonormality relations,

$$c_a = \overline{\chi^{(a)*} \chi} = \frac{1}{h} \sum_{k}^{class} N_k \chi^{(a)}(\mathcal{C}_k^{-1}) \chi(\mathcal{C}_k) \,. \tag{4.1}$$

Knowing characters is all that is needed to figure out what any reducible representation decomposes into!

As an example, 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

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

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- 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 D₄. Dihedral group D₄, 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: D₄ = $\langle g, \sigma | g^4 = \sigma^2 = e, g\sigma = \sigma g^3 \rangle$
 - (a) Find all conjugacy classes.
 - (b) Determine the dimensions of irreducible representations using the relationship

$$\sum_{i} d_i^2 = |G|, \tag{4.2}$$

where d_i is the dimension of *i*th irreducible representation.

- (c) Determine the remaining items of the character table.
- (d) Compare with the character table of quaternions, example 4.1. Are they the same or different?
- (e) Determine the indicators for all irreps of D₄. 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 [3] 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 (4.2), 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.

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- (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 $E_0 \cos(\omega t)$ is added to the system, with 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 $B_0 \cos(\omega t)$ 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 D₄ symmetry. In addition they interact with each other with the term $\lambda W(|\mathbf{r}_1 - \mathbf{r}_2|)$.

- (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)

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.

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. You can learn 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 of 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!).

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Not all finite groups are as simple or easy to figure out as D₃. For example, the order of the Ree group ${}^{2}F_{4}(2)'$ is 212(26+1)(24-1)(23+1)(2-1)/2 = 17971200.

5.2 William G. Harter

Who is Bill 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, 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.

5.3 Discussion

2017-09-25 Lin Xin kin9@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 $g \in SO(3)$ is a rotation, and $D(i)\mathbf{r} = -\mathbf{r}$ is the inversion transformation, then rotation combined with the inversion g i is an improper rotation $g i \in O(3)$. 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] 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).

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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).

- (a) What is the order of the group T_d? Show that the group is isomorphic to i) the group of permutations S₄; 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(φ) = +1), improper (det R(φ) = -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?

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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 "breezing" 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 $P^3 = P_1^3 + P_2^3$. Construct P_{ij}^3 . Verify that they are idempotent.
 - (d) Compute the $[2\times2]$ 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.
 - (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.

group theory - week 6

For fundamentalists

Georgia Tech PHYS-7143

Homework HW6

due Tuesday, October 3, 2017

== 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 6.1 3-disk symbolic dynamics	2 points
Exercise 6.2 Reduction of 3-disk symbolic dynamics to binary	3 points
Exercise 6.3 3-disk fundamental domain cycles	2 points
Exercise 6.4 C_2 -equivariance of Lorenz system	3 points

Bonus points

Exercise 6.5 Proto-Lorenz system

10 points

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

2017-09-26 Predrag Lecture 11 Symmetries and dynamics

So far we have covered what any QM fixated Group Theory textbook since 1930's and on covers. Today to turn to what we actually use group theory for *today*, *here*, in Howey, and for that there is no book but ChaosBook.org.

Many fundamental problems of fluid dynamics and more generally non-linear field theories are studied in experimental settings equipped with symmetries. That is the subject of *dynamical systems theory* (of which classical, quantum and stochastic mechanics and field theories are but specialized branches). We start gently, with perhaps the simplest physical example, the three disk game of pinball.

Read ChaosBook.org Chapter 10 Flips, slides and turns. There is also Chaos-Book.org Appendix 10 Discrete symmetries of dynamics that you probably do not need. You already know much of the material covered in the text, so best to go straight to

example 10.7 Subgroups, cosets of D_3 ,

example 11.6 3-disk game of pinball - symmetry-related orbits,

example 11.7 3-disk game of pinball - cycle symmetries,

example 11.10 3-disk game of pinball in the fundamental domain,

and then work your way backward, if there is something you do not understand off the bat..

2017-09-28 Predrag Lecture 12 Fundamental domain

Lorenz flow example. Read ChaosBook.org Chapter 11 World in a mirror. Maybe start with example 10.6 Equivariance of the Lorenz flow, example 11.8 Desymmetrization of Lorenz flow, and then work your way back if needed.

The reading and the homework for this week, is augmented by - if you find that helpful - by 'live' online blackboard lectures: click here.

6.1 Discussion

Some discussion of eigenfunctions over fundamental domains - maybe of interest to Kevin, but feel free to ignore...

2017-10-05 Predrag Heilman and Strichartz [1] *Homotopies of Eigenfunctions and the Spectrum of the Laplacian on the Sierpinski Carpet*, arXiv:0908.2942, is not an obvious read for us, but they compute a spectrum on a square domain, and we might have to be mindful of it: "Since all of our domains are invariant under the D₄ symmetry group, we can simplify the eigenfunction computations by reducing to a fundamental domain. On this domain we impose appropriate boundary conditions according to the rep-resentation type. For the 1-dimensional representation, we restrict to the sector $0 \le \theta \le \pi/4$. Recall that the functions will extend evenly when reflected about $\theta = 0$ in the 1++ and 1– cases, and oddly in the 1-+ and 1+- cases. Note that performing an even extension across a ray is equivalent to imposing Neumann boundary conditions on that ray. Similarly,

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the odd extension is equivalent to Dirichlet conditions. For the 2-dimensional representation our fundamental domain is the sector $0 \le \theta \le \pi/2$, and we impose Neumann boundary conditions on the ray $\theta = 0$ and Dirichlet conditions on the ray $\theta = \pi/2$. Note that our fundamental domains are simply connected. "

This seems to be saying that one gets the 2-dimensional representation by doubling the fundamental domain and mixing boundary conditions. Do you understand that?

- **2016-02-21 Boris** Here is my present understanding of the fundamental domains issue: If you want simple boundary conditions like Dirichlet or Neumann you stick to 1d representations only. They connect eigenfunction to itself at the fundamental domain boundaries otherwise you would need to connect pair of functions (would be something like boundary conditions for spinor in case of 2d representations.) So what you do is the following: take the largest abelian subgroup $Z_2 \times Z_2$ (for D₄) and split its spectrum with respect to its fundamental domain defined as 1/4 of the square (twice the fundamental domain of the full group). Then your see that Dirichlet-Dirichlet and Neumann-Neumann Hamiltonians still have Z_2 symmetry so your split them further into the Hamiltonians of the 1/8 fundamental domain. But Dirichlet-Neumann remains 1/4th of the square.
- **2016-02-22 Predrag** Your argument is in the spirit of Harter's class operators construction of higher-dimensional representations by using particular chains of subgroups, but I am not able to visualize how that larger fundamental domain (of the lower-order subgroup) folds back into the small fundamental domain of the whole group. How I think of the fundamental domain is explained in my online lectures, Week 14, in particular the snippet Regular representation of permuting tiles. Unfortunately if I had more time, that would have been shorter, this goes on and on, Week 15, lecture 29. *Discrete symmetry factorization*, and by the time the dust settles, I have the symmetry factorization of the determinants that we need, but I do not have a gut feeling for the boundary conditions that you do, when it comes to higher-dimensional irreps.

Copied here are a few snippets from this week's lecture notes, needed here just because exercises refer to them - read the full lecture notes instead.

Definition: Flow invariant subspace. A typical point in fixed-point subspace \mathcal{M}_H moves with time, but, due to equivariance

$$f(gx) = gf(x), \tag{6.1}$$

its trajectory $x(t) = f^t(x)$ remains within $f(\mathcal{M}_H) \subseteq \mathcal{M}_H$ for all times,

$$hf^{t}(x) = f^{t}(hx) = f^{t}(x), \quad h \in H,$$
(6.2)

i.e., it belongs to a *flow invariant subspace*. This suggests a systematic approach to seeking compact invariant solutions. The larger the symmetry subgroup, the smaller \mathcal{M}_H , easing the numerical searches, so start with the largest subgroups H first.



Figure 6.1: (a) The pair of full-space 9-cycles, the counter-clockwise $\overline{121232313}$ and the clockwise $\overline{131323212}$ correspond to (b) one fundamental domain 3-cycle $\overline{001}$.

We can often decompose the state space into smaller subspaces, with group acting within each 'chunk' separately:

Definition: Invariant subspace. $\mathcal{M}_{\alpha} \subset \mathcal{M}$ is an *invariant* subspace if

$$\{\mathcal{M}_{\alpha} \mid gx \in \mathcal{M}_{\alpha} \text{ for all } g \in G \text{ and } x \in \mathcal{M}_{\alpha}\}.$$
(6.3)

 $\{0\}$ and \mathcal{M} are always invariant subspaces. So is any Fix(H) which is point-wise invariant under action of G.

Definition: Irreducible subspace. A space \mathcal{M}_{α} whose only invariant subspaces under the action of G are $\{0\}$ and \mathcal{M}_{α} is called *irreducible*.

Example 6.1. *Equivariance of the Lorenz flow.* The velocity field in Lorenz equations [2]

$$\begin{bmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{bmatrix} = \begin{bmatrix} \sigma(y-x) \\ \rho x - y - xz \\ xy - bz \end{bmatrix} = \begin{pmatrix} -\sigma & \sigma & 0 \\ \rho & -1 & 0 \\ 0 & 0 & -b \end{pmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0 \\ -xz \\ xy \end{bmatrix}$$
(6.4)

is equivariant under the action of cyclic group $C_2 = \{e, C^{1/2}\}$ acting on \mathbb{R}^3 by a π rotation about the *z* axis,

$$C^{1/2}(x, y, z) = (-x, -y, z).$$
 (6.5)

Example 6.2. Desymmetrization of Lorenz flow: (continuation of example 6.1) Lorenz equation (6.4) is equivariant under (6.5), the action of order-2 group $C_2 = \{e, C^{1/2}\}$, where $C^{1/2}$ is [x, y]-plane, half-cycle rotation by π about the *z*-axis:

$$(x, y, z) \to C^{1/2}(x, y, z) = (-x, -y, z).$$
 (6.6)

 $(C^{1/2})^2 = 1$ condition decomposes the state space into two linearly irreducible subspaces $\mathcal{M} = \mathcal{M}^+ \oplus \mathcal{M}^-$, the *z*-axis \mathcal{M}^+ and the [x, y] plane \mathcal{M}^- , with projection operators onto the two subspaces given by

$$\mathbf{P}^{+} = \frac{1}{2}(1+C^{1/2}) = \begin{pmatrix} 0 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{P}^{-} = \frac{1}{2}(1-C^{1/2}) = \begin{pmatrix} 1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 0 \end{pmatrix}.$$
 (6.7)

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Table 6.1: D_3 correspondence between the binary labeled fundamental domain prime cycles \tilde{p} and the full 3-disk ternary labeled cycles p, together with the D_3 transformation that maps the end point of the \tilde{p} cycle into the irreducible segment of the p cycle. White spaces in the above ternary sequences mark repeats of the irreducible segment; for example, the full space 12-cycle 1212 3131 2323 consists of 1212 and its symmetry related segments 3131, 2323. The multiplicity of p cycle is $m_p = 6n_{\tilde{p}}/n_p$. The shortest pair of fundamental domain cycles related by time reversal (but no spatial symmetry) are the 6-cycles $\overline{001011}$ and $\overline{001101}$.

\tilde{p}	p	$\mathbf{g}_{ ilde{p}}$	\tilde{p}	p	$\mathbf{g}_{ ilde{p}}$
0	12	σ_{12}	000001	121212131313	σ_{23}
1	123	C	000011	121212 313131 232323	C^2
01	1213	σ_{23}	000101	121213	e
001	121 232 313	C	000111	121213 212123	σ_{12}
011	121 323	σ_{13}	001011	121232 131323	σ_{23}
0001	1212 1313	σ_{23}	001101	121231 323213	σ_{13}
0011	1212 3131 2323	C^2	001111	121231 232312 313123	C
0111	1213 2123	σ_{12}	010111	121312313231232123	C^2
00001	12121 23232 31313	C	011111	121321 323123	σ_{13}
00011	12121 32323	σ_{13}	0000001	1212121 2323232 3131313	C
00101	12123 21213	σ_{12}	0000011	1212121 3232323	σ_{13}
00111	12123	e	0000101	1212123 2121213	σ_{12}
01011	12131 23212 31323	C	0000111	1212123	e
01111	12132 13123	σ_{23}			

so

$$\begin{pmatrix} \dot{x}_{-} \\ \dot{y}_{-} \end{pmatrix} = \begin{pmatrix} -\sigma & \sigma \\ \rho & -1 \end{pmatrix} \begin{pmatrix} x_{-} \\ y_{-} \end{pmatrix} + \begin{pmatrix} 0 \\ -z x_{-} \end{pmatrix}$$
$$\dot{z}_{+} = -b z_{+} + \frac{1}{4} (x_{+} + x_{-}) (y_{+} + y_{-}) ,$$
(6.8)

where $z_+ = z$. As $(\dot{x}_+, \dot{y}_+) = (0, 0)$, values of (x_+, y_+) are conserved parts of the initial condition. We define the fundamental domain by the (arbitrary) condition $\dot{x}_- \ge 0$, and whenever exits the domain,we replace the function dependence by the corresponding fundamental domain coordinates,

$$(x_-, y_-) = C^{1/2}(\hat{x}_-, \hat{y}_-) = (-\hat{x}_-, -\hat{y}_-)$$
 if $x_- < 0$,

and record that we have applied $C^{1/2}$ (that is the 'reconstruction equation' in the case of a discrete symmetry). When we integrate (6.8), the trajectory coordinates $(\hat{x}_{-}(t), \hat{y}_{-}(t))$ are discontinuous whenever the trajectory crosses the fundamental domain border. That, however, we do not care about - the only thing we need are the Poincaré section points and the Poincaré return map in the fundamental domain.

Poincaré section hypersurface can be specified implicitly by a single condition, through a function U(x) that is zero whenever a point x is on the Poincaré section,

$$\hat{x} \in \mathcal{P} \quad \text{iff} \quad U(\hat{x}) = 0.$$
 (6.9)

In order that there is only one copy of the section in the fundamental domain, this condition has to be invariant, $U(g\hat{x}) = U(\hat{x})$ for $g \in G$, or, equivalently, the normal to it has to be equivariant

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$$\partial_j U(g\hat{x}) = g\partial_j U(\hat{x}) \quad \text{for} \quad g \in G.$$
 (6.10)

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Figure 6.2: (a) Lorenz flow cut by y = x Poincaré section plane \mathcal{P} through the z axis and both $E_{1,2}$ equilibria. Points where flow pierces into section are marked by dots. To aid visualization of the flow near the E_0 equilibrium, the flow is cut by the second Poincaré section, \mathcal{P}' , through y = -x and the z axis. (b) Poincaré sections \mathcal{P} and \mathcal{P}' laid side-by-side. (E. Siminos)

There are two kinds of compact (finite-time) orbits. Periodic orbits $x(T_p) = x(T_p)$ are either self dual under rotation $C^{1/2}$, or appear in pairs related by $C^{1/2}$; in the fundamental domain there is only one copy $\hat{x}(T_p) = \hat{x}(T_p)$ of each. Relative periodic orbits (or 'pre-periodic orbits') $\hat{x}(T_p) = C^{1/2}x(T_p)$ they are periodic orbits.

As the flow is C_2 -invariant, so is its linearization $\dot{x} = Ax$. Evaluated at E_0 , A commutes with $C^{1/2}$, and the E_0 stability matrix A decomposes into [x, y] and z blocks.

The 1-dimensional M^+ subspace is the fixed-point subspace, with the *z*-axis points left point-wise invariant under the group action

$$\mathcal{M}^{+} = \operatorname{Fix}\left(C_{2}\right) = \left\{x \in \mathcal{M} \mid g \, x = x \text{ for } g \in \{e, C^{1/2}\}\right\}$$
(6.11)

(here x = (x, y, z) is a 3-dimensional vector, not the coordinate x). A C_2 -fixed point x(t)in Fix (C_2) moves with time, but according to (6.2) remains within $x(t) \in \text{Fix}(C_2)$ for all times; the subspace $\mathcal{M}^+ = \text{Fix}(C_2)$ is flow invariant. In case at hand this jargon is a bit of an overkill: clearly for (x, y, z) = (0, 0, z) the full state space Lorenz equation (6.4) is reduced to the exponential contraction to the E_0 equilibrium,

$$\dot{z} = -b\,z\,.\tag{6.12}$$

However, for higher-dimensional flows the flow-invariant subspaces can be high-dimensional, with interesting dynamics of their own. Even in this simple case this subspace plays an important role as a topological obstruction: the orbits can neither enter it nor exit it, so the number of windings of a trajectory around it provides a natural, topological symbolic dynamics.

The \mathcal{M}^- subspace is, however, not flow-invariant, as the nonlinear terms $\dot{z} = xy - bz$ in the Lorenz equation (6.4) send all initial conditions within $\mathcal{M}^- = (x(0), y(0), 0)$ into the full, $z(t) \neq 0$ state space $\mathcal{M}/\mathcal{M}^+$.

By taking as a Poincaré section any $C^{1/2}$ -equivariant, non-self-intersecting surface that contains the *z* axis, the state space is divided into a half-space fundamental domain



Figure 6.3: (a) Lorenz attractor plotted in $[\hat{x}, \hat{y}, z]$, the doubled-polar angle coordinates (6.13), with points related by π -rotation in the [x, y] plane identified. Stable eigenvectors of E_0 : $e^{(3)}$ and $e^{(2)}$, along the *z* axis (6.12). Unstable manifold orbit $W^u(E_0)$ (green) is a continuation of the unstable $e^{(1)}$ of E_0 . (b) Blow-up of the region near E_1 : The unstable eigenplane of E_1 defined by $\operatorname{Re} e^{(2)}$ and $\operatorname{Im} e^{(2)}$, the stable eigenvector $e^{(3)}$. The descent of the E_0 unstable manifold (green) defines the innermost edge of the strange attractor. As it is clear from (a), it also defines its outermost edge. (E. Siminos)

 $\tilde{\mathcal{M}} = \mathcal{M}/C_2$ and its 180° rotation $C^{1/2}\tilde{\mathcal{M}}$. An example is afforded by the \mathcal{P} plane section of the Lorenz flow in figure 6.1. Take the fundamental domain $\tilde{\mathcal{M}}$ to be the half-space between the viewer and \mathcal{P} . Then the full Lorenz flow is captured by re-injecting back into $\tilde{\mathcal{M}}$ any trajectory that exits it, by a rotation of π around the *z* axis.

As any such $C^{1/2}$ -invariant section does the job, a choice of a 'fundamental domain' is here largely mater of taste. For purposes of visualization it is convenient to make the double-cover nature of the full state space by $\tilde{\mathcal{M}}$ explicit, through any state space redefinition that maps a pair of points related by symmetry into a single point. In case at hand, this can be easily accomplished by expressing (x, y) in polar coordinates (x, y) = $(r \cos \theta, r \sin \theta)$, and then plotting the flow in the 'doubled-polar angle representation:'

$$(\hat{x}, \hat{y}, z) = (r \cos 2\theta, r \sin 2\theta, z) = ((x^2 - y^2)/r, 2xy/r, z),$$
(6.13)

as in figure 6.1 (a). In contrast to the original *G*-equivariant coordinates [x, y, z], the Lorenz flow expressed in the new coordinates $[\hat{x}, \hat{y}, z]$ is *G*-invariant. In this representation the $\tilde{\mathcal{M}} = \mathcal{M}/C_2$ fundamental domain flow is a smooth, continuous flow, with (any choice of) the fundamental domain stretched out to seamlessly cover the entire $[\hat{x}, \hat{y}]$ plane.

