Applied Mathematics IV

Pei-Ming Ho
pmho@phys.ntu.edu.tw
Department of Physics
National Taiwan University
Taipei 106, Taiwan, R.O.C.
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This semester we will discuss about PDE and other stuffs which were not covered by Applied Math I, II or III. This may include some Lie algebra and differential geometry.

The textbook is *Mathews and Walker: Mathematical Methods of Physics*, to be abbreviated as M&W below. This note is provided as a supplement, not a substitute, to the textbook.

Another standard textbook is *Arfken and Weber: Mathematical Methods for Physicists*, 6th ed. (Elsevier Academic Press), to be abbreviated as A&W below. You are encouraged to consult materials in there.

A good textbook on Differential Geometry which you can study by yourself is: *Schutz: Geometrical Methods of Mathematical Physics*, to be abbreviated as S below.

But it is not necessary to buy the latter two books. We will also provide links to notes on the course webpage:
http://homepage.ntu.edu.tw/ pmho/ApplMath4/Syllabus.htm

We will use *Einstein's summation convention* in this note.

Chapter 1

Special Functions

1.1 Introduction

Some functions are special and arise naturally in elementary problems. Here are a few possible reasons how some functions are "special".

- It arises as part of the eigenfxs of the Laplace op.

$$\nabla^2\phi + \lambda\phi = 0. \tag{1.1}$$

  The Laplace op. in flat space $\nabla^2 = \sum_i \partial_i^2$ appears in almost every elementary problem in physics (wave eq, diffusion eq, Schrödinger eq., etc.)
  In Cartesian coordinates, $e^{i\vec{k}\cdot\vec{x}}$ is special. (And hence sin, cos are special.)
  In spherical coordinates, Legendre polynormials are special.

- It has a geometrical meaning.
- It has some interesting algebraic properties.
- They form a complete basis for a certain space of functions.

More generally, variations of this eq., say, $(\nabla^2 - V(\vec{r}))\phi + \lambda\phi = 0$ for certain V's and curved spaces that are important for physicists/mathematicians, can also lead to study of special functions.

We will not expect anyone to memorize or to be able to derive all the equations listed below. The purpose of listing all these equations is to give you an idea about what kind of identities exist for a typical special function. In the future, when you need to use these properties of a certain special function, you will not panic and know what kind of tools you may have to solve the problem at hand.

1.2 Legendre Polynomials

Orthogonality:

$$\int_{-1}^{1} dx P_m(x) P_n(x) = \frac{2}{2n+1}\delta_{mn}. \tag{1.2}$$

Examples:

$$P_0 = 1 \tag{1.3}$$
$$P_1 = x \tag{1.4}$$
$$P_2 = \frac{1}{2}(3x^2 - 1) \tag{1.5}$$
$$P_3 = \frac{1}{2}(5x^3 - 3x) \tag{1.6}$$

Boundary condition:

$$P_n(1) = 1 \qquad \forall n.$$

General formula:

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n. \tag{1.7}$$

Generating function:

$$g(t,x) = \sum_{n=0}^{\infty} P_n(x)t^n = \frac{1}{\sqrt{1-2xt+t^2}}. \tag{1.8}$$

Recurrence relations:

$$(n+1)P_{n+1}(x) - (2n+1)xP_n(x) + nP_{n-1}(x) = 0 \tag{1.9}$$

$$(1-x^2)P_n'(x) = -nxP_n(x) + nP_{n-1}(x). \tag{1.10}$$

Differential equation:

$$(1-x^2)y'' - 2xy' + n(n+1)y = 0. \tag{1.11}$$

1.3 Hermite Polynomials

Orthogonality:

$$\int_{-\infty}^{\infty} dx e^{-x^2} H_m(x)H_n(x) = 2^n n!\sqrt{\pi}\delta_{mn}. \tag{1.12}$$

Examples:

The coefficient of the x^n term in H_n is 2^n.

$$H_0 = 1 \tag{1.13}$$

$$H_1 = 2x \tag{1.14}$$

$$H_2 = 4x^2 - 2 \tag{1.15}$$

$$H_3 = 8x^3 - 12x \tag{1.16}$$

Symmetry:

$$H_n(-x) = (-1)^n H_n(x). \tag{1.17}$$

General formula:

$$H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}. \tag{1.18}$$

Generating function:

$$e^{2xt-t^2} = \sum_{n=0}^{\infty}\frac{t^n}{n!}H_n(x). \tag{1.19}$$

Recurrence relations:

$$H_{n+1} = 2xH_n - 2nH_{n-1} \tag{1.20}$$

$$H_n'(x) = 2nH_{n-1}(x) \tag{1.21}$$

Differential equation:

$$y'' - 2xy' + 2ny = 0. \tag{1.22}$$

1.4 Laguerre Polynomial

Orthogonality:

$$\int_0^\infty dx e^{-x} L_m(x) L_n(x) = \delta_{mn}. \tag{1.23}$$

Example:

Boundary condition:

$L_n(0) = 1 \qquad \forall n.$

$$L_0 = 1 \tag{1.24}$$
$$L_1 = 1 - x \tag{1.25}$$
$$L_2 = 1 - 2x + \frac{1}{2}x^2 \tag{1.26}$$
$$L_3 = 1 - 3x + \frac{3}{2}x^2 - \frac{1}{6}x^3 \tag{1.27}$$

General formula:

$$L_n = \frac{e^x}{n!}\frac{d^n}{dx^n}\left(x^n e^{-x}\right). \tag{1.28}$$

Generating function:

$$g(x,z) = \sum_{n=0}^{\infty} z^n L_n = \frac{e^{-\frac{xz}{1-z}}}{1-z}. \tag{1.29}$$

Recurrence relations:

$$(n+1)L_{n+1} = (2n+1-x)L_n - nL_{n-1}, \tag{1.30}$$
$$xL_n'(x) = nL_n(x) - nL_{n-1}(x), \tag{1.31}$$

Differential equation:

$$xy'' + (1-x)y' + ny = 0. \tag{1.32}$$

1.5 Bessel Functions

General formula:

$$J_m(x) = \sum_{\ell=0}^{\infty} \frac{(-1)^\ell x^{2\ell+m}}{2^{2\ell+m}\ell!(m+\ell)!}. \tag{1.33}$$

Normalization:

$\int_0^\infty dx\, J_n(x) = 1.$

Generating function:

$$e^{x(t-1/t)/2} = \sum_{n=-\infty}^{\infty} t^n J_n(x). \tag{1.34}$$

From this we have

$e^{ix\cos\theta} = \sum_{n=-\infty}^{\infty} i^n e^{in\theta} J_n(x).$

Recurrance relation:

$$\frac{d}{dx}\left(x^m J_m(x)\right) = x^m J_{m-1}(x). \tag{1.35}$$

Differential equation:

$$x^2y'' + xy' + (x^2 - m^2)y = 0. \tag{1.36}$$

Other identities:

$$J_{-m}(x) = (-1)^m J_m(x), \tag{1.37}$$

$$J_m(x) \to \frac{(x/2)^m}{\Gamma(m+1)}, \qquad x \to 0, \tag{1.38}$$

$$J_n(x+y) = \sum_{m=-\infty}^{\infty} J_m(x) J_{n-m}(y), \tag{1.39}$$

$$J_n(x) = \frac{1}{\pi}\int_0^\pi d\theta\, \cos(x\sin\theta - n\theta), \tag{1.40}$$

$$J_m(x) \to \sqrt{\frac{2}{\pi x}}\cos\left(x - \frac{m\pi}{2} - \frac{\pi}{4}\right), \qquad x \to \infty. \tag{1.41}$$

More identities:

$$\sum_{m=-\infty}^{\infty} J_m(x) = 1, \tag{1.42}$$

$$\int_0^1 dx\, x\, J_k(z_{km}x) J_k(z_{kn}x) = \tfrac{1}{2} J_{k+1}^2(z_{km})\delta_{mn}, \tag{1.43}$$

$$\int_0^\infty dr\, r\, J_m(kr) J_m(k'r) = \tfrac{1}{k}\delta(k-k'), \tag{1.44}$$

where $z_{km} = m$-th zero of $J_k(x)$.

The defintion of Bessel function J_n can be extended to the case when the index is real J_ν, $\nu \in \mathbb{R}$.

These functions $J_\nu(x)$ are sometimes called Bessel functions of the first kind. There are also Bessel functions of the second kind $Y_\nu(x)$, which are also called Neumann functions $N_\nu(x)$. They can be defined by

$$N_\nu(x) = \frac{J_\nu(x)\cos(\nu\pi) - J_{-\nu}(x)}{\sin(\nu\pi)}.$$

This is ill-defined for $\nu =$ integer. In that case we take the limit $\nu \to n$. $N_\nu(x)$ is the other independent solution of the same differential equation (1.36) with $m \to \nu$. Hankel functions are just a change of basis

$$H_\nu^{(1)}(x) = J_\nu(x) + iN_\nu(x), \qquad H_\nu^{(2)}(x) = J_\nu(x) - iN_\nu(x). \tag{1.45}$$

The description above allows the argument x of the Bessel function J_ν(x) to be complex. When it is purely imaginary, we get the modified Bessel functions

$$I_\nu(x) = i^{-\nu} J_\nu(ix), \qquad K_\nu(x) = \frac{\pi}{2} i^{\nu+1} H^{(1)}(ix). \tag{1.46}$$

They satisfy the differential equation

$$x^2 y'' + xy' - (x^2 + \nu^2)y = 0. \tag{1.47}$$

1.6 Other Special Functions

In this section we briefly introduce gamma function $\Gamma(x)$, beta function $B(x, y)$, and hypergeometric functions.

1.6.1 Gamma Function and Beta Function

The gamma function can be defined as

$$\Gamma(x) = \int_0^\infty dt\, t^{x-1} e^{-t}. \tag{1.48}$$

Using integration by parts, one can show from this that

$$\Gamma(x) = (x-1)\Gamma(x-1). \tag{1.49}$$

For an integer n, $\Gamma(n) = (n-1)!$.

Another useful property is

$$\Gamma(x)\Gamma(-x) = -\frac{\pi}{x\sin(\pi x)}. \tag{1.50}$$

Beta function is defined by

$$B(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}. \tag{1.51}$$

1.6.2 Hypergeometric Function

Differential equation:

$$x(1-x)y'' + [c-(a+b+1)x]y' - aby = 0. \tag{1.52}$$

A regular solution is

$${}_2F_1(a,b;c;x) = 1 + \frac{ab}{1!c}z + \frac{a(a+1)b(b+1)}{2!c(c+1)}z^2 + \dots. \tag{1.53}$$

Another independent solution is

$$x^{1-c}{}_2F_1(a+1-c, b+1-c; 2-c; x). \tag{1.54}$$

Properties:

$$\frac{d}{dx}{}_2F_1(a,b;c;x) = \frac{ab}{c}{}_2F_1(a+1,b+1;c+1;x), \tag{1.55}$$

$${}_2F_1(a,b;c;x) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)}\int_0^1 dt\, \frac{t^{b-1}(1-t)^{c-b-1}}{(1-tx)^a}. \tag{1.56}$$

The generalized hypergeometric functions are

$${}_pF_q\left[\begin{array}{c} a_1, a_2, \cdots, a_p \\ b_1, b_2, \cdots, b_q \end{array}; x\right] = \sum_{k=0}^\infty \frac{(a_1)_k (a_2)_k \cdots (a_p)k}{(b_1)_k (b_2)_k \cdots (b_q)_k}\frac{x^k}{k!}, \tag{1.57}$$

where

$$(a)_k = \frac{\Gamma(a+k)}{\Gamma(a)} = a(a+1)(a+2)\cdots(a+k-1). \tag{1.58}$$

1.7 Exercises:

1. Expand the function

$$f(x) = \begin{cases} +1, & 0 < x < 1 \\ -1, & -1 < x < 0. \end{cases} \tag{1.59}$$

as an infinite series of Legendre polynomials $P_n(x)$.

2. Evaluate the sum

$$\sum_{n=0}^{\infty} \frac{x^{n+1}}{n+1} P_n(x). \tag{1.60}$$

Hint: Use the generating function.

3. Use the Grahamm-Schmidt orthogonalization to work out the first few Hermite polynomials $H_n(x)$ for $n = 0, 1, 2$, assuming that $H_n(x)$ is a polynomial of order n of the form $H_n(x) = 2^n x^n + \cdots$. (The measure of integral is e^{-x^2}.)

4. (Fourier-Bessel transform)
Using (1.44), we define the Fourier-Bessel transform (or Hankel transform)

$$f(r) = \int_0^\infty dk\, k\, J_n(kr) F(k), \qquad F(k) = \int_0^\infty dr\, r\, J_n(kr) f(r). \tag{1.61}$$

Find $F(k)$ for $f(r) = e^{-ar}/r$.

Hint: Use the generating function.