(E. Siminos and J. Halcrow)

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References

- S. M. Heilman and R. S. Strichartz, "Homotopies of eigenfunctions and the spectrum of the Laplacian on the Sierpinski carpet", Fractals 18, 1–34 (2010).
- [2] E. N. Lorenz, "Deterministic nonperiodic flow", J. Atmos. Sci. 20, 130–141 (1963).

Exercises

6.1. **3-disk symbolic dynamics.** As periodic trajectories will turn out to be our main tool to breach deep into the realm of chaos, it pays to start familiarizing oneself with them now by sketching and counting the few shortest prime cycles. Show that the 3-disk pinball has $3 \cdot 2^{n-1}$ itineraries of length *n*. List periodic orbits of lengths 2, 3, 4, 5, \cdots . Verify that the shortest 3-disk prime cycles are 12, 13, 23, 123, 132, 1213, 1232, 1323, 12123, \cdots . Try to sketch them. (continued in exercise 6.3)

A comment about exercise 6.1, exercise 6.2, and exercise 6.3: If parts of these problems seem trivial - they are. The intention is just to check that you understand what these symbolic dynamics codings are - the main message is that the really smart coding (fundamental domain) is 1-to-1 given by the group theory operations that map a point in the fundamental domain to where it is in the full state space. This observation you might not find deep, but it is - instead of *absolute* labels, in presence of symmetries one only needs to keep track of *relative* motions, from domain to domain, does not matter which domain in absolute coordinates - that is what group actions do. And thus the word '*relative*' creeps into this exposition.

- 6.2. Reduction of 3-disk symbolic dynamics to binary. (continued from exercise 6.1)
 - (a) Verify that the 3-disk cycles $\{\overline{12}, \overline{13}, \overline{23}\}, \{\overline{123}, \overline{132}\}, \{\overline{1213} + 2 \text{ perms.}\}, \{\overline{121232313} + 5 \text{ perms.}\}, \{\overline{121323} + 2 \text{ perms.}\}, \dots,$
 - correspond to the fundamental domain cycles $\overline{0}, \overline{1}, \overline{01}, \overline{001}, \overline{011}, \cdots$ respectively.
 - (b) Check the reduction for short cycles in table 6.1 by drawing them both in the full 3-disk system and in the fundamental domain, as in figure 6.1.
 - (c) Optional: Can you see how the group elements listed in table 6.1 relate irreducible segments to the fundamental domain periodic orbits?

(continued in exercise 6.3)

6.3. **3-disk fundamental domain cycles.** Try to sketch $\overline{0}$, $\overline{1}$, $\overline{01}$, $\overline{001}$, $\overline{011}$, \cdots . in the fundamental domain, and interpret the symbols $\{0, 1\}$ by relating them to topologically distinct types of collisions. Compare with table 6.1. Then try to sketch the location of periodic points in the Poincaré section of the billiard flow. The point of this exercise is that while in the configuration space longer cycles look like a hopeless jumble, in the Poincaré section they are clearly and logically ordered. The Poincaré section is always to be preferred to projections of a flow onto the configuration space coordinates, or any other subset of state space coordinates which does not respect the topological organization of the flow.

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6.4. C₂-equivariance of Lorenz system. Verify that the vector field in Lorenz equations (6.4)

$$\dot{x} = v(x) = \begin{bmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{bmatrix} = \begin{bmatrix} \sigma(y-x) \\ \rho x - y - xz \\ xy - bz \end{bmatrix}$$
(6.14)

is equivariant under the action of cyclic group $C_2 = \{e, C^{1/2}\}$ acting on \mathbb{R}^3 by a π rotation about the z axis,

$$C^{1/2}(x, y, z) = (-x, -y, z),$$

as claimed in example 6.1.

- 6.5. **Proto-Lorenz system.** Here we quotient out the C_2 symmetry by constructing an explicit "intensity" representation of the desymmetrized Lorenz flow.
 - 1. Rewrite the Lorenz equation (6.4) in terms of variables $(u, v, z) = (x^2 y^2, 2xy, z)$

$$(u, v, z) = (x^2 - y^2, 2xy, z),$$
 (6.15)

show that it takes form

$$\begin{bmatrix} \dot{u} \\ \dot{v} \\ \dot{z} \end{bmatrix} = \begin{bmatrix} -(\sigma+1)u + (\sigma-r)v + (1-\sigma)N + vz \\ (r-\sigma)u - (\sigma+1)v + (r+\sigma)N - uz - Nz \\ v/2 - bz \end{bmatrix}$$

$$N = \sqrt{u^2 + v^2}.$$
(6.16)

- 2. Show that this is the (Lorenz)/ C_2 quotient map for the Lorenz flow, i.e., that it identifies points related by the π rotation (6.6).
- 3. Show that (6.15) is invertible. Where does the inverse not exist?
- 4. Compute the equilibria of proto-Lorenz and their stabilities. Compare with the equilibria of the Lorenz flow.
- 5. Plot the strange attractor both in the original form (6.4) and in the proto-Lorenz form (6.16)



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for the Lorenz parameter values $\sigma = 10$, b = 8/3, $\rho = 28$. Topologically, does it resemble more the Lorenz, or the Rössler attractor, or neither? (plot by J. Halcrow)

- 7. Show that a periodic orbit of the proto-Lorenz is either a periodic orbit or a relative periodic orbit of the Lorenz flow.
- 8. Show that if a periodic orbit of the proto-Lorenz is also periodic orbit of the Lorenz flow, their Floquet multipliers are the same. How do the Floquet multipliers of relative periodic orbits of the Lorenz flow relate to the Floquet multipliers of the proto-Lorenz?
- 9 Show that the coordinate change (6.15) is the same as rewriting

$$\dot{r} = \frac{r}{2} (-\sigma - 1 + (\sigma + \rho - z) \sin 2\theta + (1 - \sigma) \cos 2\theta)$$

$$\dot{\theta} = \frac{1}{2} (-\sigma + \rho - z + (\sigma - 1) \sin 2\theta + (\sigma + \rho - z) \cos 2\theta)$$

$$\dot{z} = -bz + \frac{r^2}{2} \sin 2\theta. \qquad (6.17)$$

in variables

$$(u,v) = (r^2 \cos 2\theta, r^2 \sin 2\theta)$$

i.e., squaring a complex number z = x + iy, $z^2 = u + iv$.

group theory - week 7

Lorenz to Van Gogh

Georgia Tech PHYS-7143

Homework HW7

due Thursday, October 12, 2017

== 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 7.1 Product of two groups	2 points
Exercise 7.2 Space group	2 points
Work through example 24.2 Unrestricted symbolic dynamics	6 points

Total of 12 points = 100 % score. Extra points accumulate, can help you later if you miss a few problems.

2017-10-03 Predrag Lecture 13 Fundamentalist vision

How I think of the fundamental domain is explained in my online lectures, Week 14, in particular the snippet Regular representation of permuting tiles. Unfortunately - if I had more time, that would have been shorter, this goes on and on, Week 15, lecture 29. *Discrete symmetry factorization*, and by the time the dust settles, I do not have a gut feeling for the boundary conditions when it comes to higher-dimensional irreps (see also last week's sect. 6.1 *Discussion*).

2017-10-05 Predrag Lecture 14 Diffusion confusion

Read ChaosBook.org Chapter 24 *Deterministic diffusion*. You also might find my online lectures, Week 13 helpful. I have also added ChaosBook.org Appendix A24 *Deterministic diffusion*, but you probably do not need to read that.

Exercises

- 7.1. **Product of two groups.** Let G_1 and G_2 be two finite groups. The elements of the product set $\overline{G} = G_1 \times G_2$ are defined as pairs $(g_1, g_2), g_1 \in G_1 g_2 \in G_2$.
 - (a) Show that G is a group with the multiplication operation $(g_1, g_2) \cdot (g'_1, g'_2) = (g_1g'_1, g_2g'_2)$.

Let D_1 be an irreducible representation of G_1 and let D_2 be an irreducible representation of G_2 . For each $g = (g_1, g_2) \in G$ define $D(g) = D_1(g_1) \times D_2(g_2)$

(b) Show that $D = D_1 \times D_2$ is an irreducible representation of G. What are the characters of D?

7.2. Space group.

- (a) Show that for any space group, the translations by vectors from Bravais lattice form a normal subgroup.
- (b) Can rotations of the lattice at a fixed point constitute a normal subgroup of a space group?

(B. Gutkin)

group theory - week 8

Space groups

Georgia Tech PHYS-7143

Homework HW8

due Tuesday, October 17, 2017

== 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 8.1 Band structure of a square lattice

Bonus points Exercise 8.2 *Tight binding model*

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

8 points

8 points

• F • • • • •

2017-10-12 Predrag Lecture 15 Space groups

Gutkin lecture notes Lecture 7 Applications III. Energy Band Structure, Sects. 1. Lattice symmetries and 2. Band structure. Also good reads: Dresselhaus et al. [11] (click here) chapter 9. Space Groups in Real Space, and Cornwell [9] (click here) chapter 7. Crystallographic Space Groups. Walt De Heer learned this stuff from Herzberg [15] Molecular Spectra and Molecular Structure. Condensed matter people like Kittel [21] Introduction to Solid State Physics, but I am not a fan, because simple group theoretical facts are there presented as condensed matter phenomena. Quinn and Yi [24] Solid State Physics: Principles and Modern Applications introduction to space groups looks compact and sensible.

If you are curious about graphene, work out Gutkin lecture notes Lecture 7 *Applications III. Energy Band Structure*, Sect. 7.3 *Band structure of graphene*.

This week's notes are long, because I'm fascinated why –of all fields of physics where problems are formulated on lattices– only condensed matter utilizes the theory of irreps of space groups. For the course itself, read sect. 8.1 *Space groups* and sect. 8.1.1 *Wallpaper groups* - the rest is speculations, mostly.

Why do I care? In this course we are learning theory of space groups as applied to quantum mechanics of crystals - rather than diagonalizing the Hamiltonian and computing energy levels, one works on the reciprocal lattice, and computes energy bands (continuum limit of finely spaced discrete eigenvalues of finite, periodic lattices). If fluctuations from strict periodicity are small, one can often identify the crystal by measuring the intensities of Bragg peaks.

Then there are other kinds of lattices. In computational field theory (classical and quantum) one discretizes the space-time, often on a cubic lattice; one example is worked out here in sect. 8.2 *Elastodynamic equilibria of 2D solids*. The there are Ising models in one, two, three dimensions, problems like deterministic diffusion on periodic lattices of scatterers, coupled maps lattices. None of that literature *ever* (to best of my knowledge) reduces the computations to the reciprocal space Brilluion zone. Why?

The funny thing is - I *know* the answer since 1976, but the siren song of classical crystallography is so enchanting that it has blinded me with science. I think that is due to a deep and under-appreciated "chaos / turbulence" physics underlying these problems. If deviations from the strict periodic structure are *small* (the basic "long wavelength" assumption of sect. 8.2), the "integrable" thinking in terms of normal modes applies, and you should use the crystallography described here. If the symmetry of the law you are studying is a space group, but the deviations of typical solutions are *large* (our deterministic diffusion, Ising models, ...), we have to think again. One fundamental thing we learned in studies of transitions to chaos is that the traditional Fourier analysis is useless - it just yields broad, shapeless continuous spectra. The powerful way to think about these problems is Poincaré's qualitative theory of solutions of differential equations : analyse the geometry of their flows in their *state space*. I know for a fact (from a study of cat maps and spatiotemporal cat maps - those I would have to explain one-on-one, as the papers are unpublished) that in that case the translational eigenfunctions are hyperbolic sinhes and coshes, rather than the sines and cosines we

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are used to as C_n eigenfunctions. For finite discrete symmetries you saw that irreps were fine for linear problems, like coupled arrays of springs, but symmetry reduction for a nonlinear problem like Lorenz equations required quite different techniques. For space group symmetries the analogous nonlinear problems seem still quite unexplored.

8.1 Space groups

A space group, a subgroup of the group of rotations and translations in three dimensions, is the set of transformations that leave a crystal invariant. A space group operator is commonly denoted as

$$\{R|\mathbf{t}\},\tag{8.1}$$

where t belongs to the infinite set of discrete translations, and R is one of the finite number of discrete orientation (point group) symmetries. Translation symmetry, i.e., the periodicity of a crystal, manifests itself physically through phonons, magnons, and other smooth, long-wavelength deformations. Discrete orientation symmetry manifests itself through macroscopic anisotropies of crystals, and its natural faces. The experimental challenge is to determine the crystal structure, typically by diffraction (study of the *reciprocal lattice*). It is a challenge, as one measures only the intensities of Bragg peaks, not their phases, but the answer should be one of the 230 space groups listed in the *International Tables for Crystallography*, the "Bible" of crystallographers.

Unless you have run into a quasicrystal :)

Understanding the Bible requires much more detail than what we can cover in a week or two (it could take a lifetime), and has been written up many places. I found Dresselhaus *et al.* [11] Chapter *9. Space Groups in Real Space* (click here) quite clear on matrix representation of space groups. (The MIT course 6.734 online version contains much of the same material.) I also found Béatrice Grenier's overview over crystallography helpful. Many online tools are available to ease the task, for example the FullProf suite of crystallographic programs. The Bible was completed in 19th century, but the field is undergoing a revival, as the study of topological insulators requires diving deeper into crystallography than simply looking up the tables.

The translation group T, the set of translations t that put the crystallographic structure in coincidence with itself, constitutes the *lattice*. T is a normal subgroup of G. It defines the *Bravais lattice*. Translations are of the form

$$t = t_n = n_1 a_1 + n_2 a_2 + n_3 a_3, \qquad n_i \in \mathbb{Z}.$$

The basis vectors a_j span the *unit cell*. There are 6 simple (or primitive) unit cells that contain a single point, specified by the lengths of the unit translations a, b, c and pairwise angles α, β, γ between them. The most symmetric among them is the *cubic* cell, with a = b = c and $\alpha = \beta = \gamma = 90^{\circ}$.

The lattice unit cell is always a *generating region* (a tile that tiles the entire space), but the smallest generating region *–the fundamental domain–* may be smaller than the lattice unit. At each lattice point the identical group of "atoms" constitutes the *motif.* A *primitive cell* is a minimal region repeated by lattice translations. The lattice and the motif completely characterize the crystal.

The cosets by translation subgroup T (the set all translations) form the *factor* (AKA *quotient*) group G/T, isomorphic to the point group g (rotations). All irreducible representations of a space group G can be constructed from irreducible representations of g and T. This step, however, is tricky, as, due to the non-commutativity of translations and rotations, the quotient group G/T is not a normal subgroup of the space group G.

The quantum-mechanical calculations are executed by approximating the infinite crystal by a triply-periodic one, and going go to the *reciprocal* space by deploying C_{N_j} discrete Fourier transforms. This implements the G/T quotienting by translations and reduces the calculation to a finite *Brilluoin zone*. That is the content of the '*Bloch theorem*' of condensed matter physics. Further work is then required to reduce the calculations to the point group irreps.

Point symmetry operations leave at least one point fixed. They are (a) inversion through a point, (b) rotation around an axis, (c) roto-inversion around an axis and through a point and (d) reflection through a mirror plane. The rotations have to be compatible with the translation symmetry: in 3 spatial dimensions they can only be of orders 1, 2, 3, 4, or 6. They can be proper (det = +1) or improper (det = -1).

The spectroscopists' Schoenflies notation labels point groups as: cyclic C_n , dihedral $C_{n'}$, tetrahedral T and octahedral O rotation point groups, of order n = 1, 2, 3, 4, 6, respectively. The superscript ' refers to either v (parallel mirror plane) or h (perpendicular mirror plane). The crystallographer's preferred classification is, however, the international crystallographic (Hermann-Mauguin) notation.

8.1.1 Wallpaper groups

Pedagogically, it pays to start with a discussion of two-dimensional space groups, or *wallpaper groups* (there are 17 of those).

For wallpaper groups the Hermann-Mauguin notation begins with either p or c, for a primitive cell or a face-centred cell. This is followed by a digit, n, indicating the highest order of rotational symmetry: 1-fold (none), 2-fold, 3-fold, 4-fold, or 6-fold. The first, resp. second of the next two symbols indicates the symmetry relative to one translation axis of the pattern, referred to as the main, resp. second one. The symbols are either m, g, or 1, for mirror, glide reflection, or none.

Section 9.3 Two-Dimensional Space Groups of Dresselhaus et al. [11] discusses the most symmetric of the wallpaper groups, the tiling of a plane by squares, which in the international crystallographic notation is denoted by #11, with point group p4mm. We work out this space group in exercise 8.1. The largest invariant subgroup of C_{4v} is C_4 . In that case, the space group is p4, or #10. Prefix p indicates that the unit cell is primitive (not centered). This is a 'simple', or symmorphic group, which makes calculations easier. There is, however, the third, non-symmorphic two-dimensional square space group p4g or #12 (p4gm), see Table B.10 of ref. [11]. If someone can explain its 'Biblical' diagram to me, I would be grateful. The wiki explanation, reproduced here as figure 8.1 (b), is the best one that I have found so far, but I'm still scratching my head:) The Bravais lattice 'unit cell' is a square in all three cases. In the crystallographic literature the ChaosBook's 'fundamental domain' makes an appearance only in the reciprocal lattice, as the Brilloun zone depicted for p4mm in figure 8.1 (a). However, the 'wallpaper groups' wiki does call 'fundamental domain' the smallest part of



Figure 8.1: The shaded (or yellow) area indicates a *fundamental domain*, i.e., the smallest part of the pattern whose repeats tile the entire plane. (a) For the most symmetric 2D square lattice, with point group p4mm, the fundamental domain is indicated by the shaded triangle $\Gamma \Lambda RSX \Delta \Gamma$ which constitutes 1/8 of the Brillouin zone, and contains the basic wave vectors and the high symmetry points (Fig. 10.2 of Dresselhaus *et al.* [11]). (b) For the 2D square lattice with the glide and reflect point group p4g the fundamental domain is indicated by the yellow triangle (Figure drawn by M. von Gagern).

the configuration pattern that, when repeated, tiles the entire plane.

The quantum-mechanical calculations are carried out in the reciprocal space, in our case with the full Γ point, k = 0, wave vector symmetry (see Table 10.1 of ref. [11]), and 'Large Representations'.

Sect. 10.5 Characters for the Equivalence Representation look like those for the point group, sort of.

8.1.2 One-dimensional line groups

One would think that the one-dimensional *line groups*, which describe systems exhibiting translational periodicity along a line, such as carbon nanotubes, would be simpler still. But even they are not trivial – there are 13 of them.

The normal subgroup of a line group L is its translational subgroup T, with its factor group L/T isomorphic to the *isogonal point group* P of discrete symmetries of its 1-dimensional unit cell $x \in (-a/2, a/2]$. In the reciprocal lattice k takes on the values in the first Brillouin zone interval $(-\pi/a, \pi/a]e$. In *Irreducible representations of the symmetry groups of polymer molecules*. I, Božović, Vujičić and Herbut [7] construct all the reps of the line groups whose isogonal point groups are $C_n, C_{nv}, C_{nh}, S_{2n}$, and D_n . For some of these line groups the irreps are obtained as products of the reps of the translational subgroup and the irreps of the isogonal point group.

According to W. De Heer, the Mintmire, Dunlap and White [23] paper *Are Fullerene tubules metallic*? which took care of chiral rotations for nanotubes by a tight-binding calculation, played a key role in physicists' understanding ofline groups.

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8.1.3 Time reversal symmetry

Consequences of time-reversal symmetry on line groups are discussed by Božović [6]; In the case when the Hamiltonian is invariant under time reversal [14], the symmetry group is enlarged: $L + \theta L$. It is interesting to learn if the degeneracy of the levels is doubled or not.