5. (Spherical Bessel function)
Try to solve the following differential equation

$$x^2 y'' + 2xy' + (x^2 - n(n+1))y = 0 \tag{1.62}$$

by using the ansatz $y = x^\alpha J_\nu(x)$ and $y = x^\alpha Y_\nu(x)$. Show that the result is

$$j_n(x) = \sqrt{\frac{\pi}{2x}} J_{n+1/2}(x), \qquad y_n(x) = \sqrt{\frac{\pi}{2x}} Y_{n+1/2}(x). \tag{1.63}$$

6. What linear homogeneous second-order differential equation has

$$x^\alpha J_{\pm n}(\beta x^\gamma) \tag{1.64}$$

as solutions? Give the general solution of

$$y'' + x^2 y = 0. \tag{1.65}$$

7. Find an approximate expression for the Gamma function $\Gamma(-x)$ for large positive x.

Use Stirling's formula and (1.50).

Chapter 2

PDE

Read A&W: Sec.9.1 PDE: introduction pp. 535-537.

We will mostly be concerned with 2nd order *linear* partial differential equations. They are of the form:

$$\mathcal{D}\phi = \rho, \tag{2.1}$$

where $\mathcal{D}$ is a differential operator, such as the Laplacian ∇^2, and ρ is a given function, usually referred to as the "source". The goal is usually to find ϕ for given ρ. Typically there are infinitely solutions, because any solution of the homogeneous equation

$$\mathcal{D}\varphi = 0 \tag{2.2}$$

can be used to generate new solutions of (2.1) by

$$\phi \to \phi + c\varphi \tag{2.3}$$

for any constant c. One has to specify suitable boundary conditions in order to single out a unique solution.

In Electrostatics, ϕ can be the electric potential and ρ the charge density. There are various uniqueness theorems corresponding to different ways of specifying boundary conditions for the solution to be unique.

Another type of PDE we will be interested in is the eigenvalue problem

$$(\mathcal{D} - \lambda)\phi = 0, \tag{2.4}$$

where λ is a number to be found together with the function ϕ. The goal is to find the solution pair (λ, ϕ). Usually we want to find all possible (λ, ϕ) pairs. Again the boundary condition has to be specified first. In principle, the operator $\mathcal{D}$ is not well defined until you specify the class of functions for it to acts on.

We will see that these two types of problems (2.1), (2.4) are connected through the notion of Green's function.

2.1 Review

2.1.1 Orthogonal Functions

The space of functions is a linear space. It is convenient to choose

eigenfunctions (w. certain BC's) for the operator $\mathcal{D}$ that appears in your PDE as the basis of this linear space.

Using separation of variables (Sec. 2.4), we can often reduce the linear space $\mathcal{V}$ appearing in a PDE problem to a tensor product of linear spaces of one-variable functions. That is, $\mathcal{V} = \mathcal{V}_1 \otimes \mathcal{V}_2 \otimes \cdots$, or $f(x_1, x_2, \cdots) = \sum_i f_1^{(i)}(x_1) f_2^{(i)}(x_2) \cdots$. Thus we will focus on ordinary diff. op's. in this section, although most of the principles can be generalized to partial diff. op's.

2.1.2 Sturm-Liouville Differential Operator

For ODE's, or PDE's after separation of variables, we are often dealing with *Sturm-Liouville differential operators* (so we hope)

$$\mathcal{D} = \frac{1}{\mu(x)} \left[-\frac{d}{dx} p(x) \frac{d}{dx} + q(x) \right], \tag{2.5}$$

where $\mu(x)$ is the *weight function*. The *inner product* should be defined as

$$\langle f|g\rangle = \int dx \mu(x) f^*(x) g(x). \tag{2.6}$$

The boundary condition should be chosen such that $\mathcal{D}$ is Hermitian.

2.1.3 Completeness of Eigenfunctions

Recall that the complete set of eigenvectors of a Hermitian matrix M constitute a basis of the linear space on which M acts. Recall also that one can always choose this basis to be orthonormal. Eigenvectors with different eigenvalues are automatically orthogonal:

$$\langle v_i|M|v_j\rangle = \lambda_i \langle v_i|v_j\rangle = \lambda_j \langle v_i|v_j\rangle \Rightarrow \langle v_i|v_j\rangle \propto \delta_{ij}. \tag{2.7}$$

Eigenvectors with the same eigenvalues (degeneracy) can be chosen to be orthogonal to each other by the method of Gram and Schmidt.

Eigenvectors ϕ_n of a *Sturm-Liouville operator* constitute a *complete* basis of the linear space of fxs $\mathcal{V}$ (on which $\mathcal{D}$ is self-adjoint), assuming suitable choice of $p(x), q(x), \mu(x)$ as well as BC's. (We don't need to consider eigenfx's which do not belong to $\mathcal{V}$.) It is complete in the sense that any well behaved (piecewise continuous function with a finite number of finite discontinuities) F can be approximated to arbitrary accuracy by a series $\sum_n a_n \phi_n$. That is,

$$\lim_{m\to\infty} \int_{x_0}^{x_1} dx \mu(x) \left(F(x) - \sum_{n=0}^{m} a_n \phi_n(x) \right)^2 = 0. \tag{2.8}$$

For an *orthonormal* basis ϕ_n, i.e., $\langle \phi_m|\phi_n\rangle = \delta_{mn}$, the coefficients a_n are

$$a_n = \langle \phi_n|F\rangle \equiv \int dx \mu(x) \phi_n^*(x) F(x). \tag{2.9}$$

2.1.4 Exercises:

1. Construct a complete, orthonormal basis for the 2 dim. unit sphere by combining the associated Legendre polynormials $P_\ell^m(\theta)$ as a basis for the θ-dependence, and $e^{im\phi}$ as a basis for the ϕ-dependence. The resulting functions $\{Y_\ell^m(\theta,\phi)\}$ are called spherical harmonics.

2. The PDE
$$\left(P(x)\frac{d^2}{dx^2}+Q(x)\frac{d}{dx}+R(x)-\lambda S(x)\right)\phi(x)=0$$
can be viewed as an eigenvalue problem for a Sturm-Liouville op. $\mathcal{D}$. What are the fx's $\mu(x), p(x), q(x)$ defining $\mathcal{D}$?

The eigenvalue problem of an op. $\mathcal{D}$ is to look for solutions $\phi(x)$ of the eq. $(\mathcal{D}-\lambda)\phi(x)=0$ for any $\lambda\in\mathbb{R}$ or $\mathbb{C}$. The set of values of λ is called the *spectrum*.