Johnston [19] Group theory in solid state physics is one of the many reviews that discusses Wigner's time-reversal theorems for a many-electron system, including the character tests for time-reversal degeneracy, the double space groups, and the time-reversal theorems (first discussed by Herring [14] in *Effect of time-reversal symmetry* on energy bands of crystals).

8.2 Elastodynamic equilibria of 2D solids

Artificial lattices are often introduced to formulate classical field theories (described by partial differential equations) and quantum field theories (described by path integrals) as finite-dimensional problems, either for theoretical reasons (QM in a periodic box), or in order to port them to computers. For example, lattice QCD approximates Quantum Chromodynamics by a 4-dimensional cubic crystal. What follows is a simple example of such formulation of a classical field theory, taken from Mehran Kardar's MIT course, Lecture 23.

Consider a perfect two-dimensional solid at T = 0. The equilibrium configuration of atoms forms a lattice,

$$\boldsymbol{r}_0(m,n)=m\boldsymbol{e}_1+n\boldsymbol{e}_2\,,$$

where e_1 and e_2 are basis vectors, $a = |e_j|$ is the lattice spacing, and $\{m, n\}$ are integers. At finite temperatures, the atoms fluctuate away from their equilibrium position, moving to

$$\boldsymbol{r}(m,n) = \boldsymbol{r}_0(m,n) + \boldsymbol{u}(m,n) \,,$$

As the low temperature distortions do not vary substantially over nearby atoms, one can define a coarse-grained distortion field u(x), where $x = (x_1, x_2)$ is treated as continuous, with an implicit short distance cutoff of the lattice spacing a. Due to translational symmetry, the elastic energy depends only on the strain matrix,

$$u_{ij}(\boldsymbol{x}) = \frac{1}{2} \left(\partial_i u_j + \partial_j u_i \right) \,.$$

Kardar picks the triangular lattice, as its elastic energy is isotropic (i.e., invariant under lattice rotations, see Landau and Lifshitz [22]). In terms of the Lamé coefficients λ and μ ,

$$\beta H = \frac{1}{2} \int d^2 \boldsymbol{x} \left(2\mu \, u_{ij} u_{ij} + \lambda \, u_{ii} u_{jj} \right)$$

$$= -\frac{1}{2} \int d^2 \boldsymbol{x} \, u_i \left[2\mu \, \Box \, \delta_{ij} + (\mu + \lambda) \, \partial_i \partial_j \right] u_j \,. \tag{8.2}$$

(here we have assumed either infinite or doubly periodic lattice, so no boundary terms from integration by parts), with the equations of motion something like (FIX!)

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$$\partial_t^2 u_i = \left[2\mu \,\Box \,\delta_{ij} + (\mu + \lambda) \,\partial_i \partial_j\right] u_j \,. \tag{8.3}$$

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(Note that Kardar keeps time continuous, but discretizes space. In numerical computations time is discretized as well.) The symmetry of a square lattice permits an additional term proportional to $\partial_x^2 u_x^2 + \partial_y^2 u_y^2$. In general, the number of independent elastic constants depends on the dimensionality and rotational symmetry of the lattice in question. In two dimensions, square lattices have three independent elastic constants, and triangular lattices are "elastically isotropic" (i.e., elastic properties are independent of direction and thus have only two [22]).

The Goldstone modes associated with the broken (PC: why "broken"?) translational symmetry are *phonons*, the normal modes of vibrations. Eq. (8.3) supports two types of lattice normal modes, transverse and longitudinal.

The order parameter describing broken translational symmetry is

$$\rho_{\boldsymbol{C}}(\boldsymbol{x}) = e^{i \boldsymbol{G} \cdot \boldsymbol{r}(\boldsymbol{x})} = e^{i \boldsymbol{G} \cdot \boldsymbol{u}(\boldsymbol{x})}$$

where G is any reciprocal lattice vector. Since, by definition, $G \cdot r_0$ is an integer multiple of 2π , $\rho_G = 1$ at zero temperature. Due to the fluctuations,

$$\langle \rho_{\boldsymbol{G}}(\boldsymbol{x}) \rangle = \langle e^{i \boldsymbol{G} \cdot \boldsymbol{u}(\boldsymbol{x})} \rangle$$

decreases at finite temperatures, and its correlations decay as $\langle \rho_{\boldsymbol{G}}(\boldsymbol{x}) \rho_{\boldsymbol{G}}^*(\boldsymbol{0}) \rangle$. This is the order parameter ChaosBook and Gaspard use in deriving formulas for deterministic diffusion. Kardar computes this in Fourier space by approximating $\boldsymbol{G} \cdot \boldsymbol{q}$ with its angular average $G^2 q^2/2$, ignoring the rotationally symmetry-breaking term $\cos \boldsymbol{q} \cdot \boldsymbol{x}$, and getting only the asymptotics of the correlations right (the decay is algebraic).

The translational correlations are measured in diffraction experiments. The scattering amplitude is the Fourier transform of ρ_{G} , and the scattered intensity at a wave-vector q is proportional to the structure factor. At zero temperature, the structure factor is a set of delta-functions (Bragg peaks) at the reciprocal lattice vectors.

The orientational order parameter that characterizes the broken rotational symmetry of the crystal can be defined as

$$\Psi(\boldsymbol{x}) = e^{6i\theta(\boldsymbol{x})}$$

where $\theta(\mathbf{x})$ is the angle between local lattice bonds and a reference axis. The factor of 6 accounts for the equivalence of the 6 possible C_{3v} orientations of the triangular lattice. (Kardar says the appropriate choice for a square lattice is $\exp(4i\theta(\mathbf{x}))$ - shouldn't the factor be 8, the order of C_{4v} ?) The order parameter has unit magnitude at T = 0, and is expected to decrease due to fluctuations at finite temperature. The distortion $u(\mathbf{x})$ leads to a change in bond angle given by

$$\theta(\boldsymbol{x}) = -\frac{1}{2} \left(\partial_x u_y - \partial_y u_x \right) \,.$$

(This seems to be dimensionally wrong? For detailed calculations, see the above Kardar lecture notes.)

8.3 Literature, reflections

2017-10-17 Predrag The story of quantum scattering off crystals, I believe, starts with the Bouckaert, Smoluchowski and Wigner (1936) paper [5].

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To understand the order of the full group O_h of symmetries of the cube, exercise 5.1 a.ii, it is instructive to look at figure 8.2 (figs. 8.8 and 8.12 in Joshi [20]). When a cube is a building block that tiles a 3D cubic lattice, it is referred to as the 'elementary' or 'Wigner-Seitz' cell, and its Fourier transform is called 'the first Brillouin zone' in 'the reciprocal space'. The special points and the lines of symmetry in the Brillouin zone are shown in figure 8.2 (a). The tetrahedron $\Gamma X M R$, an 1/48th part of the Brillouin zone, is the fundamental domain, as the action of the 48 elements of the point group O_h on it tiles the Brillouin zone without any gaps or overlaps.



Figure 8.2: (a) The special points and the lines of symmetry in the first Brillouin zone of a simple cubic lattice define its fundamental domain, the tetrahedron ΓXMR . (b) Just not to get any ideas that this is easy: the fundamental domain for the first Brillouin zone of a bcc lattice. (From Joshi [20].)

2016-10-17 Predrag OK, I'll confess. The reason why it is lovely to teach graduate level physics is that one is allowed to learn new things while doing it. I'll now sketch one, perhaps wild, direction that you are completely free to ignore.

Here is the problem of space groups in the nutshell. The Euclidean invariance on Newtonian space-time (including its subgroups, such as the discrete space groups), and the Poincaré invariance of special-relativistic space-time is a strange brew: the space is non-compact (homogeneity), while rotations are compact (isotropy). That leads to the conceptually awkward situation of mixing a group of additions (translations) with a group of multiplications (rotations). To work with such group we *first* translate objects to the *origin* and *then* rotate them with the respect to the origin. That's not nice, because by translation invariance any point is as good as any other, there is no preferred origin. There is no reason why one should translate first, rotate second. What one needs is a formalism that implements translations and rotations on the same footing.

If I understand Hestenes [16] right (also David Finkelstein and perhaps Holger Beck Nielsen have told me things in this spirit) a way to accomplish that is to replace the flat translational directions by a compact manifold where translations and rotations are non-commuting multiplicative group operations.

A part of the Hestenes program is redoing crystallography. I have read Hestenes [17] paper (but not the Hestenes and Holt [18] follow up). It looks very interesting,
but I will spare you from my comments here, as I do not know how to make this formalism work for our purposes (character; explicit computations), so I should not waste your time on that. If you do have a look at his, or at Coxeter [10] discussion of planar tilings, please do report back to me.

- 2016-10-19 Predrag Graphene is a two-dimensional sheet of carbon in which the carbon atoms are arranged in a honeycomb lattice: each carbon atom is connected to three neighbors. It was exfoliated by Schafhaeutl [3, 26] in 1840 (more recently, a con man got a Nobel Prize for that), and formally defined for chemists by Boehm [4] in 1986. In 1947 Wallace [30] calculated the electronic structure of graphene, as a preliminary exercise to calculating electronic structure of graphite, and noted that the velocity of the electrons was independent of their energies: they all travel at the same speed (about 100 km per second, about 1/3000 of the speed of light): plot of the energy of the electrons in graphene as a function of its momentum (which is inversely proportional to its wavelength) is V shaped since the energy of the electron is linearly proportional to its momentum (Wallace [30] Eq. 3.1). The energy of a free electron is proportional to the square of its momentum, but not so in a crystal. As this is reminiscent of massless elementary particles like photons and neutrino's, it has been renamed since 'Dirac cones', but Dirac has nothing whatsoever to do with that. To learn more, talk to people from the Claire Berger and Walt De Heer's group [2] - I have extracted above history of graphene from De Heer's notes (the "con man" is my own angle on what went down with this particular Nobel prize).
- **2017-10-01 Predrag** Martin Mourigal found the Presqu'île Giens, May 2009 *Contribution of Symmetries in Condensed Matter* Summer School very useful. Villain [29] *Symmetry and group theory throughout physics* gives a readable overview. The overheads are here, many of them are of potential interest. Mourigal recommends

Canals and Schober [8] *Introduction to group theory*. It is very concise and precise, a bastard child of Bourbaki and Hamermesh [13]. Space groups show up only once, on p. 24: "By working with the cosets we have effectively factored out the translational part of the problem."

Ballou [1] An introduction to the linear representations of finite groups appears rather formal (and very erudite).

Grenier, B. and Ballou [12] Crystallography: Symmetry groups and group representations.

The word crystal stems from Greek 'krustallas' and means "solidified by the cold."

Schober [27] *Symmetry characterization of electrons and lattice excitations* gives an eminently readable discussion of space groups.

Rodríguez-Carvajal and Bourée [25] Symmetry and magnetic structures

Schweizer [28] *Conjugation and co-representation analysis of magnetic structures* deals with black, white and gray groups that Martin tries not to deal with, so all Mourigal groups are gray. Villain discusses graphene in the Appendix A of *Symmetry and group theory throughout physics* [29].

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Figure 8.3: Square lattice of atoms

Exercises

- 8.1. **Band structure of a square lattice.** A charged particle (without spin) moves in a potential created by an infinite square lattice of atoms, see figure 8.3.
 - (a) What are the symmetry groups of the Bravais and reciprocal lattices?
 - (b) Plot the 1st Brillouin zone. What is its symmetry? What is the corresponding fundamental domain?

Let k be quasi-momentum and $E_n(k)$ the energy of the *n*th band.

- (c) At which points of the Brillouin zone is the group $G^{(k)}$ (the group which leaves vector k invariant) nontrivial? What is it?
- (d) What is the symmetry of $E_n(\mathbf{k})$ as a function of \mathbf{k} ? At which points of the Brillouin zone is the group velocity $\nabla E_n(\mathbf{k})$ equal 0?
- (e) At which points of the Brillouin zone neighboring bands (generically) stick to each other? How many bands can stick? Explain from the group theory prospective.
- (f) Assume now that the lattice is slightly squeezed along one of the axis. What will be the new symmetry of the system and its 1st Brillouin zone? Will the sticking between bands be lifted or persiss?

(B. Gutkin)

- 8.2. Tight binding model. Verify your solution of exercise 8.1 within the 2-state tight binding model. Assume that particle can hop either from corner to corner of the square lattice with coefficient t_1 or from corner to the middle of the square with coefficient t_2 (and vice versa).
 - (a) Show the obtained energy bands $E_i(\mathbf{k})$ as both contour- and 3-dimensional plots.
 - (b) Compare with the results from exercise 8.1.

group theory - week 9

Continuous groups

Georgia Tech PHYS-7143

Homework HW9

due Tuesday, October 24, 2017

== 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 9.1 Irreps of $SO(2)$	2 points
Exercise 9.2 Reduction of product of two $SO(2)$ irreps	1 point
Exercise 9.3 Irreps of $O(2)$	2 points
Exercise 9.4 Reduction of product of two $O(2)$ irreps	1 point
Exercise 9.5 A fluttering flame front	4 points

Bonus points

Exercise 9.6 O(2) fundamental domain for Kuramoto-Sivashinsky equation (difficult) 10 points

Total of 10 points = 100 % score.

2017-10-17 Predrag Lecture 16 Continuous groups

This lecture is not taken from any particular book, it's about basic ideas of how one goes from finite groups to the continuous ones that any physicist should know. The main idea comes from discrete groups. We have worked one example out in week 2, the discrete Fourier transform of example 2.4 *Projection operators for cyclic group* C_N . The cyclic group C_N is generated by the powers of the rotation by $2\pi/N$, and in general, in the $N \to \infty$ limit one only needs to understand the algebra of T_{ℓ} , generators of infinitesimal transformations, $D(\theta) = 1 + i \sum_{\ell} \theta_{\ell} T_{\ell}$. Applied to functions, they turn out to be partial derivatives.

2017-10-19 Predrag Lecture 17 Lie groups. Matrix representations

The $N \to \infty$ limit of C_N gets you to the continuous Fourier transform as a representation of $U(1) \simeq SO(2)$, but from then on this way of thinking about continuous symmetries gets to be increasingly awkward. So we need a fresh restart; that is afforded by matrix groups, and in particular the unitary group $U(n) = U(1) \otimes SU(n)$, which contains all other compact groups, finite or continuous, as subgroups.

Reading: Chen, Ping and Wang [6] *Group Representation Theory for Physicists*, Sect 5.2 *Definition of a Lie group, with examples*.

Reading: C. K. Wong Group Theory notes, Chap 6 1D continuous groups, Sects. 6.1-6.3 Irreps of SO(2). In particular, note that while geometrically intuitive representation is the set of rotation $[2 \times 2]$ matrices, they split into pairs of 1-dimensional irreps. Also, not covered in the lectures, but worth a read: Sect. 6.6 completes discussion of Fourier analysis as continuum limit of cyclic groups C_n , compares SO(2), discrete translations group, and continuous translations group.

Sect. 9.1 that follows is a very condensed extract of chapters 3 *Invariants and reducibility* and 4 *Diagrammatic notation* from *Group Theory - Birdtracks, Lie's, and Exceptional Groups* [8]. I am usually reluctant to use birdtrack notations in front of graduate students indoctrinated by their professors in the 1890's tensor notation, but today I'm emboldened by the very enjoyable article on *The new language of mathematics* by Dan Silver [16]. 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 Crimsons of their youth. You chill to beats younger than Windows 98, to grime, to trap, to hardvapour, to birdtracks.

9.1 Lie groups for pedestrians

[...] which is an expression of consecration of angular momentum.

- Mason A. Porter's student

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Figure 9.1: Circle group $S^1 = SO(2)$, the symmetry group of a circle with directed rotations, is a compact group, as its natural parametrization is either the angle $\phi \in [0, 2\beta)$, or the perimeter $x \in [0, L)$.

Definition: A Lie group is a topological group G such that (i) G has the structure of a smooth differential manifold, and (ii) the composition map $G \times G \to G : (g, h) \to gh^{-1}$ is smooth, i.e., \mathbb{C}^{∞} differentiable.

Do not be mystified by this definition. Mathematicians also have to make a living. The compact Lie groups that we will deploy here are a generalization of the theory of $SO(2) \simeq U(1)$ rotations, i.e., Fourier analysis. By a 'smooth differential manifold' one means objects like the circle of angles that parameterize continuous rotations in a plane, figure 9.1, or the manifold swept by the three Euler angles that parameterize SO(3) rotations.

By 'compact' one means that these parameters run over finite ranges, as opposed to parameters in hyperbolic geometries, such as Minkowsky SO(3, 1). The groups we focus on here are compact by default, as their representations are linear, finite-dimensional matrix subgroups of the unitary matrix group U(d).

Example 1. Circle group. A circle with a direction, figure 9.1, is invariant under rotation by any angle $\theta \in [0, 2\pi)$, and the group multiplication corresponds to composition of two rotations $\theta_1 + \theta_2 \mod 2\pi$. The natural representation of the group action is by a complex numbers of absolute value 1, i.e., the exponential $e^{i\theta}$. The composition rule is then the complex multiplication $e^{i\theta_2}e^{i\theta_1} = e^{i(\theta_1+\theta_2)}$. The circle group is a *continuous group*, with infinite number of elements, parametrized by the continuous parameter $\theta \in [0, 2\pi)$. It can be thought of as the $n \to \infty$ limit of the cyclic group C_n . Note that the circle divided into n segments is *compact*, in distinction to the infinite lattice of integers \mathbb{Z} , whose limit is a *line* (noncompact, of infinite length).

An element of a $[d \times d]$ -dimensional matrix representation of a *Lie group* continuously connected to identity can be written as

$$g(\boldsymbol{\phi}) = e^{i\boldsymbol{\phi}\cdot T}, \qquad \boldsymbol{\phi}\cdot T = \sum_{a=1}^{N} \phi_a T_a, \qquad (9.1)$$

where $\phi \cdot T$ is a *Lie algebra* element, T_a are matrices called 'generators', and $\phi = (\phi_1, \phi_2, \dots, \phi_N)$ are the parameters of the transformation. Repeated indices are summed

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throughout, and the dot product refers to a sum over Lie algebra generators. Sometimes it is convenient to use the Dirac bra-ket notation for the Euclidean product of two real vectors $x, y \in \mathbb{R}^d$, or the product of two complex vectors $x, y \in \mathbb{C}^d$, i.e., indicate complex *x*-transpose times *y* by

$$\langle x|y\rangle = x^{\dagger}y = \sum_{i}^{d} x_{i}^{*}y_{i} \,. \tag{9.2}$$

Finite unitary transformations $\exp(i\phi \cdot T)$ are generated by sequences of infinitesimal steps of form

$$g(\boldsymbol{\delta}\boldsymbol{\phi}) \simeq 1 + i\boldsymbol{\delta}\boldsymbol{\phi} \cdot T, \quad \boldsymbol{\delta}\boldsymbol{\phi} \in \mathbb{R}^N, \quad |\boldsymbol{\delta}\boldsymbol{\phi}| \ll 1,$$
 (9.3)

where T_a , the *generators* of infinitesimal transformations, are a set of linearly independent $[d \times d]$ hermitian matrices (see figure 9.2 (b)).

The reason why one can piece a global transformation from infinitesimal steps is that the choice of the "origin" in coordinatization of the group manifold sketched in figure 9.2 (a) is arbitrary. The coordinatization of the tangent space at one point on the group manifold suffices to have it everywhere, by a coordinate transformation g, i.e., the new origin y is related to the old origin x by conjugation $y = g^{-1}xg$, so all tangent spaces belong the same class, they are geometrically equivalent.