2.1.5 Homework Assignment

1. A&W: Exercise (10.2.3).
2. A&W: Exercise (10.2.8). (Liouville substitution)
3. A&W: Exercise (10.3.5). (Gram-Schmidt)
4. The exercise 1. in Sec. 2.1.1.
5. Construct a complete basis for the space of fx's $\mathcal{V}_a$ on the interval $[0,\pi]$ with the BC $f+af'=0$ at both ends for a given number $a\in\mathbb{R}$, as eigenfx's of the diff. op. $\frac{d^2}{dx^2}$.

2.2 Linear Algebra

The first thing to note about a diff. eq. of the form
$$\mathcal{D}\phi=\rho \tag{2.10}$$
is that this equation is formally the same as an equation in linear algebra, with $\mathcal{D}=$ matrix (linear map), and $|\phi\rangle$ and $|\rho\rangle$ being vectors.

We will use $|\cdot\rangle$ to represent elements in a vector space $\mathcal{V}$ and $\langle\cdot|$ elements in the dual space $\mathcal{V}^*$. So we rewrite (2.10) as
$$\mathcal{D}|\phi\rangle=|\rho\rangle. \tag{2.11}$$

The space of functions is a linear space. If $|f_1\rangle, |f_2\rangle\in\mathcal{V}$, their superposition $(a|f_1\rangle+b|f_2\rangle)\in\mathcal{V}$.

The differential operator $\mathcal{D}$ acts on a function to give another function, and its action is linear:
$$\mathcal{D}(a|f_1\rangle+b|f_2\rangle)=a\mathcal{D}|f_1\rangle+b\mathcal{D}|f_2\rangle. \tag{2.12}$$

Thus $\mathcal{D}$ is a linear map acting on the linear space of functions. This is the most salient feature of linear PDE's, and we will see that it is useful to view it as a problem in linear algebra.

Feynman: The same equations have the same solutions.

lattice:

Putting the problem on a lattice, the diff. op. becomes a difference operator. $|\phi\rangle$ and $|\rho\rangle$ become columns with finite number of elements. One can imagine that the original problem is the continuum limit of this problem of linear algebra.

The linear space of functions on a lattice has the natural basis in which each basis vector $|e_n\rangle$ is the function which is 1 at the n-th point and 0 everywhere else. A function can be expanded in this basis as $|f\rangle = |e_n\rangle f_n$, where f_n is the value of the function at the n-th point. (The continuum limit of f_n is $f(x)$.) We have the following correspondence:

$$n \leftrightarrow x, \quad f_n \leftrightarrow f(x), \quad \sum_n \leftrightarrow \int dx, \quad \delta_{mn} \leftrightarrow \delta(x-x'), \tag{2.13}$$

$$|f\rangle = f_n|n\rangle \leftrightarrow f(x) = \int dx' f(x')\delta(x-x'), \tag{2.14}$$

$$\langle f|g\rangle = \sum_n f_n^* g_n \leftrightarrow \int dx f(x)^* g(x), \tag{2.15}$$

$$|f\rangle\langle g| = f_m g_n^* |m\rangle\langle n|, \quad f_m g_n^* \leftrightarrow f(x)g(x')^*. \tag{2.16}$$

change of basis

One can also choose a different basis for the linear space $\mathcal{V}$ related to the previous basis by a linear map M: $|e_n\rangle = |E_a\rangle M_{an}$. In the new basis, a function is $|f\rangle = |E_a\rangle F_a$, with $F_a = M_{an} f_n$ In the continuum limit, it is $(n \to x, a \to k)$

$$F(k) = \int dx\, u(k,x) f(x). \tag{2.17}$$

This is the Fourier transform if $u(k,x) \propto exp(ikx)$. Thus, functions do not have to be represented as $f(x)$ (in terms of the basis $\delta(x-x')$). They are vectors in a linear space and how they look depends on which basis you choose. (The linear space is infinite dimensional; we will worry about convergence later.)

eigenfunctions

Sec.10.1 Self-Adjoint ODEs pp. 622-634.

Understanding that a diff. eq. is a problem in linear algebra, we can apply techniques in linear algebra. If $\mathcal{D}$ is *Hermitian*, it is associated with a convenient basis of the linear space $\mathcal{V}$, i.e., its eigenvectors.

$\mathcal{D}$ is *Hermitian* if $\mathcal{D}^\dagger = \mathcal{D}$. See below.

$$\mathcal{D}|e_n\rangle = \lambda_n |e_n\rangle. \tag{2.18}$$

The number of eigenvectors equals the dimension of the linear space $\mathcal{V}$. We can always choose the eigenvectors to satisfy

$$\langle e_m|e_n\rangle = \delta_{mn}, \tag{2.19}$$

and then we have the identity

$$|e_n\rangle\langle e_n| = I, \tag{2.20}$$

$\mathcal{V}^*$ is the *dual space* of $\mathcal{V}$ if there is a nondegenerate bilinear map $\langle\alpha|\beta\rangle \in \mathbb{C}$ $\forall|\alpha\rangle \in \mathcal{V}, \langle\beta| \in \mathcal{V}^*$.
If $\mathcal{V}$ is equipped with a (positive-definite) *norm* $\| \, |\alpha\rangle \, \|^2$, $\mathcal{V}$ is the dual of itelf.
By $\langle e_n|$ we denote the element in $\mathcal{V}^*$ which satisfies $\langle e_m|e_n\rangle = \delta_{mn}$.
More generally, by $\langle\alpha|$ we mean $\langle e_n|\alpha_n^*$ if $|\alpha\rangle = \alpha_n|e_n\rangle$, so that

where I is the identity operator.

Green's fx.

For problems involving the op. $\mathcal{D}$, it is convenient to represent fx's in the basis $|e_a\rangle$ of eigenfx's

$$|\rho\rangle = |e_n\rangle\rho_n, \qquad \rho_n = \langle e_n|\rho\rangle. \tag{2.21}$$

The solution to the diff. eq. is then

$$|\phi\rangle = |e_n\rangle\phi_n, \qquad \phi_n = \lambda_{\underline{n}}^{-1}\rho_{\underline{n}}. \tag{2.22}$$

(Underlined indices are not summed over.) That is

$$|\phi\rangle = \mathcal{D}^{-1}|\rho\rangle = G|\rho\rangle, \tag{2.23}$$

where G is called the *Green's function* or *propagator*

$$G = \frac{|e_n\rangle\langle e_n|}{\lambda_n}. \tag{2.24}$$

Apparently, if $\mathcal{D}$ is Hermitian, G is also Hermitian. If G is also a real fx. $G(x_1, x_2) \in \mathbb{R}$, it will be symmetric $G(x_1, x_2) = G(x_2, x_1)$. (See a more explicit proof on Arfken and Weber: **Symmetry of Green's function** on p. 595, p. 596.)

$M = |e_m\rangle M_{mn}\langle e_n|$ represents the matrix with elements M_{mn}.
One can think of $|e_n\rangle$ as the basis of columns, and $\langle e_n|$ as the basis of rows.
The *Hermitian conjugate* $M^\dagger$ of an operator M is defined by $\langle\alpha|M|\beta\rangle = \langle M^\dagger\alpha|\beta\rangle$.

2.3 Boundary Condition

Read A&W: Sec.9.1 PDE: Classes of PDEs and Characteristics, Boundary Conditions pp. 538-543.

Usually $\mathcal{V}$ is a restricted class of functions for certain physical reasons. For example, if ϕ represents the electric potential inside a conducting shell, ϕ should vanish on the boundary, and should be finite everywhere except at places where the charge density ρ diverges.

Terminology:

Dirichlet boundary condition: ϕ given on the boundary.

Neumann boundary condition: $\partial_n\phi$ given on the boundary.

Cauchy boundary condition: both ϕ and $\partial_n\phi$ given on the boundary.

In general, we can also have boundary conditions which specify the value of $a\phi + b\partial_n\phi$.

inner product

The inner product of $\mathcal{V}$ and its dual $\mathcal{V}^*$ is usually of the form

$$\langle f|g\rangle \int dx\mu(x)f(x)^*g(x), \tag{2.25}$$

where μ is usually a function (the *measure* or *weight fx*) although in principle it can be a differential operator.

Example: $i\frac{d}{dx}$ is a self-adjoint operator on $\mathcal{V}$ if $\mathcal{V}$ is restricted to functions with suitable BC such that $f^*g|_{x_0}^{x_1} = 0$, where x_0 and x_1 are boundaries of the interval on which functions in $\mathcal{V}$ are defined.

The *adjoint* (*Hermitian conjugate*) of an operator is defined by

$$\langle f|\mathcal{D}g\rangle = \langle \mathcal{D}^\dagger f|g\rangle, \tag{2.26}$$

that is

$$\int dx\mu f^*(x)\mathcal{D}g(x) = \int dx\mu(\mathcal{D}^\dagger f)^* g(x). \tag{2.27}$$

The derivation of the adjoint involves integration by parts and thus there is usually a boundary term involved. For an operator to be self-adjoint (Hermitian), i.e., $\mathcal{D}^\dagger = \mathcal{D}$, the boundary term has to be taken care of by suitable boundary conditions and choice of measure μ.

2.3.1 Uniqueness and Existence

Sometimes suitable choice of boundary conditions leads to a unique solution for the diff. eq. (2.10). This is often guaranteed by physical laws and well-defined physical setup. For example, $x(0)$ and $\dot{x}(0)$ uniquely determines $x(t > 0)$ via the evolution eq. $\ddot{x} = -V'(x)$.

To discuss this topic, we classify PDE's into 3 classes: *elliptic, parabolic*, and *hyperbolic*. A diff. op.

$$\mathcal{D} = a\frac{\partial^2}{\partial x^2} + 2b\frac{\partial^2}{\partial x\partial y} + c\frac{\partial^2}{\partial y^2} + d\frac{\partial}{\partial x} + e\frac{\partial}{\partial y} + f \tag{2.28}$$

is elliptic, parabolic or hyperbolic depending on whether $b^2 - ac$ is $< 0, = 0$ or > 0. By change of variables, we can change a, b and c. But the sign of the determinant is invariant.

This classification can be roughly understood when trying to solve the diff. eq.

$$\mathcal{D}f = \left(a\frac{\partial^2}{\partial x^2} + 2b\frac{\partial^2}{\partial x\partial y} + c\frac{\partial^2}{\partial y^2}\right) f = 0 \tag{2.29}$$

If a, b, c are fx's of x, y, here we consider an infinitesimal region of x, y in which a, b, c are roughly constant.

by using the ansatz

$$f(x, y) = F(\alpha x + y). \tag{2.30}$$

For this ansatz to satisfy (2.29), we need

$$a\alpha^2 + 2b\alpha + c = 0. \tag{2.31}$$

For the hyperbolic case, this eq. has two sol's α_+, α_-, and the general sol. to (2.29) is

$$f = F_+(\alpha_+ x + y) + F_-(\alpha_- x + y). \tag{2.32}$$

For the parabolic case, there is only one sol. α_0. We can try another ansatz

$$f(x, y) = g(x, t)F(\alpha_0 x + y) \tag{2.33}$$

and find the general sol. of the diff. eq.

$$f = F_0(\alpha_0 x + y) + g(x, t)F_1(\alpha_0 x + y), \tag{2.34}$$

where $g(x,t)$ is any linear combination of x and y.

The elliptic case admits no solution for this ansatz.

elliptic

The prototype of an elliptic diff. op. is

$$\mathcal{D} = -\frac{\partial^2}{\partial x_i^2}. \tag{2.35}$$

(The minus sign is a convention.)

Suppose $\mathcal{D}$ is of the form $\mathcal{D} = \sum_i d_i^\dagger d_i$. If there are two solutions to (2.10), we have $\mathcal{D}|f\rangle = 0$ for the difference f of the two solutions. Then

$$0 = \langle f|\mathcal{D}f\rangle = \langle d_i f|d_i f\rangle = \|\, d_i|f\rangle\|^{\,2}. \tag{2.36}$$

This expression is always positive definite if the inner product is positive definite. The inner product is *positive definite* if the norm of a vector $|v\rangle$, i.e. $\langle v|v\rangle$, is zero only if $|v\rangle = 0$.

If the inner product is positive definite, this is possible only if $d_i|f\rangle = 0\ \forall i$. Together with the boundary condition, which is $f = 0$ for Dirichlet boundary condition and $f' = 0$ for Neumann boundary condition, this may lead to the conclusion that $f = 0$. (Recall the proof of uniqueness for electric potential with equipotential boundary conditions.)

parabolic

The standard form of a parabolic diff. op. is

$$\mathcal{D} = -\frac{\partial^2}{\partial x^2} + \frac{\partial}{dt}. \tag{2.37}$$

This op. appears in diffusion eqs.

hyperbolic

The standard form of a hyperbolic diff. op. is

$$\mathcal{D} = \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} = \left(\frac{\partial}{\partial t} - \frac{\partial}{\partial x}\right)\left(\frac{\partial}{\partial t} + \frac{\partial}{\partial x}\right). \tag{2.38}$$

For the uniqueness problem, we should study the homogeneous diff. eq. for the difference of two sol's. The most general solution to the wave eq. $\mathcal{D}f = 0$ is

$$f = f_+(x+t) + f_-(x-t). \tag{2.39}$$

The notion of causality in special relativity is helpful for you to decide whether a boundary condition is suitable or not.

characteristics

If a, b, c are not constant, we can still define two vectors (dt, dx) at each point (t, x), called characteristics, according to

$$a\left(\frac{dt}{dx}\right)^2 + 2b\frac{dt}{dx} + c = 0. \tag{2.40}$$

These are the directions that information propagates. Causality is defined by integrating these vectors into curves.