Unitary and orthogonal groups are defined as groups that preserve 'length' norms, $\langle gx|gx\rangle = \langle x|x\rangle$, and infinitesimally their generators (9.3) induce no change in the norm, $\langle T_ax|x\rangle + \langle x|T_ax\rangle = 0$, hence the Lie algebra generators T_a are hermitian for,

$$T_a^{\dagger} = T_a \,. \tag{9.4}$$

The flow field at the state space point x induced by the action of the group is given by the set of N tangent fields

$$t_a(x)_i = (T_a)_{ij} x_j \,, \tag{9.5}$$

which span the *d*-dimensional group tangent space at state space point x, parametrized by $\delta\phi$.

For continuous groups the Lie algebra, i.e., the algebra spanned by the set of N generators T_a of infinitesimal transformations, takes the role that the |G| group elements play in the theory of discrete groups (see figure 9.2).

9.1.1 Invariants

One constructs the irreps of finite groups by identifying matrices that commute with all group elements, and using their eigenvalues to decompose arbitrary representation of the group into a unique sum of irreps. The same strategy works for the compact Lie groups, (9.9), and is indeed the key idea that distinguishes the invariance groups classification developed in *Group Theory - Birdtracks, Lie's, and Exceptional Groups* [8] from the 19th century Cartan-Killing classification of Lie algebras.

Definition. The vector $q \in V$ is an *invariant vector* if for any transformation $g \in \mathcal{G}$

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$$q = Gq. (9.6)$$

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Figure 9.2: (a) Lie algebra fields $\{t_1, \dots, t_N\}$ span the tangent space of the group orbit \mathcal{M}_x at state space point x, see (9.5) (figure from WikiMedia.org). (b) A global group transformation $g: x \to x'$ can be pieced together from a series of infinitesimal steps along a continuous trajectory connecting the two points. The group orbit of state space point $x \in \mathbb{R}^d$ is the N-dimensional manifold of all actions of the elements of group G on x.

Definition. A tensor $x \in V^p \otimes \overline{V}^q$ is an *invariant tensor* if for any $g \in G$

$$x_{b_1\dots b_q}^{a_1 a_2\dots a_p} = G^{a_1}{}_{c_1} G^{a_2}{}_{c_2}\dots G_{b_1}{}^{d_1}\dots G_{b_q}{}^{d_q} x_{d_1\dots d_q}^{c_1 c_2\dots c_p} .$$
(9.7)

If a bilinear form $m(\bar{x}, y) = x^a M_a{}^b y_b$ is invariant for all $g \in \mathcal{G}$, the matrix

$$M_a{}^b = G_a{}^c G^b{}_d M_c{}^d \tag{9.8}$$

is an *invariant matrix*. Multiplying with G_b^e and using the unitary, we find that the invariant matrices *commute* with all transformations $g \in \mathcal{G}$:

$$[G,\mathbf{M}] = 0. \tag{9.9}$$

Definition. An *invariance group* G is the set of all linear transformations (9.7) that preserve the primitive invariant relations (and, by extension, *all* invariant relations)

$$p_1(x,\bar{y}) = p_1(Gx,\bar{y}G^{\mathsf{T}}) p_2(x,y,z,...) = p_2(Gx,Gy,Gz...), \qquad (9.10)$$

Unitarity guarantees that all contractions of primitive invariant tensors, and hence all composed tensors $h \in H$, are also invariant under action of \mathcal{G} . As we assume unitary \mathcal{G} , it follows that the list of primitives must always include the Kronecker delta.

Example 2. If $p^a q_a$ is the only invariant of \mathcal{G}

$$p'^{a}q'_{a} = p^{b}(G^{\dagger}G)_{b}{}^{c}q_{c} = p^{a}q_{a}, \qquad (9.11)$$

then \mathcal{G} is the full *unitary group* U(n) (invariance group of the complex norm $|x|^2 = x^b x_a \delta^a_b$), whose elements satisfy

$$G^{\dagger}G = 1. \tag{9.12}$$

Example 3. If we wish the z-direction to be invariant in our 3-dimensional space, q = (0, 0, 1) is an invariant vector (9.6), and the invariance group is O(2), the group of all rotations in the x-y plane.

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9.1.2 Discussion

- 2017-11-07 Qimen Xu Please explain when one keeps track of the order of tensorial indices?
- **2017-11-07 Predrag** In a tensor, upper, lower indices are separately ordered and that order matters. The simplest example: if some indices form an antisymmetric pair, writing them in wrong order gives you a wrong sign. In a matrix representation of a group action, one has to distinguish between the "in" set of indices the ones that get contracted with the initial tensor, and the "out" set of indices that label the tensor after the transformation. Only if the matrix is Hermitian the order does not matter. If you understand Eq. (3.22) in birdtracks.eu, you get it. Does that answer your question?

9.1.3 Infinitesimal transformations, Lie algebras

A unitary transformation G infinitesimally close to unity can be written as

$$G_a{}^b = \delta^b_a + iD^b_a \,, \tag{9.13}$$

where D is a hermitian matrix with small elements, $|D_a^b| \ll 1$. The action of $g \in \mathcal{G}$ on the conjugate space is given by

$$(G^{\dagger})_b{}^a = G^a{}_b = \delta^a_b - iD^a_b.$$
(9.14)

D can be parametrized by $N \le n^2$ real parameters. *N*, the maximal number of independent parameters, is called the *dimension* of the group (also the dimension of the Lie algebra, or the dimension of the adjoint rep).

Here we shall consider only infinitesimal transformations of form G = 1 + iD, $|D_b^a| \ll 1$. We do not study the entire group of invariant transformation, but only the transformations connected to the identity. For example, we shall not consider invariances under coordinate reflections.

The generators of infinitesimal transformations (9.13) are hermitian matrices and belong to the $D_b^a \in V \otimes \overline{V}$ space. However, not any element of $V \otimes \overline{V}$ generates an allowed transformation; indeed, one of the main objectives of group theory is to define the class of allowed transformations.

This subspace is called the *adjoint* space, and its special role warrants introduction of special notation. We shall refer to this vector space by letter A, in distinction to the defining space V. We shall denote its dimension by N, label its tensor indices by $i, j, k \dots$, denote the corresponding Kronecker delta by a thin, straight line,

$$\delta_{ij} = i - j, \qquad i, j = 1, 2, \dots, N,$$
(9.15)

and the corresponding transformation generators by

$$(C_A)_i, {}^a_b = \frac{1}{\sqrt{a}} (T_i)^a_b = i - \underbrace{\int}^a_b a, b = 1, 2, \dots, n$$

 $i = 1, 2, \dots, N.$

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Matrices T_i are called the *generators* of infinitesimal transformations. Here a is an (uninteresting) overall normalization fixed by the orthogonality condition

$$(T_i)^a_b(T_j)^b_a = \operatorname{tr}(T_iT_j) = a\,\delta_{ij}$$

$$- \underbrace{\bigcirc}_{a \ } = a \ - \underbrace{\frown}_{a \ }. \tag{9.16}$$

For every invariant tensor q, the infinitesimal transformations G = 1 + iD must satisfy the invariance condition (9.6). Parametrizing D as a projection of an arbitrary hermitian matrix $H \in V \otimes \overline{V}$ into the adjoint space, $D = \mathbf{P}_A H \in V \otimes \overline{V}$,

$$D_b^a = \frac{1}{a} (T_i)_b^a \epsilon_i , \qquad (9.17)$$

we obtain the *invariance condition* which the *generators* must satisfy: they *annihilate* invariant tensors:

$$T_i q = 0. (9.18)$$

To state the invariance condition for an arbitrary invariant tensor, we need to define the action of generators on the tensor reps. By substituting $G = 1 + i\epsilon \cdot T + O(\epsilon^2)$ and keeping only the terms linear in ϵ , we find that the generators of infinitesimal transformations for tensor reps act by touching one index at a time:

$$(T_{i})_{b_{1}...b_{q}}^{a_{1}a_{2}...a_{p}}, \frac{d_{q}...d_{1}}{c_{p}...c_{2}c_{1}} = (T_{i})_{c_{1}}^{a_{1}}\delta_{c_{2}}^{a_{2}}\ldots\delta_{c_{p}}^{a_{p}}\delta_{b_{1}}^{d_{1}}\ldots\delta_{b_{q}}^{d_{q}}$$
$$+\delta_{c_{1}}^{a_{1}}(T_{i})_{c_{2}}^{a_{2}}\ldots\delta_{c_{p}}^{a_{p}}\delta_{b_{1}}^{d_{1}}\ldots\delta_{b_{q}}^{d_{q}} + \ldots + \delta_{c_{1}}^{a_{1}}\delta_{c_{2}}^{a_{2}}\ldots(T_{i})_{c_{p}}^{a_{p}}\delta_{b_{1}}^{d_{1}}\ldots\delta_{b_{q}}^{d_{q}}$$
$$-\delta_{c_{1}}^{a_{1}}\delta_{c_{2}}^{a_{2}}\ldots\delta_{c_{p}}^{a_{p}}(T_{i})_{b_{1}}^{d_{1}}\ldots\delta_{b_{q}}^{d_{q}} - \ldots - \delta_{c_{1}}^{a_{1}}\delta_{c_{2}}^{a_{2}}\ldots\delta_{c_{p}}^{a_{p}}\delta_{b_{1}}^{d_{1}}\ldots(T_{i})_{b_{q}}^{d_{q}}.$$
 (9.19)

This forest of indices vanishes in the birdtrack notation, enabling us to visualize the formula for the generators of infinitesimal transformations for any tensor representation:

$$\overrightarrow{T} = \overrightarrow{T} + \overrightarrow{T} = \overrightarrow{T}, \quad (9.20)$$

with a relative minus sign between lines flowing in opposite directions. The reader will recognize this as the Leibnitz rule.

The invariance conditions take a particularly suggestive form in the birdtrack notation. Equation (9.18) amounts to the insertion of a generator into all external legs of the diagram corresponding to the invariant tensor q:



The insertions on the lines going into the diagram carry a minus sign relative to the insertions on the outgoing lines.

As the simplest example of computation of the generators of infinitesimal transformations acting on spaces other than the defining space, consider the adjoint rep. Where does the ugly word "adjoint" come from in this context is not obvious, but remember it this way: this is the one distinguished representation, which is intrinsic to the Lie algebra, with the explicit matrix elements $(T_i)_{jk}$ of the adjoint rep given by the the fully antisymmetric structure constants iC_{ijk} of the algebra (i.e., its multiplication table under the commutator product). It's the continuous groups analogoue of the multiplication table, or the regular representation for the finite groups. The factor *i* ensures their reality (in the case of hermitian generators T_i), and we keep track of the overall signs by always reading indices *counterclockwise* around a vertex:

$$-iC_{ijk} =$$

$$(9.22)$$

$$= - \qquad (9.23)$$

As all other invariant tensors, the generators must satisfy the invariance conditions (9.21):

Redrawing this a little and replacing the adjoint rep generators (9.22) by the structure constants, we find that the generators obey the *Lie algebra* commutation relation

$$(9.24)$$

In other words, the Lie algebra commutator

$$T_i T_j - T_j T_i = i C_{ijk} T_k . (9.25)$$

is simply a statement that T_i , the generators of invariance transformations, are themselves invariant tensors. Now, honestly, do you prefer the three-birdtracks equation (9.24), or the mathematician's page-long definition of the adjoint rep? It's a classic example of bad notation getting into way of understanding a relation of beautiful simplicity. The invariance condition for structure constants C_{ijk} is likewise



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Rewriting this with the dot-vertex (9.22), we obtain

This is the Lie algebra commutator for the adjoint rep generators, known as the *Jacobi relation* for the structure constants

$$C_{ijm}C_{mkl} - C_{ljm}C_{mki} = C_{iml}C_{jkm}.$$
(9.27)

Hence, the Jacobi relation is also an invariance statement, this time the statement that the structure constants are invariant tensors.

9.1.4 Discussion

2017-10-17 Lin Xin Please explain the $M_{\mu\nu,\delta\rho}$ generators of SO(n).

2017-11-07 Predrag Let me know if you understand the derivation of Eqs. (4.51) and (4.52) in birdtracks.eu. Does that answer your question?

9.2 Birdtracks - updated history

Predrag Cvitanović

November 7, 2017

Young tableaux and (non-Hermitian) Young projection operators were introduced by Young [20] in 1933 (Tung monograph [19] is a standard exposition). In 1937 R. Brauer [3] introduced diagrammatic notation for δ_{ij} in order to represent "Brauer algebra" permutations, index contractions, and matrix multiplication diagrammatically. R. Penrose's papers were the first to cast the Young projection operators into a diagrammatic form. In 1971 monograph [13] Penrose introduced diagrammatic notation for symmetrization operators, Levi-Civita tensors [15], and "strand networks" [12]. Penrose credits Aitken [1] with introducing this notation in 1939, but inspection of Aitken's book reveals a few Brauer diagrams for permutations, and no (anti)symmetrizers. Penrose's [14] 1952 initial ways of drawing symmetrizers and antisymmetrizers are very aesthetical, but the subsequent developments gave them a distinctly ostrich flavor [14]. In 1974 G. 't Hooft introduced a double-line notation for U(n) gluon group-theory weights [18]. In 1976 Cvitanović [7] introduced analogous notation for SU(N), SO(n)and Sp(n). For several specific, few-index tensor examples, diagrammatic Young projection operators were constructed by Canning [5], Mandula [11], and Stedman [17].

The 1975–2008 Cvitanović diagrammatic formulation of the theory of all semisimple Lie groups [8] as a way to compute group theoretic wights without any recourse to symbols goes conceptually and profoundly beyond the Penrose notation (indeed, Cvitanović "birdtracks" bear no resemblance to Penrose's "fornicating ostriches" [14]).

A chapter in Cvitanović 2008 monograph [8] sketches how birdtrack (diagrammatic) Young projection operators for arbitrary irreducible representation of SU(N)

could be constructed (this text is augmented by a 2005 appendix by Elvang, Cvitanović and Kennedy [9] which, however, contains a significant error). Keppeler and Sjödahl [10] systematized the construction by offering a simple method to construct Hermitian Young projection operators in the birdtrack formalism. Their iteration is easy to understand, and the proofs of Hermiticity are simple. However, in practice, the algorithm is inefficient - the expression balloon quickly, the Young projection operators soon become unwieldy and impractical, if not impossible to implement.

The Alcock-Zeilinger algorithm, based on the simplification rules of ref. [2], leads to explicitly Hermitian and drastically more compact expressions for the projection operators than the Keppeler-Sjödahl algorithm [10]. Alcock-Zeilinger fully supersedes Cvitanović's formulation, and any future full exposition of reduction of SU(N) tensor products into irreducible representations should be based on the Alcock-Zeilinger algorithm.

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Exercises

9.1. Irreps of SO(2). Matrix

$$T = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$
(9.28)

is the generator of rotations in a plane.

(a) Use the method of projection operators to show that for rotations in the kth Fourier mode plane, the irreducible 1D subspaces orthonormal basis vectors are

$$\mathbf{e}^{(\pm k)} = \frac{1}{\sqrt{2}} \left(\pm \mathbf{e}_1^{(k)} - i \, \mathbf{e}_2^{(k)} \right) \,.$$

How does T act on $e^{(\pm k)}$?

(b) What is the action of the $[2 \times 2]$ rotation matrix

$$D^{(k)}(\theta) = \begin{pmatrix} \cos k\theta & -\sin k\theta \\ \sin k\theta & \cos k\theta \end{pmatrix}, \qquad k = 1, 2, \cdots$$

on the $(\pm k)$ th subspace $e^{(\pm k)}$?

- (c) What are the irreducible representations characters of SO(2)?
- 9.2. Reduction of a product of two SO(2) irreps. Determine the Clebsch-Gordan series for SO(2). Hint: Abelian group has 1-dimensional characters. Or, you are just multiplying terms in Fourier series.

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9.3. **Irreps of O**(2). O(2) is a group, but not a Lie group, as in addition to continuous transformations generated by (9.28) it has, as a group element, a parity operation

$$\sigma = \left[\begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right]$$

which cannot be reached by continuous transformations.

- (a) Is this group Abelian, i.e., does T commute with $R(k\theta)$? Hint: evaluate first the $[T, \sigma]$ commutator and/or show that $\sigma D^{(k)}(\theta)\sigma^{-1} = D^{(k)}(-\theta)$.
- (b) What are the equivalence (i.e., conjugacy) classes of this group?
- (c) What are irreps of O(2)? What are their dimensions?
 - Hint: O(2) is the $n \to \infty$ limit of D_n , worked out in exercise 4.4 *Irreducible representations of dihedral group* D_n . Parity σ maps an SO(2) eigenvector into another eigenvector, rendering eigenvalues of any O(2) commuting operator degenerate. Or, if you really want to do it right, apply Schur's first lemma to improper rotations

$$R^{'}(\theta) = \begin{pmatrix} \cos k\theta & -\sin k\theta \\ \sin k\theta & \cos k\theta \end{pmatrix} \sigma = \begin{pmatrix} \cos k\theta & \sin k\theta \\ \sin k\theta & -\cos k\theta \end{pmatrix}$$

to prove irreducibility for $k \neq 0$.

- (d) What are irreducible characters of O(2)?
- (e) Sketch a fundamental domain for O(2).
- 9.4. Reduction of a product of two O(2) irreps. Determine the Clebsch-Gordan series for O(2), i.e., reduce the Kronecker product $D^{(k)} \bigotimes D^{(\ell)}$.

9.5. A fluttering flame front.

(a) Consider a linear partial differential equation for a real-valued field u = u(x, t) defined on a periodic domain u(x, t) = u(x + L, t):

$$u_t + u_{xx} + \nu u_{xxxx} = 0, \qquad x \in [0, L].$$
 (9.29)

In this equation $t \ge 0$ is the time and x is the spatial coordinate. The subscripts x and t denote partial derivatives with respect to x and t: $u_t = \partial u/d\partial$, u_{xxxx} stands for the 4th spatial derivative of u = u(x, t) at position x and time t. Consider the form of equations under coordinate shifts $x \to x + \ell$ and reflection $x \to -x$. What is the symmetry group of (9.29)?

- (b) Expand u(x, t) in terms of its SO(2) irreducible components (hint: Fourier expansion) and rewrite (9.29) as a set of linear ODEs for the expansion coefficients. What are the eigenvalues of the time evolution operator? What is their degeneracy?
- (c) Expand u(x,t) in terms of its O(2) irreducible components (hint: Fourier expansion) and rewrite (9.29) as a set of linear ODEs. What are the eigenvalues of the time evolution operator? What is their degeneracy?
- (d) Interpret u = u(x, t) as a 'flame front velocity' and add a quadratic nonlinearity to (9.29),

$$u_t + \frac{1}{2}(u^2)_x + u_{xx} + \nu u_{xxxx} = 0, \qquad x \in [0, L].$$
(9.30)

This nonlinear equation is known as the Kuramoto-Sivashinsky equation, a baby cousin of Navier-Stokes. What is the symmetry group of (9.30)?

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- (e) Expand u(x, t) in terms of its O(2) irreducible components (see exercise 9.3) and rewrite (9.30) as an infinite tower of coupled nonlinear ODEs.
- (f) What are the degeneracies of the spectrum of the eigenvalues of the time evolution operator?
- 9.6. O(2) fundamental domain for Kuramoto-Sivashinsky equation. You have C_2 discrete symmetry generated by flip σ , which tiles the space by two tiles.
 - Is there a subspace invariant under this C₂? What form does the tower of ODEs take in this subspace?
 - How would you restrict the flow (the integration of the tower of coupled ODEs) to a fundamental domain?

This problem is indeed hard, a research level problem, at least for me and the grad students in our group. Unlike the beautiful full-reducibility, character-orthogonality representation theory of linear problems, in nonlinear problems symmetry reduction currently seems to require lots of clever steps and choices of particular coordinates, and we am not at all sure that our solution is the optimal one. Somebody looking at the problem with a fresh eye might hit upon a solution much simpler than ours. Has happened before :)

Burak Budanur's solution is written up in Budanur and Cvitanović [4] Unstable manifolds of relative periodic orbits in the symmetry-reduced state space of the Kuramoto-Sivashinsky system sect. 3.2 O(2) symmetry reduction, eq. (17) (get it here).

9.7. Lie algebra from invariance. Derive the Lie algebra commutator and the Jacobi identity as particular examples of the invariance condition, using both index and birdtracks notations. The invariant tensors in question are "the laws of motion," i.e., the generators of infinitesimal group transformations in the defining and the adjoint representations.

group theory - week 10

$\mathbf{O}(2)$ symmetry sliced

Georgia Tech PHYS-7143

Homework HW10

due Thursday, November 2, 2017

== 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	10.1 Conjugacy classes of SO(3)	2 points (+ 2 bonus points,	if complete)
Exercise	10.2 The character of $SO(3)$ 3-dimen	sional representation	1 point
Exercise	10.3 The orthonormality of $SO(3)$ characteristics of $SO(3)$ characterist	aracters	2 point
Exercise	10.4 $U(1)$ equivariance of two-mode.	s system for finite angles	3 points
Exercise	10.6 $SO(2)$ or harmonic oscillator sl	ice	2 points

Bonus points

Exercise 10.5 Integrate the two-modes system	4 point
Exercise 10.7 Invariant subspace of the two-modes system	1 point
Exercise 10.8 Slicing the two-modes system	1 point
Exercise 10.9 The symmetry reduced two-modes flow	(difficult) 6 points

Total of 10 points = 100 % score.

2017-10-24 Predrag Lecture 18 Lie groups, algebras Bridging the step from discrete to continuous compact groups: invariant integration measures, characters, character orthonormality and completeness relations.

Reading: ChaosBook.org Chap. *Continuous symmetry factorization*, only Sect 26.1 *Compact groups*.

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Reading: sect. 10.3 Two-modes SO(2)-equivariant flow. For the long version, see ChaosBook.org Chap. *Relativity for cyclists*, and ChaosBook.org Chap. *Slice & dice*, Sect. 13.1 Only dead fish go with the flow to Sect. 13.5 First Fourier mode slice. This is difficult material, so it is OK if you do not get it this time around. None of this will be on the final - the main point is that once you face a nonlinear problem, nothing is easy - not even rotations on a circle.

2017-10-26 Predrag Solutions week 10

10.1 Literature

C. K. Wong *Group Theory* notes, Chap 6 *1D continuous groups*, works out in full detail the representations and Haar measures for 1-dimensional Lie groups, and explains the difference between rotations and translations.

Chen, Ping and Wang [1] *Group Representation Theory for Physicists*, Sect 5.3 *Lie algebras* and Sect 5.4 *Finite transformations* work out several SU(2) and O(3) examples. Sects 5.5, 5.6 and 5.7 also merit a quick read.

In his group theory notes D. Vvedensky, chapter 8, sect. 8.3 Axis–angle representation of proper rotations in three dimensions, has a very nice discussion of the (10.2) parametrization of the SO(3) 3-dimensional group manifold: the parameter space corresponds to the interior of a sphere of radius π , and the over the classes of SO(3) is given by integral over spherical shells. In sect. 8.4 he derives the Haar measure (without calling it so).

In sect. 8.5 Vvedensky says: "For SO(2), we were able to determine the characters of the irreducible representations directly, i.e., without having to determine the basis functions of these representations. The structure of SO(3), however, does not allow for such a simple procedure, so we must determine the basis functions from the outset." That I disagree with; in birdtracks.eu sect. 15.1 *Reps of SU*(2) I construct the irreps and label them by their Young tableaus with no recourse to spherical harmonics.

10.2 SO(3) character orthogonality

In 3 Euclidean dimensions, a rotation around z axis is given by the SO(2) matrix

$$R_3(\varphi) = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0\\ \sin\varphi & \cos\varphi & 0\\ 0 & 0 & 1 \end{pmatrix} = \exp\varphi \begin{pmatrix} 0 & -1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 0 \end{pmatrix} .$$
(10.1)

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An arbitrary rotation in \mathbb{R}^3 can be represented by

$$R_{\boldsymbol{n}}(\varphi) = e^{-i\varphi \,\boldsymbol{n} \cdot \boldsymbol{L}} \qquad \boldsymbol{L} = (L_1, L_2, L_3), \qquad (10.2)$$

where the unit vector n determines the plane and the direction of the rotation by angle φ . Here L_1, L_2, L_3 are the generators of rotations along x, y, z axes respectively,

$$L_{1} = i \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \quad L_{2} = i \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad L_{3} = i \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (10.3)$$

with Lie algebra relations

$$[L_i, L_j] = i\varepsilon_{ijk}L_k \,. \tag{10.4}$$

All SO(3) rotations (10.2) by the same angle θ around different rotation axis n are conjugate to each other,

$$e^{i\phi\boldsymbol{n}_{2}\cdot\boldsymbol{L}}e^{i\theta\boldsymbol{n}_{1}\cdot\boldsymbol{L}}e^{-i\phi\boldsymbol{n}_{2}\cdot\boldsymbol{L}} = e^{i\theta\boldsymbol{n}_{3}\cdot\boldsymbol{L}}, \qquad (10.5)$$

with $e^{i\phi} n_2 \cdot L$ and $e^{-i\theta} n_2 \cdot L$ mapping the vector n_1 to n_3 and back, so that the rotation around axis n_1 by angle θ is mapped to a rotation around axis n_3 by the same θ . The conjugacy classes of SO(3) thus consist of rotations by the same angle about all distinct rotation axes, and are thus labelled the angle θ . As the conjugacy class depends only on θ , the characters can only be a function of θ . For the 3-dimensional special orthogonal representation, the character is

$$\chi = 2\cos(\theta) + 1. \tag{10.6}$$

For an irrep labeled by j, the character of a conjugacy class labeled by θ is

$$\chi^{(j)}(\theta) = \frac{\sin(j+1/2)\theta}{\sin(\theta/2)}$$
(10.7)

To check that these characters are orthogonal to each other, one needs to define the group integration over a parametrization of the SO(3) group manifold. A group element is parametrized by the rotation axis n and the rotation angle $\theta \in (-\pi, \pi]$, with n a unit vector which ranges over all points on the surface of a unit ball. Note however, that a π rotation is the same as a $-\pi$ rotation (n and -n point along the same direction), and the n parametrization of SO(3) is thus a 2-dimensional surface of a unit-radius ball with the opposite points identified.

The Haar measure for SO(3) requires a bit of work, here we just use note that after the integration over the solid angle (characters do not depend on it), the Haar measure is

$$dg = d\mu(\theta) = \frac{d\theta}{2\pi} (1 - \cos(\theta)) = \frac{d\theta}{\pi} \sin^2(\theta/2).$$
(10.8)

With this measure the characters are orthogonal, and the character orthogonality theorems follow, of the same form as for the finite groups, but with the group averages replaced by the continuous, parameter dependent group integrals

$$\frac{1}{G|}\sum_{g\in G} \to \int_G dg$$

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exercise 10.1

exercise 10.2

exercise 11.1

exercise 10.3



Figure 10.1: Two-modes flow before (a) and after (b) symmetry reduction by first Fourier mode slice. Here a long trajectory (red and blue) starting on the unstable manifold of the TW_1 (red), until it falls on to the strange attractor (blue) and the shortest relative periodic orbit $\overline{1}$ (magenta). Note that the relative equilibrium becomes an equilibrium, and the relative periodic orbit becomes a periodic orbit after the symmetry reduction.

The good news is that, as explained in ChaosBook.org Chap. *Relativity for cyclists* (and in *Group Theory - Birdtracks, Lie's, and Exceptional Groups* [2]), one never needs to actually explicitly construct a group manifold parametrizations and the corresponding Haar measure.

10.3 Two-modes **SO**(2)-equivariant flow

Consider the pair of U(1)-equivariant complex ODEs

$$\dot{z}_1 = (\mu_1 - i e_1) z_1 + a_1 z_1 |z_1|^2 + b_1 z_1 |z_2|^2 + c_1 \overline{z}_1 z_2$$

$$\dot{z}_2 = (\mu_2 - i e_2) z_2 + a_2 z_2 |z_1|^2 + b_2 z_2 |z_2|^2 + c_2 z_1^2, \qquad (10.9)$$

with z_1 , z_2 complex, and all parameters real valued.

This system is a generic example of a few-modes truncation of a Fourier representation of some physical flow, such as fluid dynamics convection flow, truncated in such a way that the model exhibits the same symmetries as the full original problem, while being drastically simpler to study. It is a merely a toy model with no physical interpretation, just like the iconic Lorenz flow. We use it to illustrate the effects of continuous symmetry on chaotic dynamics.

We refer to this toy model as the *two-modes* system. It belongs to the family of simplest ODE systems that we know that (a) have a continuous U(1) / SO(2), but no discrete symmetry (if at least one of $e_j \neq 0$). (b) models 'weather', in the same sense that Lorenz equation models 'weather', (c) exhibits chaotic dynamics, (d) can be easily visualized, in the dimensionally lowest possible setting required for chaotic dynamics, with the full state space of dimension d = 4, and the SO(2)-reduced dynamics taking place in 3 dimensions, and (e) for which the method of slices reduces the symmetry by a single global slice hyperplane.

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The model has an unreasonably high number of parameters. After some experimentation we fix or set to zero various parameters, and in the numerical examples that follow, we settle for parameters set to

$$\mu_1 = -2.8, \ \mu_2 = 1, \ e_1 = 0, \ e_2 = 1,$$

$$a_1 = -1, \ a_2 = -2.66, \ b_1 = 0, \ b_2 = 0, \ c_1 = -7.75, \ c_2 = 1, \ (10.10)$$

unless explicitly stated otherwise. For these parameter values the system exhibits chaotic behavior. Experiment! If you find a more interesting behavior for some other parameter values, please let us know. The simplified system of equations can now be written as a 3-parameter $\{\mu_1, c_1, a_2\}$ two-modes system,

$$\dot{z}_1 = \mu_1 z_1 - z_1 |z_1|^2 + c_1 \overline{z}_1 z_2 \dot{z}_2 = (1 - i) z_2 + a_2 z_2 |z_1|^2 + z_1^2.$$
(10.11)

In order to numerically integrate and visualize the flow, we recast the equations in real variables by substitution $z_1 = x_1 + i y_1$, $z_2 = x_2 + i y_2$. The two-modes system (10.9) is now a set of four coupled ODEs

$$\begin{aligned} \dot{x}_1 &= (\mu_1 - r^2) x_1 + c_1 (x_1 x_2 + y_1 y_2), \qquad r^2 = x_1^2 + y_1^2 \\ \dot{y}_1 &= (\mu_1 - r^2) y_1 + c_1 (x_1 y_2 - x_2 y_1) \\ \dot{x}_2 &= x_2 + y_2 + x_1^2 - y_1^2 + a_2 x_2 r^2 \\ \dot{y}_2 &= -x_2 + y_2 + 2 x_1 y_1 + a_2 y_2 r^2. \end{aligned}$$
(10.12)

Try integrating (10.12) with random initial conditions, for long times, times much beyond which the initial transients have died out. What is wrong with this picture? Figure 10.3 (a) is a mess. As we show here, the attractor is built up by a nice 'stretch & fold' action, hidden from the view by the continuous symmetry induced drifts. That is fixed by 'quotienting' model's SO(2) symmetry, and reducing the dynamics to a 3-dimensional symmetry-reduced state space, figure 10.3 (b).

References

- [1] J.-Q. Chen, J. Ping, and F. Wang, *Group Representation Theory for Physicists* (World Scientific, Singapore, 1989).
- [2] P. Cvitanović, Group Theory Birdtracks, Lie's, and Exceptional Groups (Princeton Univ. Press, Princeton, NJ, 2008).

Exercises

10.1. **Conjugacy classes of SO**(3): Show that all SO(3) rotations (10.2) by the same angle θ around any rotation axis *n* are conjugate to each other:

$$e^{i\phi\boldsymbol{n}_{2}\cdot\boldsymbol{L}}e^{i\theta\boldsymbol{n}_{1}\cdot\boldsymbol{L}}e^{-i\phi\boldsymbol{n}_{2}\cdot\boldsymbol{L}} = e^{i\theta\boldsymbol{n}_{3}\cdot\boldsymbol{L}}$$
(10.13)

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exercise 10.5

exercise 10.6 exercise 10.7 exercise 10.8 Check this for infinitesimal ϕ , and argue that from that it follows that it is also true for finite ϕ . Hint: use the Lie algebra commutators (10.4).

10.2. The character of SO(3) 3-dimensional representation: Show that for the 3-dimensional special orthogonal representation (10.2), the character is

$$\chi = 2\cos(\theta) + 1.$$
 (10.14)

Hint: evaluating the character explicitly for $R_x(\theta)$, $R_y(\theta)$ and $R_z(\theta)$.

10.3. **The orthonormality of SO**(3) **characters:** Verify that given the Haar measure (10.8), the characters (10.7) are orthogonal:

$$\langle \chi(j)|\chi(j')\rangle = \int_{G} dg \,\chi^{(j)}(g^{-1}) \,\chi^{(j')}(g) = \delta_{jj'} \,. \tag{10.15}$$

10.4. U(1) equivariance of two-modes system for finite angles: Show that the vector field in two-modes system (10.9) is equivariant under (9.1), the unitary group U(1) acting on $\mathbb{R}^4 \cong \mathbb{C}^2$ as the k = 1 and 2 modes:

$$g(\theta)(z_1, z_2) = (e^{i\theta} z_1, e^{i2\theta} z_2), \quad \theta \in [0, 2\pi).$$
(10.16)

- 10.5. Integrate the two-modes system: Integrate (10.12) and plot a long trajectory of twomodes in the 4d state space, (x_1, y_1, y_2) projection, as in figure 10.3 (a). To save you time (typing in (10.12) is tedious), we have prepared for you python code, and online graded problem set here. If you do this exercise, please get started early, in order to make sure that the autograder is working, and forward to us the grades that you receive from the autograder.
- 10.6. SO(2) or harmonic oscillator slice: Construct a moving frame slice for action of SO(2) on \mathbb{R}^2

 $(x, y) \mapsto (x \cos \theta - y \sin \theta, x \sin \theta + y \cos \theta)$

by, for instance, the positive y axis: x = 0, y > 0. Write out explicitly the group transformation that brings any point back to the slice. What invariant is preserved by this construction?

- 10.7. Invariant subspace of the two-modes system: Show that $(0, 0, x_2, y_2)$ is a flow invariant subspace of the two-modes system (10.12), i.e., show that a trajectory with the initial point within this subspace remains within it forever.
- 10.8. **Slicing the two-modes system:** Choose the simplest slice template point that fixes the 1. Fourier mode,

$$\hat{x}' = (1, 0, 0, 0).$$
 (10.17)

(a) Show for the two-modes system (10.12), that the velocity within the slice, and the phase velocity along the group orbit are

$$\hat{v}(\hat{x}) = v(\hat{x}) - \dot{\phi}(\hat{x})t(\hat{x})$$
 (10.18)

$$\dot{\phi}(\hat{x}) = -v_2(\hat{x})/\hat{x}_1$$
 (10.19)

- (b) Determine the chart border (the locus of point where the group tangent is either not transverse to the slice or vanishes).
- (c) What is its dimension?

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- (d) What is its relation to the invariant subspace of exercise 10.7?
- (e) Can a symmetry-reduced trajectory cross the chart border?
- 10.9. The symmetry reduced two-modes flow: Pick an initial point $\hat{x}(0)$ that satisfies the slice condition for the template choice (10.17) and integrate (10.18) & (10.19). Plot the three dimensional slice hyperplane spanned by (x_1, x_2, y_2) to visualize the symmetry reduced dynamics. Does it look like figure 10.3 (b)?

group theory - week 11

${\rm SU}(2)$ and ${\rm SO}(3)$

Georgia Tech PHYS-7143

Homework HW11

due Tuesday, November 7, 2017

== 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 11.1 The characters of $SO(3)$ representations	1 point
Exercise 11.2 Lie algebra of $SO(4)$ and $SU(2) \otimes SU(2)$	6 points
Exercise 11.5 SO(n) Clebsch-Gordan series for $V \otimes V$.	3 points

Bonus points

Exercise 11.3 Real and pseudo-real representations of SO(3)	4 points
Exercise 11.4 Total spin of N particles	5 points

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

2017-10-31 Predrag Lecture 20 SU(2) and SO(3)

Gutkin notes, Lect. 9 SU(2), SO(3) and their representations, Sects. 1-3.2; sect. 11.1 SU(2) - SO(3) correspondence below.

2017-11-02 Predrag Lecture 21 SO(3) birdtracks

Birdtrack notation [1] is explained here.

You can fetch clippings on irreps of SU(n) and SO(n) from Predrag's monograph [1] here. Go through Sect. 2.2 *First example:* SU(n), Sect. 6.1 *Symmetrization*, Sect. 6.2 *Antisymmetrization*, Sect. 9.1 *Two-index tensors*. Skim through Sect. 9.2 *Three-index tensors*, and Table 9.1. There is also a glimpse of a some birdtracking (still to be written up) in sect. 11.2 Irreps of SO(n).

Reading for the next week: Sect. 9.3 Young tableaux.

11.1 SU(2) - SO(3) correspondence

Notes by Kimberly Y. Short

Angular momentum $L = r \times p$ has three components, the operators that generate SU(2) and satisfy $[L_1, L_2] = iL_3$. If we define $e = L_1 + iL_2$, $f = L_1 - iL_2$, and $h = 2L_3$, then we have the following algebra:

$$[h, e] = 2e, \quad [h, f] = -2f, \quad [e, f] = h$$
 (11.1)

where

$$e = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad f = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad h = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
(11.2)

Matrices e and f act as the raising and lowering (also called 'ladder') operators L_{\pm} in this representation. (The set $\{e, f, h\}$ forms an '*sl*₂-triple'.)

We observe that there are $n^2 - 1 = 3$ such operators satisfying this algebra, which is the Lie algebra of SU(n), where n = 2. The eigenvalues of h are integers separated by 2, and the eigenvalues of L_3 must be half-integers separated by 1. Consequently, the representation with highest L_3 eigenvalue given by l must have dimension 2l + 1(note: 2l is λ_{max} for h).

Further, $L^2 = L \cdot L$ commutes with L_1 , L_2 , and L_3 and hence, by Schur's Lemma, $L^2 = \lambda \mathbb{I}$ in this representation, so every vector is an eigenvector of L^2 . For example, we've seen in quantum mechanics,

$$L^2 Y_l^m = l(l+1)\hbar^2 Y_l^m$$
(11.3)

And since the spherical harmonics $Y_l^m(\theta, \phi)$ constitute an orthonormal basis of the Hilbert space of square-integrable functions, any vector can be expanded in a basis of $Y_l^m(\theta, \phi)$. L_{\pm} act on Y_l^m in the following way:

$$L_{\pm}Y_{l}^{m} = \hbar\sqrt{l(l+1) - m(m\pm 1)} Y_{l}^{m\pm 1}.$$
(11.4)

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An element of SU(2) can be written as

$$e^{i\sigma_j\alpha_j/2} \tag{11.5}$$

where σ_j is a Pauli matrix and α_j is a number. (The exponentiation of the Pauli matrices gives SU(2).) What is the importance of the 1/2 factor in the argument of the exponential. First, consider a generic position vector $\mathbf{r} = x\hat{e}_i + y\hat{e}_j + z\hat{e}_k$. We may construct a matrix of the form

$$\sigma \cdot r = \sigma_x x + \sigma_y y + \sigma_z z$$

$$= \begin{pmatrix} 0 & x \\ x & 0 \end{pmatrix} + \begin{pmatrix} 0 & -iy \\ iy & 0 \end{pmatrix} + \begin{pmatrix} z & 0 \\ 0 & -z \end{pmatrix}$$

$$= \begin{pmatrix} z & x - iy \\ x + iy & -z \end{pmatrix}$$
(11.6)

The determinant,

det
$$\begin{pmatrix} z & x - iy \\ x + iy & -z \end{pmatrix} = -(x^2 + y^2 + z^2) = -x^2$$
 (11.7)

is an expression for the length of a vector.