For a region in 2D space, consider a segment of boundary given by $(x(s), y(s))$, where the parameter s is chosen such that $1 = \left(\frac{dx}{ds}\right)^2 + \left(\frac{dy}{ds}\right)^2$. Now we try to understand how much information we can get from the Cauchy BC on the boundary. Given f on the boundary, we can get

$$\frac{df}{ds} = \frac{dx}{ds}\frac{\partial f}{\partial x} + \frac{dy}{ds}\frac{\partial f}{\partial y}. \tag{2.41}$$

In addition, the normal derivative of f is also given in the Cauchy BC:

$$\partial_n f = \frac{dx}{ds}\frac{\partial f}{\partial y} - \frac{dy}{ds}\frac{\partial f}{\partial x}. \tag{2.42}$$

From the two eqs above, one can determine the 1st derivatives $\frac{\partial f}{\partial x}$ and $\frac{\partial f}{\partial y}$, in terms of the given functions $\frac{df}{ds}$ and $\partial_n f$. The next step is to check whether we can also (uniquely) determine the 2nd derivatives on the boundary using the PDE (2.29). If yes, this BC is suitable for this 2nd order PDE. The eqs at hand are

$$\begin{aligned} a\partial_x^2 f + 2b\partial_x\partial_y f + c\partial_y^2 f &= \text{some function of}(x, y, \partial_x f, \partial_y f), && (2.43)\\ \frac{dx}{ds}\partial_x^2 f + \frac{dy}{ds}\partial_x\partial_y f &= \frac{d}{ds}\partial_x f, && (2.44)\\ \frac{dx}{ds}\partial_x\partial_y f + \frac{dy}{ds}\partial_y^2 f &= \frac{d}{ds}\partial_y f. && (2.45) \end{aligned}$$

These linear relations have a unique sol. only if the coeffients on the LHS form a matrix with nonzero determinant. The determinant is

$$a\left(\frac{dy}{ds}\right)^2 - 2b\frac{dx}{ds}\frac{dy}{ds} + c\left(\frac{dx}{ds}\right)^2. \tag{2.46}$$

If the determinant vanishes, the BC is not suitable. This happens when the tangent of the boundary satisfies

$$\frac{dy}{dx} = \frac{b \pm \sqrt{b^2 - ac}}{a}. \tag{2.47}$$

Note that this is the same as the direction of propagation in the hyperbolic case.

2.3.2 Comment on BC

Let us make a digression here. In the Lagrangian formulation, a physical system is defined by an action

$$S = \int dt L, \tag{2.48}$$

where L is the Lagrangian. The equation of motion, called the Euler-Lagrange equation in this context, is the condition that extremizes the action. This is the *principle of least action*.

For a nonrelativistic particle,

$$L = K - V = \frac{1}{2}m\dot{x}^2 - V(x). \tag{2.49}$$

For the wave equation

$$\left(\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right)\phi(t,x) = 0, \tag{2.50}$$

the suitable Lagrangian is

$$L = \int dx\mathcal{L} = \frac{1}{2}\left(\dot{\phi}^2 - \phi'^2\right). \tag{2.51}$$

To derive the Euler-Lagrange eq., we variate the action

$$\delta S = \int dtdx\left(\delta\dot{\phi}\dot{\phi} - \delta\phi'\phi'\right) = \int dtdx\delta\phi(-\ddot{\phi} + \phi'') - \int dt\left[\delta\phi\phi'\right]_{x_0}^{x_1}, \tag{2.52}$$

where x_0 and x_1 are the boundary coordinates. This not only gives the wave eq., but also a clue about the BC. The least action principle demands that your choice of BC must guarantee that the boundary term vanishes. For example: Dirichlet BC, Neumann BC, and periodic BC are all acceptable here. Different choices of BC correspond to different physical settings.

For spaces without boundary, e.g. a sphere or a torus, the BC is replaced by the requirement that the field is finite and continuous everywhere on the space. (We will still call them BC's.) When we choose the coordinate system in such a way that the topology of space is not manifest (e.g. polar coordinates for $\mathbb{R}^2$), we also need to impose suitable BC's to ensure the continuity.

BC's change the spectrum of eigenvalues of $\mathcal{D}$. For example, imposing a periodic BC on $\mathbb{R}$ is the same as replacing $\mathbb{R}$ by S^1. The spectrum of ∂_x^2 is changed from $\mathbb{R}$ to $\mathbb{Z}$.

2.3.3 Exercises:

1. Derive the Laplacian for flat space in spherical coordinates.
2. Derive the Laplacian for the metric $ds^2 = -dt^2 + a^2(t)(dx^2 + dy^2 + dz^2)$. This is the metric for a spatially flat FRW universe.

2.4 Separation of Variables

Fourier transform naturally arises from the wave eq. in flat spacetime with Cartesian coordinates. The Laplace operator is

$$\nabla^2 = \partial_i^2. \tag{2.53}$$

This is probably the simplest example of separation of variables. The 3D flat space is viewed as a product space $\mathbb{R}^3 = \mathbb{R}\times\mathbb{R}\times\mathbb{R}$. The space of functions on $\mathbb{R}^3$ is then $\mathcal{A}\otimes\mathcal{A}\otimes\mathcal{A}$, where $\mathcal{A}$ is the space of functions on $\mathbb{R}$. Eigenfunctions on $\mathcal{A}^{\otimes 3}$ is then $e^{ik_x x}e^{ik_y y}e^{ik_z z} = e^{ik\cdot x}$. What we learned in Sec.2.2 leads to the

Read A&W: Sec.9.3 Separation of Variables pp. 554-560.
Read A&W: Sec.9.8 Heat Flow, or Diffusion, PDE pp. 611-618
See M&W for more examples. (attached)

use of Fourier transform. Similarly, separation of variables applied to spherical coordinates and cylindrical coordinates leads to different bases of functions on flat space.

The most important technique in deriving the basis of eigenfunctions is the separation of variables. Separation of variables helps us to reduce a PDE to ODE's.

If an isometry is realized as the translation of a coordinate (e.g. x, y, z in Catesian coordinates, ϕ, z in cylindrical coordinates and ϕ in spherical coordinates), the eigenfunctions derived by separation of variables are labelled by an additive quantum number corresponding to an operator that generates the translation.