Now consider a unitary transformation of this matrix. For example,

$$U(\sigma \cdot r)U^{\dagger} = \sigma_{x}(\sigma \cdot r)\sigma_{x}$$

$$= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} z & x - iy \\ x - iy & z \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} -z & x + iy \\ x - iy & z \end{pmatrix}$$
(11.8)

Taking this determinant, we find the same expression as before:

det
$$\begin{pmatrix} -z & x+iy\\ x-iy & z \end{pmatrix} = -(x^2+y^2+z^2) = -x^2$$
 (11.9)

We observe that, like SO(3), SU(2) preserves the lengths of vectors.

The correspondence between SO(3) and SU(2) can be made more explicit. To see this, consider an SU(2) transformation on a two-component object called a *spinor* ψ where

$$\psi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \,, \tag{11.10}$$

and

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$$x = \frac{1}{2}(\beta^2 - \alpha^2), \quad y = -\frac{i}{2}(\alpha^2 + \beta^2), \quad z = \alpha\beta.$$
 (11.11)

One may check that an SU(2) transformation on ψ is equivalent to an SO(3) transformation on \boldsymbol{x} . From this equivalence, one sees that an SU(2) transformation has three

real parameters that correspond to the three rotation angles of SO(3). If we label the "angles" for the SU(2) transformation by α , β , and γ , we observe, for a "rotation" about \hat{x}

$$U_x(\alpha) = \begin{pmatrix} \cos \alpha/2 & i \sin \alpha/2 \\ i \sin \alpha/2 & \cos \alpha/2 \end{pmatrix}.$$
 (11.12)

Likewise for an SU(2) transformation about \hat{y} :

$$U_y(\beta) = \begin{pmatrix} \cos\beta/2 & \sin\beta/2 \\ -\sin\beta/2 & \cos\beta/2 \end{pmatrix}$$
(11.13)

And for the final rotation, the SU(2) transformation about \hat{z} :

$$U_z(\gamma) = \begin{pmatrix} e^{i\gamma/2} & 0\\ 0 & e^{-i\gamma/2} \end{pmatrix}$$
(11.14)

Compare these three matrices to the corresponding SO(3) rotation matrices:

$$R_x(\zeta) = \begin{pmatrix} 1 & 0 & 0\\ 0 & \cos\zeta & \sin\zeta\\ 0 & -\sin\zeta & \cos\zeta \end{pmatrix}, \quad R_y(\phi) = \begin{pmatrix} \cos\phi & 0 & \sin\phi\\ 0 & 1 & 0\\ -\sin\phi & 0 & \cos\phi \end{pmatrix}$$
$$R_z(\theta) = \begin{pmatrix} \cos\theta & \sin\theta & 0\\ -\sin\theta & \cos\theta & 0\\ 0 & 0 & 1 \end{pmatrix} \quad (11.15)$$

They're equivalent! Result: Half the rotation angle generated by SU(2) corresponds to a rotation generated by SO(3).

In this context, the eigenvalue equation for L_3 and for L^2 are differential equations whose solutions are the spherical harmonics Y_l^m which take the form

$$e^{im\phi}P_l^m(\cos\theta), \quad -l \le m \le l$$
 (11.16)

in spherical coordinates and which determine the shape of electron orbitals and their probabilities to be found in a given region.

In quantum mechanics, the possible results of a measurement are determined by the possible eigenvalues of an operator. As such, the possible measurable values of the z-component of angular momentum correspond to the allowed values of L_3 . The measurement outcomes are not arbitrary; the largest one, l, must be a half-integer, and there are 2l + 1 eigenvectors. Applying the lowering operator L_- one-by-one, we can find the possible outcomes to be $m \in \{l, l - 1, ..., -l\}$. The angular dependence of the corresponding wave function goes as $\sim e^{im\phi} P_l^m(\cos \theta)$. In addition, higher values of l correspond to higher energy, so the different values of l correspond to different electron orbitals in order of increasing energy.

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Young tableaux		=	•	+		+		
Dimensions	n^2	=	1	+	$\frac{n(n-1)}{2}$	+	$\frac{(n+2)(n-1)}{2}$	
Projectors		$=\frac{1}{r}$	\mathbf{C}	C+		+	$\left\{ \boxed{{1}}} - \frac{1}{n} \right\} $	$\subset \}$

Table 11.1: SO(n) Clebsch-Gordan series for $V \otimes V$.

11.2 Irreps of **SO**(*n*)

The dimension of SO(n) is given by the trace of the adjoint projection operator:

$$N = \operatorname{tr} \mathbf{P}_A = \Theta = \frac{n(n-1)}{2}$$
. (11.17)

Dimensions of the other reps are listed in table 11.1.

References

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

Exercises

11.1. The characters of SO(3) representations: Show that for an irrep labeled by j, the character of a conjugacy class labeled by θ

$$\chi^{(j)}(\theta) = \frac{\sin(j+1/2)\theta}{\sin(\theta/2)}$$
(11.18)

can be obtained by taking the trace of $R_z^i(\theta)$. Verify that for j = 1 this character is the three dimensional special orthogonal representation character (10.6).

11.2. Lie algebra of SO(4) and SU(2) \otimes SU(2). One particle Hamiltonian with a central potential has in general SO(3) symmetry group. It turns out, however, that for Coulomb potential the symmetry group is actually larger - SO(4), rather than SO(3). This explains why the energy level degeneracies in the hydrogen atom are anomalously large. So SO(4) and its representations are of a special importance in atomic physics.

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(a) Show that the Lie algebra $\mathfrak{so}(4)$ of the group SO(4) is generated by real antisymmetric 4×4 matrices.

(b) What is the dimension of $\mathfrak{so}(4)$?

A natural basis in $\mathfrak{so}(4)$ is provided by antisymmetric matrices $M_{\mu\nu}$, $\mu, \nu \in \{1, 2, 3, 4, \mu \neq \nu\}$, generators of SO(4) rotations which leave invariant the $\mu\nu$ -plane. The elements of these matrices are given by

$$(M_{\mu\nu})_{ij} = \delta_{i\mu}\delta_{j\nu} - \delta_{j\mu}\delta_{i\nu} \tag{11.19}$$

(c) Check that these matrices satisfy the following commutation relationship:

$$[M_{ab}, M_{cd}] = M_{ad}\delta_{bc} + M_{bc}\delta_{ad} - M_{ac}\delta_{bd} - M_{bd}\delta_{ac}.$$

- (d) Show that Lie algebras of the groups SO(4) and $SU(2) \times SU(2)$ are isomorphic. Path:
 - (d.i) Define matrices

$$J_k = \frac{1}{2} \varepsilon_{kij} M_{i,j}, \qquad K_k = M_{k4}, \quad k = 1, 2, 3$$

and

$$\mathcal{A}_k = rac{1}{2} \left(J_k + K_k
ight) \quad ext{and} \quad \mathcal{B}_k = rac{1}{2} \left(J_k - K_k
ight) \,.$$

- (d.ii) Show that A and B satisfy the same commutation relations as two copies of $\mathfrak{su}(2)$.
- (e) How does one construct irreps of $\mathfrak{so}(4)$ out of irreps of $\mathfrak{su}(2)$?
- (f) Are groups SO(4) and $SU(2) \otimes SU(2)$ isomorphic to each other?

(B. Gutkin)

11.3. **Real and pseudo-real representations of SO**(3). Recall (Gutkin notes, Lect. 4 *Representation Theory II*, Sect. 5 *5. Three types of representations*) that there are exist three types of representation which can be distinguished by the indicator:

$$\int_{G} d\mu(g)\chi_{l}(g^{2}) = \begin{cases} +1 & \text{real} \\ 0 & \text{complex} \\ -1 & \text{pseudo-real} \end{cases}$$
(11.20)

Determine for which values of l = 0, 1/2, 1, 3/2, 2... the representation D_l of SO(3) is real or pseudo-real.

Hint: The characters and Haar measure (10.8) of SO(3) are given by

$$\chi_l(g) = \frac{\sin\left(\left[l + \frac{1}{2}\right]\theta\right)}{\sin\left(\frac{1}{2}\theta\right)}, \qquad d\mu(g) = \frac{d\theta}{\pi}\sin^2(\theta/2) \tag{11.21}$$

where θ is rotation angle for the group element g.

(B. Gutkin)

11.4. Total spin of N particles. Consider a system of four particles with spin 1/2. Assuming that all (except spin) degrees of freedom are frozen the Hilbert space of the system is given by $V = V_{1/2} \otimes V_{1/2} \otimes V_{1/2} \otimes V_{1/2}$, with $V_{1/2}$ being two-dimensional space for each spin. $V = \bigoplus V_s$ can be decomposed then into different sectors V_s having the total spin s i.e., $\hat{S}^2 v = s(s+1)v$, for any $v \in V_s$. Here $\hat{S}^2 = (\sum_{i=1}^4 \hat{s}_i)^2$ and $\hat{s}_i = (\hat{s}_i^x, \hat{s}_i^y, \hat{s}_i^z)$ is spin operator for *i*-th particle.

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- (a) What are possible values *s* for the total spin of the system?
- (b) Determine dimension of the subspace of V_0 with 0 total spin. In other words: how many times trivial representation enters into product:

$$D = D_{1/2} \otimes D_{1/2} \otimes D_{1/2} \otimes D_{1/2} ?$$
(11.22)

(c) What is the answer to the above questions for N spins?

Hint: it is convenient to use (11.21) to decompose D into irreps.

(B. Gutkin)

11.5. SO(n) Clebsch-Gordan series for $V \otimes V$.

(a) Show that the product of two *n*-dimensional reps of SO(n) decomposes into three irreps:

(b) Compute the dimensions of the three irreps.

(c) Which one is the adjoint one, and why? Hint: check the invariance condition.

11.6. Splitting of degeneracies in a central potential. Hamiltonian H_0 has rotational symmetry of SO(3).

(a) What are the possible energy level degeneracies of H_0 ?

A weak perturbation V with a symmetry T_d of full tetrahedron group is added (e.g., V is a potential created by lattice of atoms with a symmetry of T_d).

- (b) What will be the degeneracies of new Hamiltonian $H_0 + V$?
- (c) Assuming that the total angular momentum of the system before the perturbation is l = 2. How the degeneracies of the corresponding energy level will be split after the perturbation is applied?

(B. Gutkin)

11.7. Quadrupole transitions.

a) Write $Q_1 = xy$, $Q_2 = zy$, $Q_3 = x^2 - y^2$ and $Q_4 = 2z^2 - x^2 - y^2$ as components of spherical tensor of rank 2. *Hint:* use spherical harmonics $Y_l^m(\theta, \varphi)$.

b) The last quantity Q_4 is known as quadrupole moment. What are the selection rules for transitions induced by Q_4 in a system with SO(3) symmetry? In other words, for which m, l and k, j the transition rates:

$$P_{m,l\to k,j} \sim \left| \langle m \, l | Q_4 | j \, k \rangle \right|^2$$

are non-zero?

c) By using Wigner-Eckart theorem write down the relationship between $|\langle m l | Q_4 | j k \rangle|^2$ and $|\langle m l | Q_1 | j k \rangle|^2$ in terms of Clebsch-Gordan coefficients.

(B. Gutkin)

2017-11-17

PHYS-7143-17 week11

group theory - week 12

Lorentz group; spin

Georgia Tech PHYS-7143

Homework HW12

due Tuesday, November 14, 2017

== 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 12.1 Lorentz spinology Exercise 12.2 Lorentz spin transformations 5 points 5 points

Total of 10 points = 100 % score.

2017-11-07 Predrag Lecture 22

 $SO(4) = SU(2) \otimes SU(2)$; Lorentz group

For SO(4) = SU(2) \otimes SU(2) see also birdtracks.eu chap. 10 Orthogonal groups, pp. 121-123; sect. 20.3.1 SO(4) or Cartan $A_1 + A_1$ algebra

For Lorentz group, read Schwichtenberg [1] Sect. 3.7

2017-11-09 Predrag Lecture 23 SO(1, 3); Spin

Schwichtenberg [1] Sect. 3.7

12.1 Spinors and the Lorentz group

A Lorentz transformation is any invertible real $[4 \times 4]$ matrix transformation Λ ,

$$x^{\prime\mu} = \Lambda^{\mu}_{\ \nu} x^{\nu} \tag{12.1}$$

which preserves the Lorentz-invariant Minkowski bilinear form $\Lambda^T \eta \Lambda = \eta$,

$$x^{\mu}y_{\mu} = x^{\mu}\eta_{\mu\nu}y^{\nu} = x^{0}y^{0} - x^{1}y^{1} - x^{2}y^{2} - x^{3}y^{3}$$

with the metric tensor $\eta = diag(1, -1, -1, -1)$.

A contravariant four-vector $x^{\mu} = (x^0, x^1, x^2, x^3)$ can be arranged [2] into a Hermitian $[2 \times 2]$ matrix in $Herm(2, \mathbb{C})$ as

$$\underline{x} = \sigma_{\mu} x^{\mu} = \begin{pmatrix} x^0 + x^3 & x^1 - ix^2 \\ x^1 + ix^2 & x^0 - x^3 \end{pmatrix}$$
(12.2)

in the hermitian matrix basis

$$\sigma_{\mu} = \bar{\sigma}^{\mu} = (\mathbb{1}_2, \boldsymbol{\sigma}) = (\sigma_0, \sigma_1, \sigma_2, \sigma_3), \quad \bar{\sigma}_{\mu} = \sigma^{\mu} = (\mathbb{1}_2, -\boldsymbol{\sigma}), \quad (12.3)$$

with σ given by the usual Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$
(12.4)

With the trace formula for the metric

$$\frac{1}{2} \operatorname{tr} \left(\sigma_{\mu} \bar{\sigma}_{\nu} \right) = \eta_{\mu\nu} \,, \tag{12.5}$$

the covariant vector x^{μ} can be recovered by

$$\frac{1}{2}\operatorname{tr}\left(\underline{x}\bar{\sigma}^{\mu}\right) = \frac{1}{2}\operatorname{tr}\left(x^{\nu}\sigma_{\nu}\bar{\sigma}^{\mu}\right) = x^{\nu}\eta_{\nu}^{\ \mu} = x^{\mu} \tag{12.6}$$

The Minkowski norm squared is given by

$$\det \underline{x} = (x^0)^2 - (x^1)^2 - (x^2)^2 - (x^3)^2 = x_\mu x^\mu , \qquad (12.7)$$

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and with (12.3)

$$\overline{x} = \begin{pmatrix} x^0 - x^3 & -x^1 + ix^2 \\ -x^1 - ix^2 & x^0 + x^3 \end{pmatrix} = \begin{pmatrix} x_0 + x_3 & x_1 - ix_2 \\ x_1 + ix_2 & x_0 - x_3 \end{pmatrix},$$
(12.8)

the Minkowski scalar product is given by

$$x^{\mu}y_{\mu} = \frac{1}{2} \operatorname{tr}(\underline{x}\,\overline{y})\,. \tag{12.9}$$

The *special linear group* $SL(2, \mathbb{C})$ in two complex dimensions is given by the set of all matrices Λ such that

$$SL(2,\mathbb{C}) = \{\Lambda \in GL(2,\mathbb{C}) \mid \det \Lambda = +1\}.$$

$$(12.10)$$

Let a matrix $\Lambda \in SL(2, \mathbb{C})$ act on $\underline{x} \in Herm(2, \mathbb{C})$ as

$$\underline{x} \mapsto \underline{x}' = \Lambda \underline{x} \Lambda^{\dagger} \tag{12.11}$$

where [†] denotes Hermitian conjugation. The Minkowski scalar product is preserved, det $\underline{x}' = \det \underline{x}$. Thus \underline{x}' can also be represented by a real linear combination of generalized Pauli matrices

$$\underline{x}' = \sigma_{\mu} x'^{\mu}$$
 with $x'_{\mu} x'^{\mu} = x_{\mu} x^{\mu}$ (12.12)

and Λ explicitly acts as a Lorentz transformation (12.1), with $\Lambda^{\mu}_{\nu} = \frac{1}{2} \operatorname{tr} (\bar{\sigma}^{\mu} \Lambda \sigma_{\nu} \Lambda^{\dagger})$. The mapping is two-to-one, as two matrices $\pm \Lambda \in SL(2, \mathbb{C})$ generate the same Lorentz transformation $\Lambda \underline{x} \Lambda^{\dagger} = (-\Lambda) \underline{x} (-\Lambda)^{\dagger}$. This Λ belong to the proper orthochronous Lorentz group $SO^+(1,3)$, and it can be shown that $SL(2,\mathbb{C})$ is simply connected and is the double universal cover of the $SO^+(1,3)$.

Consider the fully antisymmetric Levi-Civita tensor $\varepsilon = -\varepsilon^{-1} = -\varepsilon^{\mathrm{T}}$ in two dimensions

$$\varepsilon = i\sigma_2 = \begin{pmatrix} 0 & 1\\ -1 & 0 \end{pmatrix} . \tag{12.13}$$

This defines a symplectic (i.e., skew-symmetric) bilinear form $\langle u, v \rangle = -\langle v, u \rangle$ on two spinors u and v, elements of the two-dimensional complex vector (or spinor) space \mathbb{C}^2

$$u = \begin{pmatrix} u^1 \\ u^2 \end{pmatrix}, \quad v = \begin{pmatrix} v^1 \\ v^2 \end{pmatrix}, \quad (12.14)$$

equipped with the symplectic form

$$\langle u, v \rangle = u^1 v^2 - u^2 v^1 = u^{\mathsf{T}} \varepsilon v \,. \tag{12.15}$$

This symplectic form is $SL(2, \mathbb{C})$ -invariant

$$\langle u, v \rangle = u^{\mathrm{T}} \varepsilon v = \langle \Lambda u, \Lambda v \rangle = u^{\mathrm{T}} \Lambda^{\mathrm{T}} \varepsilon \Lambda v ,$$
 (12.16)

so one can interpret the group acting on spinors as $SL(2, \mathbb{C}) \cong Sp(2, \mathbb{C})$, the complex symplectic group in two dimensions

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$$\operatorname{Sp}(2,\mathbb{C}) = \left\{ \Lambda \in GL(2,\mathbb{C}) \, | \, \Lambda^{\mathsf{T}} \varepsilon \Lambda = \varepsilon \right\}.$$
(12.17)

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Summary. The group of Lorentz transformations of spinors is the group SL(2,C) of $[2 \times 2]$ complex matrices with determinant 1, i.e., the invariant tensor is the 2-index Levi-Civita ε_{AB} . The SL(2,C) matrices are parametrized by three complex dimensions and therefore six real ones (the matrices have four complex numbers and one complex constraint on the determinant). This matches the 6 dimensions of the group manifold associated with the Lorentz group SO(1,3).

Andrew M. Steane writes "A spinor is the most basic mathematical object that can be Lorentz-transformed." His *An introduction to spinors*, arXiv:1312.3824, might help you develop intuition about spinors.