2.4.1 Comments

Why Separation of Variables Work

An arbitrary function of n variables can always be written in the form

$$f(x_1, \cdots, x_n) = \sum_i f_1^{(i)}(x_1) \cdots f_n^{(i)}(x_n). \tag{2.54}$$

As an example, any function that admits a Taylor expansion is of this form

$$f(x_1, \cdots, x_n) = \sum_{m_1, \cdots, m_n} f_{m_1 \cdots m_n} x_1^{m_1} \cdots x_n^{m_n}. \tag{2.55}$$

This is merely a special case of (2.54).

Now if we choose a complete basis $\{\phi_{\alpha_a}^{(a)}(x_a)\}$ for each variable x_a ($a = 1, \cdots, n$), so that each element $f_a^{(i)}(x_a)$ in (2.54) can be expanded in that basis, the expansion (2.54) is of the form

$$f(x_1, \cdots, x_n) = \sum_{\alpha_1, \cdots, \alpha_n} f_{\alpha_1 \cdots \alpha_n} \phi_{\alpha_1}^{(1)}(x_1) \cdots \phi_{\alpha_n}^{(n)}(x_n). \tag{2.56}$$

The trick of separation of variable is to find an ordinary differential operator for each variable appearing in the partial diff. op. $\mathcal{D}$. Then we use the eigenfx's for each ordinary diff. op's as a basis of fx's of that variable. In the above we tried to convince you that we are not missing anything after putting all the bases of all variables together.

In short, if $\mathcal{V}_a$ is the space of fx's for the space $\mathcal{M}_a$, the space of fx's on the space $\mathcal{M}_1 \times \mathcal{M}_2 \times \cdots \times \mathcal{M}_n$ is $\mathcal{V}_1 \otimes \mathcal{V}_2 \otimes \cdots \otimes \mathcal{V}_n$.

Even when the space $\mathcal{M}$ under investigation is not a product space, separation of variables can still be applied, although one has to properly define $\mathcal{V}_a$'s by choosing suitable BC's.

How to Choose the Variables for Separation of Variables?

In the above we considered the Laplace op. ∇^2 in flat space in both Cartesian coordinates and spherical coordinates. (The use of Cylindrical coordinates can be found in the textbook.) Why do we need to do separation of variables in different variables? Is not one complete basis of fx's enough?

The main reason is the BC. A BC specified on a sphere ar $r = R$, or a BC like "f goes to zero at infinity", which means $f \overset{r\to\infty}{\to} 0$, suggests the use of spherical coordinates. On the other hand, a periodic BC over a box $x \in [0, L_x]$, $y \in [0, L_y]$, $z \in [0, L_z]$, for example, suggests that the Cartesian coordinates will be better.

A secondary reason is the symmetry. It is convenient to use different coordinate systems for problems with different symmetries. (This is a general statement beyond PDE's.) The bases of fx's found via separation of variables in different coordinate systems behave differently under symmetry transformations of the space. The basis of fx's for the Cartesian coord's changes in a simply way under translation

$$x \to x + a, \qquad \phi_k(x) = e^{ik\cdot x} \to e^{ik\cdot a}\phi_k(x). \tag{2.57}$$

The spherical harmonics transform in a simple way under rotations

$$\phi \to \phi + a, \qquad Y_\ell^m(\theta, \phi) \to Y_\ell^m(\theta, \phi + a) = e^{ima} Y_\ell^m(\theta, \phi). \tag{2.58}$$

More generally, under a generic rotation, the spherical harmonics transform as

$$(\theta, \phi) \to (\theta', \phi'), \qquad Y_\ell^m(\theta, \phi) \to Y_\ell^m(\theta', \phi') = M_n^m Y_\ell^n(\theta, \phi), \tag{2.59}$$

without mixing harmonics with different ℓ.

Any complete basis of fx's provides a linear representation of any symmetry of the underlying space. Generically a symmetry transformation mixes all states together. But in some bases certain symmetry transformations are realized in relatively simple ways.

Comment on Laplace Op.

The above can be extended to curved backgrounds. In Riemannian geometry, the crucial object that defines the Riemannian structure of a space is the *metric*

$$ds^2 = g_{ij}(x) dx^i dx^j. \tag{2.60}$$

This gives the definition of distance between to infinitesimally separated points (x) and $(x + dx)$. Finite distance can be defined by integration $\int ds$.

For the flat background, $g_{ij}(x) = \delta_{ij}$ in Cartesian coordinates. But we can choose any other coordinate system (e.g. spherical or cylindrical coordinate

systems). Using the chain rule $dx^i = dx^i(y) = dy^a \frac{\partial x^i}{\partial y^a}$, we can express the metric in terms of a new coordinate system y as

$$ds^2 = g'_{ab} dy^a dy^b, \qquad g'_{ab} = g_{ij} \frac{\partial x^i}{\partial y^a} \frac{\partial x^j}{\partial y^b}. \tag{2.61}$$

Since physics should not depend on the coordinate system we choose, the proper generalization of the Kinetic term for a particle is

$$K = \frac{1}{2} m \dot{x}_i^2 \Rightarrow K = \frac{1}{2} m g_{ij} \dot{x}^i \dot{x}^j. \tag{2.62}$$

For a wave, it is

$$\mathcal{L} = \frac{1}{2} \partial_\mu \phi \partial^\mu \phi \Rightarrow \mathcal{L} = \frac{1}{2} \sqrt{-g} g^{\mu\nu} \partial_\mu \phi \partial_\nu \phi. \tag{2.63}$$

From here one can derive the Laplacian that will appear in the wave eq.

$$\nabla^2 = \frac{1}{\sqrt{g}} \partial_\mu \sqrt{g} g^{\mu\nu} \partial_\nu. \tag{2.64}$$

Comment on Helmholtz Eq.

The wave eq. in 4 Dimensional Minkowski space is

$$\ddot{\phi} - \nabla^2 \phi = 0. \tag{2.65}$$

Via Fourier transform w.r.t. t, we only need to consider sol's of the form

$$\phi = e^{i\omega t} \phi_\omega(x, y, z). \tag{2.66}$$

Then the wave eq. turns into the Helmholtz eq. (With suitable BC, the 3D Laplacian is positive definite. Otherwise ω might be complex, signaling an instability.)