References

- [1] J. Schwichtenberg, *Physics from Symmetry* (Springer, Berlin, 2015).
- [2] E. Wigner, "On unitary representations of the inhomogeneous Lorentz group", Ann. Math. **40**, 149–204 (1939).

Exercises

12.1. Lorentz spinology.

Show that

(a)

$$x^2 = x_\mu x^\mu = \det \underline{x} \tag{12.18}$$

(b)

$$x_{\mu}y^{\mu} = \frac{1}{2}(\det\left(\underline{x} + \underline{y}\right) - \det\left(\underline{x}\right) - \det\left(\underline{y}\right))$$
(12.19)

(c)

$$x_{\mu}y^{\mu} = \frac{1}{2} \text{tr} \left(\underline{x}\,\overline{y}\right),\tag{12.20}$$

where $\overline{y} = \overline{\sigma}_{\mu} y^{\mu}$

12.2. Lorentz spin transformations.

Let a matrix $\Lambda \in SL(2, \mathbb{C})$ act on hermitian matrix \underline{x} as

$$\underline{x} \mapsto \underline{x}' = \Lambda \underline{x} \Lambda^{\dagger} . \tag{12.21}$$

- (a) Check that \underline{x}' is Hermitian, and the Minkowski scalar product (12.19) is preserved.
- (b) Show that Λ explicitly acts as a Lorentz transformation $x'^{\mu} = \Lambda^{\mu}_{\ \nu} x^{\nu}$.
- (c) Show that the mapping from a $\Lambda \in SL(2,\mathbb{C})$ to the Lorentz transformation in SO(1,3) is two-to-one.

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(d) Consider the Levi-Civita tensor $\epsilon = -\epsilon^{-1} = -\epsilon^{T}$ in two dimensions,

$$\epsilon = \left(\begin{array}{cc} 0 & 1\\ -1 & 0 \end{array}\right) \,, \tag{12.22}$$

and the associated symplectic form

$$\langle u, v \rangle = u^{\mathsf{T}} \varepsilon v = u^1 v^2 - u^2 v^1 \,. \tag{12.23}$$

Show that this symplectic form is $SL(2, \mathbb{C})$ -invariant

$$\langle u, v \rangle = u^{\mathrm{T}} \varepsilon v = \langle \Lambda u, \Lambda v \rangle = u^{\mathrm{T}} \Lambda^{\mathrm{T}} \varepsilon \Lambda v .$$
 (12.24)

2017-11-17

Simple Lie algebras; SU(3)

Georgia Tech PHYS-7143

Homework HW13

due Tuesday, November 21, 2017

== 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 13.1 Root systems of simple Lie algebras5 pointsExercise 13.2 Meson octet5 points

Bonus points

Exercise 13.3 SU(3) symmetry in 3D Harmonic Oscillator 5 points

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



Figure 13.1: (a) The meson (pseudoscalars) octet. (b) The quark triplet, the anti-quark triplet and the gluon octet. (Wikipedia).

2017-11-14 Predrag Lecture 24 Representations of simple algebras

Gutkin notes, Lect. 10 *Representations of simple algebras, general construction. Application to SU*(3), Sects. 1-4.

2017-11-16 Predrag Lecture 25 Cartan construction of SU(3) irreps

Gutkin notes, Lect. 10 Representations of simple algebras, general construction. Application to SU(f3), Sect. 5.

13.1 Literature

Mathematicians map E_8 , and it is bigger than the human genome.

Exercises

13.1. Root system of simple Lie algebras.

a) Determine dimensions of Lie algebras $\mathfrak{so}(N)$, $\mathfrak{su}(N)$ and dimensions of their Cartan subalgebras. What is the number of the positive roots for these Lie algebras?

b) Show that $N \times N$ diagonal matrices H_i with zero traces and uper/lower corner $N \times N$ matrices $E^{(a,b)}$ with the elements $E^{(a,b)}_{i,j} = \delta_{ia}\delta_{ib}$ provide Cartan-Weyl basis of $\mathfrak{su}(N)$. To put it differently, show that $E^{(a,b)}$ are eigenstates for adjoint representation of H_i 's.

(B. Gutkin)

13.2. Meson octet. In Gutkin lecture notes, Lect. 11 Strong interactions: flavor SU(3), the

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meson octet, figure 13.1 (a)

$$\Phi = \begin{pmatrix} \frac{\pi^{0}}{\sqrt{2}} + \frac{\eta}{\sqrt{6}} & \pi^{+} & K^{+} \\ \pi^{-} & -\frac{\pi^{0}}{\sqrt{2}} + \frac{\eta}{\sqrt{6}} & K^{0} \\ K^{-} & \overline{K^{0}} & -\frac{2\eta}{\sqrt{6}} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{\pi^{0}}{\sqrt{2}} & \pi^{+} & 0 \\ \pi^{-} & -\frac{\pi^{0}}{\sqrt{2}} & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & K^{+} \\ 0 & 0 & K^{0} \\ K^{-} & \overline{K^{0}} & 0 \end{pmatrix} + \frac{\eta}{\sqrt{6}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} (J3.1)$$

is interpreted as arising from the adjoint representation of SU(3), i.e., the traceless part of the quark-antiquark $\mathbf{3} \otimes \mathbf{\overline{3}} = \mathbf{1} \oplus \mathbf{8}$ outer product (see figure 13.1 (b)),

$$\begin{pmatrix} u\overline{u} & u\overline{d} & u\overline{s} \\ d\overline{u} & d\overline{d} & d\overline{s} \\ s\overline{u} & s\overline{d} & s\overline{s} \end{pmatrix} .$$
(13.2)

where we have replaced in (13.1) the constituent $q \otimes \overline{q}$ combinations by the names of the elementary particles they build.

Given the quark quantum numbers

	Q	Ι	I_3	Y	B
u	2/3	1/2	1/2	1/3	1/3
d	-1/3	1/2	-1/2	1/3	1/3
s	-1/3	0	0	-2/3	1/3

verify the strangeness and charge assignments of figure 13.1 (a).

13.3. **SU**(3) **symmetry in 3D Harmonic Oscillator.** The Hamiltonian of 3D isotropic harmonic oscillator is given by

$$H = \sum_{i=1}^{3} \frac{p_i^2}{2m} + \frac{m\omega^2}{2} x_i^2 = \hbar \omega \sum_{i=1}^{3} (a_i^{\dagger} a_i + 1/2),$$

where $a_i = \sqrt{\frac{m\omega}{2\hbar}} x_i + i\sqrt{\frac{1}{2m\omega\hbar}} p_i$ is creation (a_i^{\dagger} resp. annihilation) operator satisfying $[a_i, a_i^{\dagger}] = \delta_{ij}, [a_i, a_j] = 0.$

a) Show that $a_i \to U_{i,j}a_j$, with $U \in U(3)$ is a symmetry of the Hamiltonian. In other words isotropic 3D harmonic oscillator has U(3) rather than O(3) symmetry!

b) Calculate degeneracy of the n-th level $E_n = \omega \hbar (n + 3/2)$ of the oscillator.

c) By comparison of dimensions find out which representations of ${\rm SU}(3)$ appear in the spectrum of harmonic oscillator.

(B. Gutkin)

Flavor SU(3)

Georgia Tech PHYS-7143

Homework HW14

due Tuesday, November 28

8 points

== 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 14.1 Gell-Mann–Okubo mass formula

Bonus points

Exercise 15.3 Young tableaux for SU(3)3 pointsExercise 15.4 Irrep projection operators for unitary groups5 points

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



Figure 14.1: A lattice gauge theory calculation of the light QCD spectrum. Horizontal lines and bands are the experimental values with their decay widths. The π , K and and Ξ have no error bars because they are used to set the light and strange quark masses and the overall scale respectively. From Scholarpedia.

2017-11-21 Predrag Lecture 26 Flavor SU(3)

Gutkin notes, Lect. 11 *Strong interactions: flavor* SU(3). Heisenberg isospin SU(2). Gell-Mann flavor SU(3). Gell-Mann-Okubo mass formula.

2017-11-24 Predrag (No lecture) Young tableaux

Young tableaux for SU(3) and SU(n) have not yet been covered in the lectures, but you can easily learn them yourself, from, for example, Gutkin notes, Lect. 12 *Young tableaux*. Boris Gutkin is a grownup, beyond learning new stuff, so he follows old fashioned references such as Fulton and Harris [4]. The resulting simple recipe with 0 explanation can be found, for example, here *C.G. Wohl*.

A modern exposition is given in *Group Theory* – *Birdtracks, Lie's, and Exceptional Groups*, Chapt. 9 *Unitary groups*. Currently I am a fan of the Alcock-Zeilinger algorithm [1–3], based on the simplification rules of ref. [2], which leads to explicitly Hermitian and compact expressions for the projection operators. Alcock-Zeilinger fully supersedes Cvitanović's formulation, and any future full exposition of birdtracks reduction of SU(N) tensor products into irreducible representations should be based on the Alcock-Zeilinger algorithm.

The Gell-Mann-Okubo mass sum rules [5–7] are an easy consequence of the approximate SU(3) flavor symmetry. Determination of quark masses is much harder - they are parameters of the standard model, determined by optimizing the spectrum of particle masses obtained by lattice QCD calculations as compared to the experimental baryon and meson masses. The best determination of the mass spectrum as of 2012 is given in figure 14.1. Up, down quarks are about 3 and 6 MeV, respectively, with strange quark mass about 100 MeV, all with large error brackets. As of 2017, I have not found an update to figure 14.1, but the latest on the subject can probably be traced in Georg von Hippel's latticeqcd.blogspot.com.

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References

- [1] J. Alcock-Zeilinger and H. Weigert, "Transition operators", J. Math. Phys. 58, 051702 (2016).
- [2] J. Alcock-Zeilinger and H. Weigert, "Compact Hermitian Young projection operators", J. Math. Phys. 58, 051702 (2017).
- [3] J. Alcock-Zeilinger and H. Weigert, "Simplification rules for birdtrack operators", J. Math. Phys. **58**, 051701 (2017).
- [4] W. Fulton and J. Harris, *Representation Theory* (Springer, New York, 1991).
- [5] M. Gell-Mann, *The Eightfold Way: A Theory of Strong Interaction Symmetry*, Synchrotron Laboratory Report CTSL-20 (CalTech, 1961).
- [6] M. Gell-Mann, "Symmetries of baryons and mesons", Phys. Rev. 125, 1067– 1084 (1962).
- [7] S. Okubo, "Note on unitary symmetry in strong interactions", Progr. Theor. Phys. 27, 949–966 (1962).

Exercises

14.1. **Gell-Mann–Okubo mass formula.** The mass symmetry-breaking interaction for an isospin multiplet is proportional to the 3rd component of the isospin operator, I_3 . Similarly, the symmetry-breaking interaction of SU(3) for the meson octet is given by the 8th component of the octet operator $Y = \lambda_8$. Derive the GMO mass formula for mesons

$$m_{\eta}^2 = \frac{4\,m_K^2 - m_{\pi}^2}{3}\,.\tag{14.1}$$

by eliminating the parameter for the strength of this interaction, as in Gutkin lecture notes, Lect. 11 Strong interactions: flavor SU(3).

Many particle systems. Young tableaux

Georgia Tech PHYS-7143

Homework HW15

due Tuesday, December 5

== 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 15.1 Representations of SU(3)Exercise 15.2 Young tableaux for S_5 5 points 3 points

Bonus points

Exercise 15.3 Young tableaux for $SU(3)$	3 points
Exercise 15.4 Irrep projection operators for unitary groups	5 points

Total of 20 points = 100 % score.

2017-11-28 Predrag Lecture 28 Many particle systems. Young tableaux

Gutkin notes, Lect. 12 Many particle systems.

Excerpt from Predrag's monograph [4], fetch it here: Sect. 9.3 Young tableaux.

2017-11-30 Predrag Lecture 29 Young tableaux

Excerpts from Predrag's monograph [4], fetch them here:

Sect. 2.2 *First example:* SU(n) (skim over casimirs and beyond: this example gives you a flavor of birdtracks computations, you do not need to work it out in detail),

Sect. 6.1 Symmetrization, Sect. 6.2 Antisymmetrization, Sect. 9.1 Two-index tensors, Sect. 9.2 Three-index tensors, and Table 9.1.

Reading for this week: Sect. 9.3 Young tableaux.

15.1 Literature

The clearest current exposition and the most powerful irrep reduction of SU(n) is given in the triptych of papers by Judith Alcock-Zeilinger and her thesis adviser H. Weigart, University of Cape Town:

Simplification rules for birdtrack operators [3], Compact Hermitian Young projection operators [2], and Transition operators [1].

However, you want to study these in detail only if your research leads you to study of multiparticle states.

References

- [1] J. Alcock-Zeilinger and H. Weigert, "Transition operators", J. Math. Phys. 58, 051702 (2016).
- [2] J. Alcock-Zeilinger and H. Weigert, "Compact Hermitian Young projection operators", J. Math. Phys. **58**, 051702 (2017).
- [3] J. Alcock-Zeilinger and H. Weigert, "Simplification rules for birdtrack operators", J. Math. Phys. 58, 051701 (2017).
- [4] P. Cvitanović, *Group Theory Birdtracks, Lie's, and Exceptional Groups* (Princeton Univ. Press, Princeton, NJ, 2008).

Exercises

- 15.1. **Representations of SU**(3). Any irrep of SU(3) can be labeled D(p,q) by its highest weight $\lambda = p\lambda_1 + q\lambda_2$, where $\lambda_{1,2}$ are the two fundamental weights.
 - (a) Find all irreps D(p,q) of SU(3) with the dimensions less then 20 (see lecture notes for the dimensions of D(p,q)).
 - (b) Draw the lattice Λ generated by $\lambda_{1,2}$ and mark there all the weights v (i.e., lattice nodes) which belong to irrep. D(3,0). Is D(3,0) a real irrep?
 - (c) Consider product (reducible) representation 3 ⊗ 3, where 3 = D(1,0) is the fundamental irrep. Mark all the weights v on Λ which belong to 3 ⊗ 3. Using this find out decomposition of 3 ⊗ 3 into irreps:

 $3 \otimes 3 = \Box \oplus \bigtriangleup, \qquad \Box =?, \qquad \bigtriangleup =?$

Hint: see lecture notes for similar exercise on $3 \otimes \overline{3}$.

(d) Using previous results find decomposition of $3 \otimes 3 \otimes 3$ into irreps.

(B. Gutkin)

15.2. Young tableaux for S_5 .

- (a) Draw all Young diagrams for the symmetric group S_5 . How many irreducible representations has it? Which of the diagrams correspond to one-dimensional irreps?
- (b) Find Young diagram corresponding to the irrep of S_5 with the largest dimension? Draw Young tableaux corresponding to this irrep/Young diagram. What is the dimension of this irrep?
- (c) What are the dimensions of the remaining irreps?

(B. Gutkin)

15.3. **Young tableaux for SU**(3). Solve exercise 15.1 (c,d) by using Young tableaux. *Remark:* If Young tableaux for SU(3) are not covered in the lectures, learn them yourself from, for example, *Group Theory Birdtracks, Lie's, and Exceptional Groups.* The resulting simple recipe with 0 explanation can be found, for example, here *C.G. Wohl.*

(B. Gutkin)

15.4. **Irrep projection operators for unitary groups.** Derive projection operators and dimensions for irreps of the Kronecker product of the defining and the adjoint reps of SU(n) listed in *Group Theory Birdtracks, Lie's, and Exceptional Groups*, Table 9.3. (Ignore "indices," we have not defined them.)

Wigner 3- and 6-j coefficients

Georgia Tech PHYS-7143

Homework HW16

due whenever - optional, not graded

== 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 16.1 *Gravity tensors*, part (a) Exercise 16.1 *Gravity tensors*, part (b) Exercise 16.1 *Gravity tensors*, part (c) Exercise 16.1 *Gravity tensors*, part (d) Exercise 16.1 *Gravity tensors*, part (e) Exercise 16.1 *Gravity tensors*, part (f) Exercise 16.1 *Gravity tensors*, part (g) Exercise 16.1 *Gravity tensors*, part (h)

Bonus points

Exercise 16.1 *Gravity tensors*, part (i) Exercise 16.1 *Gravity tensors*, part (j) 2 points 4 points 1 point 2 points 3 points 4 points 3 points 6 points

4 points 10 points

Total of 20 points = 100 % score.

2017-12-05 Predrag Lecture 30 Wigner 3- and 6-j coefficients

Excerpts from Predrag's monograph [4], fetch them here:

Background reading on groups, vector spaces, tensors, invariant tensors, invariance groups (my advice is to start with Sect. 5.1 *Couplings and recouplings*, then backtrack to these introductory sections as needed):

Sect. 3.2 Defining space, tensors, reps,

Sect. 3.3 Invariants,

Sect. 4.1 Birdtracks,

Sect. 4.2 Clebsch-Gordan coefficients, and

Sect. 4.3 Zero- and one-dimensional subspaces.

The final result, discussed in the day's whiteboard-side chat, is invariant and highly elegant: any group-theoretical invariant quantity can be expressed in terms of Wigner 3- and 6-j coefficients:

Sect. 5.1 Couplings and recouplings,

Sect. 5.2 Wigner 3n-j coefficients, and

Sect. 5.3 Wigner-Eckart theorem.

The rest is just bedside reading, nothing technical: Sect. 4.8 *Irrelevancy of clebsches* and Sect. 4.9 *A brief history of birdtracks*.

Course finale: Indiana Jones video (click here).

16.1 Literature

We noted in sect. 2.1 that a practically-minded physicist always has been, and continues to be resistant to gruppenpest. Apparently already in 1910 James Jeans wrote, while discussing what should a physics syllabus contain: "We may as well cut out the group theory. That is a subject that will never be of any use in physics."

Voit writes here about the "The Stormy Onset of Group Theory in the New Quantum Mechanics," citing Bonolis [2] *From the rise of the group concept to the stormy onset of group theory in the New Quantum Mechanics. A saga of the invariant characterization of physical objects, events and theories.*

Chayut [3] From the periphery: the genesis of Eugene P. Wigner's application of group theory to quantum mechanics traces the origins of Wigner's application of group theory to quantum mechanics traces the origins of Wigner's application of group theory to quantum physics to his early work as a chemical engineer, in chemistry and crystallography. "In the early 1920s, crystallography was the only discipline in which symmetry groups were routinely used. Wigner's early training in chemistry exposed him to conceptual tools which were absent from the pedagogy available to physicists for many years to come. This both enabled and pushed him to apply the group theoretic approach to quantum physics. It took many years for the approach first introduced by Wigner in the 1920s – and whose reception by the physicists was initially problematical – to assume the pivotal place it now holds." Another historical exposition is given by Scholz [6] Introducing groups into quantum theory (1926–1930).

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So what is group theory good for? By identifying the symmetries, one can apply group theory to determine good quantum numbers which describe a physical state (i.e., the irreps). Group theory then says that many matrix elements vanish, or shows how are they related to others. While group theory does determine the actual value of a matrix element of interest, it vastly simplifies its calculation.

The old fashioned atomic physics, fixated on SO(3) / SU(2), is too explicit, with too many bras and kets, too many square roots, too many deliriously complicated Clebsch-Gordan coefficients that you do not need, and way too many labels, way too explicit for you to notice that all of these are eventually summed over, resulting in a final answer much simpler than any of the intermediate steps.

I wrote my book [4] *Group Theory - Birdtracks, Lie's, and Exceptional Groups* to teach you how to compute everything you need to compute, without ever writing down a single explicit matrix element, or a single Clebsch-Gordan coefficient. There are two versions. There is a particle-physics / Feynman diagrams version that is index free, graphical and easy to use (at least for the low-dimensional irreps). The key insights are already in Wigner's book [8]: the content of symmetry is a set of invariant numbers that he calls 3n-j's. Then there are various mathematical flavors (Weyl group on Cartan lattice, etc.), elegant, but perhaps too elegant to be computationally practical.

But it is nearly impossible to deprogram people from years of indoctrination in QM and EM classes. The professors have no time to learn new stuff, and students love manipulating their mu's and nu's.

References

- S. L. Adler, J. Lieberman, and Y. J. Ng, "Regularization of the stress-energy tensor for vector and scalar particles propagating in a general background metric", Ann. Phys. 106, 279–321 (1977).
- [2] L. Bonolis, "From the Rise of the Group Concept to the Stormy Onset of Group Theory in the New Quantum Mechanics. A saga of the invariant characterization of physical objects, events and theories", Rivista Nuovo Cim. 27, 1–110 (2005).
- [3] M. Chayut, "From the periphery: the genesis of Eugene P. Wigner's application of group theory to quantum mechanics", Found. Chem. **3**, 55–78 (2001).
- [4] P. Cvitanović, Group Theory Birdtracks, Lie's, and Exceptional Groups (Princeton Univ. Press, Princeton, NJ, 2008).
- [5] R. Penrose, "Applications of negative dimensional tensors", in *Combinatorial mathematics and its applications*, edited by D. J. J.A. Welsh (Academic, New York, 1971), pp. 221–244.
- [6] E. Scholz, "Introducing groups into quantum theory (1926–1930)", Hist. Math. 33, 440–490 (2006).
- [7] S. Weinberg, Gravitation and Cosmology: Principles and Applications of the General Theory of Relativity (Wiley, New York, 1972).
- [8] E. P. Wigner, *Group Theory and Its Application to the Quantum Mechanics of Atomic Spectra* (Academic, New York, 1931).

Exercises

16.1. **Gravity tensors.** In this problem we will apply diagrammatic methods ("birdtracks") to construct and count the numbers of independent components of the "irreducible rankfour gravity curvature tensors." However, any notation that works for you is OK, as long as you obtain the same irreps and their dimensions. The goal of this exercise (longish, as much of it is the recapitulation of the material covered in the book) is to give you basic understanding for how Young tableaux work for groups other than U(n). We start with

Part 1 : U(n) Young tableaux decomposition.

(a) The Riemann-Christoffel curvature tensor of general relativity has the following symmetries (see, for example, Weinberg [7] or the Riemann curvature tensor wiki):

$$R_{\alpha\beta\gamma\delta} = -R_{\beta\alpha\gamma\delta} \tag{16.1}$$

$$R_{\alpha\beta\gamma\delta} = R_{\gamma\delta\alpha\beta} \tag{16.2}$$

$$R_{\alpha\beta\gamma\delta} + R_{\beta\gamma\alpha\delta} + R_{\gamma\alpha\beta\delta} = 0.$$
 (16.3)

Introducing a birdtrack notation for the Riemann tensor

$$R_{\alpha\beta\gamma\delta} = \frac{\beta}{\gamma} \underbrace{\mathbf{R}}_{\mathbf{\delta}}, \qquad (16.4)$$

check that we can state the above symmetries as

$$R_{\alpha\beta\gamma\delta} = -R_{\beta\alpha\gamma\delta}$$

$$R_{\alpha\beta\gamma\delta} = R_{\gamma\delta\alpha\beta}$$
(16.5)
$$R_{\alpha\beta\gamma\delta} = R_{\gamma\delta\alpha\beta}$$

$$\mathbf{R} = \mathbf{R}, \qquad (16.6)$$

$$R_{\alpha\beta\gamma\delta} + R_{\beta\gamma\alpha\delta} + R_{\gamma\alpha\beta\delta} = 0$$

$$\boxed{R} + \boxed{R} + \boxed{R} = 0. \quad (16.7)$$

The first condition says that R lies in the $\square \otimes \square$ subspace.

(b) The second condition says that R lies in the $\square \leftrightarrow \square$ interchange-symmetric subspace.



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(c) Show that the third condition (16.7) says that R has no components in the irrep:

$$\mathbf{R} + \mathbf{R} + \mathbf{R} = 3 \mathbf{R} = 0. \quad (16.9)$$

Hence, the symmetries of the Riemann tensor are summarized by the irrep projection operator [5]:

(d) Verify that the Riemann tensor is in the \square subspace

(e) Compute the number of independent components of the Riemann tensor $\mathbf{R}_{\alpha\beta\gamma\delta}$ by taking the trace of the \square irrep projection operator:

$$d_R = \operatorname{tr} \mathbf{P}_R = \frac{n^2(n^2 - 1)}{12} \ . \tag{16.12}$$

Part 2 : SO(n) Young tableaux decomposition

The Riemann tensor has the symmetries of the \square irrep of U(n). However, gravity is also characterized by the symmetric tensor $g_{\alpha\beta}$, that reduces the symmetry to a local SO(n) invariance (more precisely SO(1, n - 1), but compactness is not important here). The extra invariants built from $g_{\alpha\beta}$'s decompose U(n) reps into sums of SO(n) reps. Orthogonal group SO(n) is the group of transformations that leaves invariant a symmetric quadratic form $(q, q) = g_{\mu\nu}q^{\mu}q^{\nu}$, with a primitive invariant rank-2 tensor:

$$g_{\mu\nu} = g_{\nu\mu} = \mu \longrightarrow \nu \qquad \qquad \mu, \nu = 1, 2, \dots, n.$$
 (16.13)

If (q,q) is an invariant, so is its complex conjugate $(q,q)^* = g^{\mu\nu}q_{\mu}q_{\nu}$, and

$$g^{\mu\nu} = g^{\nu\mu} = \mu \longrightarrow \nu \tag{16.14}$$

is also an invariant tensor. The matrix $A^{\nu}_{\mu} = g_{\mu\sigma}g^{\sigma\nu}$ must be proportional to unity, as otherwise its characteristic equation would decompose the defining n-dimensional rep. A convenient normalization is

*σ*11

$$g_{\mu\sigma}g^{\sigma\nu} = \delta^{\nu}_{\mu}$$

$$\longleftrightarrow = -$$
(16.15)

As the indices can be raised and lowered at will, nothing is gained by keeping the arrows. Our convention will be to perform all contractions with metric tensors with upper indices and omit the arrows and the open dots:

$$g^{\mu\nu} \equiv \mu - \nu . \qquad (16.16)$$

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The U(n) 2-index tensors can be decomposed into a sum of their symmetric and antisymmetric parts. Specializing to the subgroup SO(n), the rule is to lower all indices on all tensors, and the symmetrization projection operator is written as

$$\begin{split} S_{\mu\nu,\rho\sigma} &= g_{\rho\rho'}g_{\sigma\sigma'}S_{\mu\nu},^{\rho'\sigma'} \\ &= \frac{1}{2}\left(g_{\mu\sigma}g_{\nu\rho} + g_{\mu\rho}g_{\nu\sigma}\right) \end{split}$$

From now on, we drop all arrows and $g^{\mu\nu}$'s and write the decomposition into symmetric and antisymmetric parts as

The new invariant tensor, specific to SO(n), is the index contraction:

$$\mathbf{T}_{\mu\nu,\rho\sigma} = g_{\mu\nu}g_{\rho\sigma}, \qquad \mathbf{T} = \int \left(\begin{array}{c} . \end{array} \right)$$
 (16.18)

Its characteristic equation

$$\mathbf{T}^2 = \bigcup \quad \bigcirc \quad \bigcirc \quad \frown = n\mathbf{T} \tag{16.19}$$

yields the trace and the traceless part projection operators. As T is symmetric, ST = T, only the symmetric subspace is reduced by this invariant.

(f) Show that SO(n) 2-index tensors decompose into three irreps:

traceless symmetric:

$$(P_2)_{\mu\nu,\rho\sigma} = \frac{1}{2} \left(g_{\mu\sigma} g_{\nu\rho} + g_{\mu\rho} g_{\nu\sigma} \right) - \frac{1}{n} g_{\mu\nu} g_{\rho\sigma} = \boxed{-\frac{1}{n}} - \frac{1}{n} \left(16.20 \right)$$

$$(P_1)_{\mu\nu,\rho\sigma} = \frac{1}{n}g_{\mu\nu}g_{\rho\sigma} = \frac{1}{n}$$

 $(P_1)_{\mu\nu,\rho\sigma} = \frac{1}{n} g_{\mu\nu} g_{\rho\sigma} = \frac{1}{n} \sum_{\nu,\sigma} (P_3)_{\mu\nu,\rho\sigma} = \frac{1}{2} (g_{\mu\sigma} g_{\nu\rho} - g_{\mu\rho} g_{\nu\sigma}) =$ singlet: (16.21)(16.22) antisymmetric:

What are the dimensions of the three irreps?

(g) In the same spirit, the U(n) irrep \square is decomposed by the SO(n) intermediate 2-index state invariant matrix

Show that the intermediate 2-index subspace splits into three irreducible reps by (16.20) – (16.22):

$$\mathbf{Q} = \frac{1}{n} \underbrace{\mathbf{Q}}_{0} + \mathbf{Q}_{S} + \mathbf{Q}_{A} + \left\{ \underbrace{\mathbf{P}}_{\mathbf{Q}} + \underbrace{\mathbf{Q}}_{\mathbf{Q}} - \frac{1}{n} \underbrace{\mathbf{Q}}_{\mathbf{Q}} + \underbrace{\mathbf{Q}}_{\mathbf{Q}} \right\} + \underbrace{\mathbf{P}}_{\mathbf{Q}} \underbrace{\mathbf{Q}}_{\mathbf{Q}} + \underbrace{\mathbf{Q}}_{$$

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Show that the antisymmetric 2-index state does not contribute

$$\mathbf{P}_{\mathbf{R}}\mathbf{Q}_A = 0. \tag{16.25}$$

(Hint: The Riemann tensor is symmetric under the interchange of index pairs.)

(h) Fix the normalization of the remaining two projection operators by computing $\mathbf{Q}_S^2, \mathbf{Q}_0^2$:

$$\mathbf{P}_0 = \frac{2}{n(n-1)} \underbrace{}_{(n-1)} \underbrace{}_{($$

$$\mathbf{P}_{S} = \frac{4}{n-2} \left\{ \mathbf{P}_{S} - \frac{1}{n} \mathbf{P}_{S} \right\}$$
(16.27)

and compute their dimensions.

This completes the SO(n) reduction of the \square U(n) irrep (16.11):

U(n)	\rightarrow	$\mathrm{SO}(n)$				
	\rightarrow		+		+	0
\mathbf{P}_R	=	\mathbf{P}_W	+	\mathbf{P}_{S}	+	\mathbf{P}_0
$\frac{n^2(n^2-1)}{12}$	=	$\frac{(n+2)(n+1)n(n-3)}{12}$	+	$\frac{(n+2)(n-1)}{2}$	+	1

(16.28)

The projection operator for the SO(n) traceless \square irrep is:

п

$$\mathbf{P}_{W} = \mathbf{P}_{R} - \mathbf{P}_{S} - \mathbf{P}_{0}$$

$$\mathbf{P}_{W} = \frac{4}{3} \mathbf{P}_{W} - \frac{4}{n-2} \mathbf{P}_{0} + \frac{2}{(n-1)(n-2)} \mathbf{P}_{0} \mathbf{P}_{0}$$

(i) The above three projection operators project out the standard, SO(n)-irreducible general relativity tensors:

Curvature scalar:

ъ

$$R = -\left(\boxed{\mathbf{R}} = R^{\mu}_{\ \nu\mu}{}^{\nu}$$
(16.30)

Traceless Ricci tensor:

п

п

$$R_{\mu\nu} - \frac{1}{n}g_{\mu\nu}R = -\left(\mathbf{R} + \frac{1}{n}\right)\left(\mathbf{R}\right)$$
(16.31)

Weyl tensor:

$$C_{\lambda\mu\nu\kappa} = (\mathbf{P}_W R)_{\lambda\mu\nu\kappa}$$

$$= \mathbf{R} - \frac{4}{n-2} \mathbf{R} + \frac{2}{(n-1)(n-2)} \mathbf{R}$$

$$= R_{\lambda\mu\nu\kappa} + \frac{1}{n-2} (g_{\mu\nu}R_{\lambda\kappa} - g_{\lambda\nu}R_{\mu\kappa} - g_{\mu\kappa}R_{\lambda\nu} + g_{\lambda\kappa}R_{\mu\nu})$$

$$- \frac{1}{(n-1)(n-2)} (g_{\lambda\kappa}g_{\mu\nu} - g_{\lambda\nu}g_{\mu\kappa})R. \qquad (16.32)$$

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The numbers of independent components of these tensors are given by the dimensions of corresponding irreducible subspaces in (16.28).

What is the lowest dimension in which the Ricci tensor contributes? the Weyl tensor contributes? Show that in 2, respectively 3 dimensions, we have

$$n = 2: \quad R_{\lambda\mu\nu\kappa} = (P_0 R)_{\lambda\mu\nu\kappa} = \frac{1}{2} (g_{\lambda\nu}g_{\mu\kappa} - g_{\lambda\kappa}g_{\mu\nu})R$$

$$n = 3: \qquad = g_{\lambda\nu}R_{\mu\kappa} - g_{\mu\nu}R_{\lambda\kappa} + g_{\mu\kappa}R_{\lambda\nu} - g_{\lambda\kappa}R_{\mu\nu} \quad (16.33)$$

$$-\frac{1}{2} (g_{\lambda\nu}g_{\mu\kappa} - g_{\lambda\kappa}g_{\mu\nu})R \quad .$$

(j) The last example of this exercise is an application of birdtracks to general relativity index manipulations. The object is to find the characteristic equation for the Riemann tensor in *four dimensions*.

The antisymmetrization tensor $A_{a_1a_2...}, {}^{b_p...b_2b_1}$ has nonvanishing components, only if all lower (or upper) indices differ from each other. If the defining dimension is smaller than the number of indices, the tensor A has no nonvanishing components:

This identity implies that for p > n, not all combinations of p Kronecker deltas are linearly independent. A typical relation is the p = n + 1 case

$$0 = \prod_{\substack{1 \ 2 \ \cdots \ n+1}}^{n} = \prod_{\substack{1 \ 2 \ \cdots \ n+1}}^{n} - \prod_{\substack{1 \ 2 \ \cdots \ n}}^{n} + \prod_{\substack{1 \ 2 \ \cdots \ n}}^{n} - \dots$$
(16.35)

Contract (16.34) with two Riemann tensors:

$$0 = \begin{array}{c} \hline R \\ \hline R \\ \hline R \end{array}, \quad (16.36)$$

and obtain the characteristic equation by expanding with (16.35):

$$0 = 2 \mathbf{R} \mathbf{R} - 4 \mathbf{R} \mathbf{R}$$
$$-4 \mathbf{R}$$
$$-4 \mathbf{R} \mathbf{R}$$
$$-4 \mathbf{R}$$
$$-4$$

This identity has been used by Adler et al., eq. (E2) in ref. [1].

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An overview, and the epilogue

This whole course has only one message:

If you have a symmetry, **USE** it!

These notes in isolation do not make much sense - the essence of teaching is unveiling of concepts on a black/white board at human pace, interacting in live time. But nevertheless the notes might be useful to you, as they are hyperlinked to the literature that develops a given topic into depth. Here is a brief summary of the course, the ideas you want to take with you:

week 1 Linear algebra

Projection operators (1.33): eigenvalues of a matrix split a vector space into subspaces.

week 2 Finite groups

Groups, permutations, group multiplication tables, rearrangement theorem, subgroups, cosets, classes.

week 3 Representation theory

Irreps, regular representation. So far, everything was intuitive: a representation of a group was bunch of 0's and 1's indicating how a group operation permutes physical objects. But now the first surprise:

Any representation of any finite group can be put into unitary form, and so complex-valued vector spaces and unitary representation matrices make their entrance.

week 4 Characters

Schur's Lemma. Unitary matrices can be diagonalized, and from that follows the Wonderful Orthogonality Theorem for Characters (coordinate independent, intrinsic numbers), and the full reducibility of any representation of any finite group.

week 5 Classes

The algebra of central or 'all-commuting' class operators, connects the reduction in terms of characters to the projection operators of week 1. The key idea:

Define a group by what objects (primitive invariant tensors) it leaves invariant.

week 6 Fundamental domain

Dynamical systems application: the Lorenz flow and its C₂ symmetry.

week 7 Lorenz to Van Gogh; Diffusion confusion

(1) Conclusion of the finite groups part of the course: Lorenz flow desymmetrization: if the system is nonlinear, its symmetry reduction is not easy.

(2) So far, everything was finite and compact. Next: two distinct ways of going infinite: (a) discrete translations, exemplified by deterministic diffusion and space groups of week 8, and (b) continuous Lie groups, exemplified by rotations of week 9.

week 8 Space groups

Translation group, Bravais lattice, wallpaper groups, reciprocal lattice, Brilluoin zone.

week 9 Continuous groups

Lie groups. Matrix representations. Invariant tensors. Lie algebra. Adjoint representation, Jacobi relation. Birdtracks.

Irreps of SO(2) and O(2) Clebsch-Gordan series (i.e., reduction of their products).

week 10 SO(3) characters; O(2) symmetry sliced

(a) Group integrals. SO(3) character orthogonality.

(b) Continuous symmetry reduction for a *nonlinear* system is much harder than discrete symmetry reduction of week 7. "Slicing" is a research level topic, will not be included in the final.

week 11 SU(2) and SO(3)

 $SU(2) \simeq SO(3)$ correspondence leads to the next rude awakening; our 3-dimensional Euclidean space is not fundamental! All irreps of SO(3) are built from 2-dimensional complex vectors, or 1/2 spins. Birdtrack notation for the smallest irreps of SO(*n*).

week 12 Lorentz group; spin

(a) We now loose compactness: even though the SO(1,3) Lorentz invariance group of the Minkowski space symmetries is not compact, its Lie algebra still closes, as for the compact SO(4).

(b) $SO(4) \simeq SU(2) \otimes SU(2)$ correspondence leads to the Minkowski 4-dimensional space not being fundamental either - all irreps of the Lorentz group are built from combinations of 2-dimensional complex vectors, or spinors.

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(c) Not included in the final: together with general relativity, this leads to replacement of the Minkowski continuum by a 4-dimensional spacetime (or quantum) foam, a candidate theory of quantum gravity.

week 13 Simple Lie algebras; SU(3)

The next profound shift:

So far all our group notions were based on tangible, spatial intuition: permutations, reflections, rotations. But now Lie groups take on a life of their own.

(a) The SO(3) theory of angular momenta generalizes to Killing-Cartan lattices, and a fully abstract enumeration of all possible semi-simple compact Lie groups.

(b) SU(2) is promoted to an *internal* isospin symmetry, decoupled from our Euclidean spatial intuition. Modern particle physics is born, with larger and larger internal symmetry groups, tacked onto higher and higher dimensional continuum spacetimes.

week 14 Flavor SU(3)

Gell-Mann–Okubo formula. The next triumph of particle physics is yet another departure; observed baryons and mesons are built up from quarks, particles by assumption unobservable in isolation.

week 15 Young tableaux

We have come full circle now: as a much simpler alternative to the Cartan-Killing construction, irreps of the *finite* symmetric group S_n classify the irreps of the *continuous* SU(n) symmetry multi-particle states.

week 16 Wigner 3- and 6-j coefficients

The goal of group theory is to predict measurable numbers, numbers independent of any particular choice of coordinate. The full reducibility says that any such number is built from 3- and 6-j coefficients: they are the total content of group theory.