Separation of variables allows you to imagine that PDE of the form

$$\nabla^2 \phi + k^2 \phi = 0 \tag{2.67}$$

arises from the PDE

$$\nabla'^2 \phi = 0 \tag{2.68}$$

in a higher dimension with

$$\nabla'^2 = \nabla^2 + \frac{\partial^2}{\partial t^2}. \tag{2.69}$$

For the ansatz

$$\phi = e^{-at} \phi_0(x), \tag{2.70}$$

the diffusion eq.

$$\nabla^2 \phi = \frac{\partial \phi}{\partial t} \tag{2.71}$$

is also of the same form.

2.4.2 Exercises:

1. For $f(x,y) = X(x)Y(y)$, derive the ODE's that $X(x)$ and $Y(y)$ should satisfy in order for $f(x,y)$ to satisfy the PDE

$$\mathcal{D}f = \lambda f, \qquad \mathcal{D} = \frac{1}{a^2(x)}(\partial_x^2 + \partial_y^2). \tag{2.72}$$

2. Find the most general fx. $f(r,\theta,\phi)$ satisfying the following conditions in terms of the complete basis of 3D space in spherical coordinates:

   - $r \in [0,\infty)$, $\lim_{r\to\infty} f(r,\theta,\phi) = 0$.
   - $r \in [a,b]$, $f(a,\theta,\phi) = A(\theta,\phi)$, $f(b,\theta,\phi) = B(\theta,\phi)$ for given fx.'s A and B.
   - $r \in [0,\infty)$, $\phi \in [0,\pi]$, $f(r,\theta,0) = f(r,\theta,\pi) = 0$.

3. Find the most general fx. $f(\rho,\phi,z)$ in cylindrical coordinates for f defined on $\rho \in [a,b]$, with the BC $f(a,\phi,z) = F_0(\phi,z)$ and $f(b,\phi,z) = F_1(\phi,z)$, where F_0 and F_1 are given fx's.

4. A long hollow conductor has a rectangular cross section with sides a and $2a$. One side of length $2a$ is charged to a potential V_0. The other 3 sides are grounded $V = 0$. Find the electric potential $V(x,y)$ for $x \in [-a,a], y \in [-a/2, a/2]$.

5. The temperature of a homogeneous sphere of radius a obeys the diffusion eq. $\nabla^2 T = \dot{T}$. ($\dot{T} = \partial_t T$.) By external means, the surface temperature of the sphere is given by $T(t, r = a) = T_0 \sin(\omega t)$. Find the temperature inside the sphere $T(t,r)$.

2.4.3 Homework Assignment

1. The exercise 1. in Sec. 2.3.3.
2. A&W: Exercise (9.3.4).
3. A&W: Exercise (9.3.5).
4. A&W: Exercise (9.3.6).
5. A&W: Exercise (9.3.8).

Chapter 3

Green's Function

Green's function was formally discussed in Sec.2.2. It satisfies the PDE

$$\mathcal{D}G(x,x') = \frac{1}{\mu(x)}\delta(x,x'), \tag{3.1}$$

so that the PDE $\mathcal{D}\phi(x) = \rho(x)$ for given ρ can be solved by

$$\phi(x) = \int dx'\mu(x')G(x,x')\rho(x'). \tag{3.2}$$

In Sec. 2.2 we have a general sol. for Green's fx. (2.24)

$$G = \frac{|\phi_n\rangle\langle\phi_n|}{\lambda_n}. \tag{3.3}$$

Here we repeat the derivation in more explicit notations.

First, we use the eigenfx's of $\mathcal{D}$ as the basis of fx's. We have

$$\mathcal{D}\phi_n(x) = \lambda_n\phi_n(x). \tag{3.4}$$

Gram and Schmidt told us that we can choose ϕ_n's to be an orthonormal basis satisfying

$$\langle\phi_m|\phi_n\rangle \equiv \int d^dx\mu(x)\phi_m^*(x)\phi_n(x) = \delta_{mn}. \tag{3.5}$$

For 3D flat space ($d=3$), $\int d^3x\mu(x) = \int dxdydz = \int drd\theta d\phi r^2\sin\theta$, etc.

As a basis, we can expand the x dependence of G in $\phi_n(x)$ as

$$G(x,x') = \sum_n g_n(x')\phi_n(x). \tag{3.8}$$

Similarly we can expand Dirac's delta fx. as

$$\frac{1}{\mu(x)}\delta(x,x') = \sum_n A_n(x')\phi_n(x). \tag{3.9}$$

Now we multiply this eq. by $\phi_m^*(x)$ and integrate $\int dx\mu(x)$. We get

$$\phi_m^*(x') = A_m(x'). \tag{3.10}$$

Read A&W: Sec.10.5 Green's Function-Eigenfunction Expansion pp. 662-674.

Read A&W: Sec.9.7 Non-homogeneous Equation-Green's Function pp. 592-610.

Dirac δ fx is defined (as a distribution) by $\int dx'\delta(x-x')f(x') = f(x)$ for any well-behaved fx f.

We can also do this for the x'-dependence of $g_n(x')$

$$g_n(x') = \sum_m g_{nm}\phi_m(x'), \tag{3.6}$$

so that

$$G(x,x') = \sum_{mn} g_{mn}\phi_m(x)\phi_n(x'). \tag{3.7}$$

But we will not need to do this for this derivation of G.

Hence we have rederived eq. (2.20)

$$\frac{1}{\mu(x)}\delta(x,x') = \sum_n \phi_n(x)\phi_n^*(x'). \tag{3.11}$$

Now we should determine $g_n(x')$ from the PDE (3.1), which gives

$$\mathcal{D}G(x,x') = \sum_n g_n(x')\lambda_n\phi_n(x) = \frac{1}{\mu(x)}\delta(x,x') = \sum_n \phi_n(x)\phi_n^*(x'). \tag{3.12}$$

It is now obvious that $g_n(x') = \phi_n^*(x')/\lambda_n$, and so

$$G(x,x') = \sum_n \frac{\phi_n(x)\phi_n^*(x')}{\lambda_n}. \tag{3.13}$$

This general expression of the Green's fx. depends on the choice of BC's since the eigenfx's ϕ_n do.

Often this infinite sum can be greatly simplified to a more compact expression.

3.0.4 Green's Function for Electrostatic Potential

The physical meaning: **Green's fx = the field of a unit point source.**

A well known example of Green's fx is

$$G(x,x') = \frac{1}{4\pi|x-x'|}, \tag{3.14}$$

which appears in electrostatics for the electric potential. The PDE $\nabla^2\phi(x) = -\rho(x)$ is solved by $\phi(x) = \int dx' G(x,x')\rho(x')$.

The Green's fx (3.14) assumes that the BC is $G(r) \overset{r\to\infty}{\to} 0$. The *method of images* can be used to find the Green's fx with some other BC's.

As we learned from Sec. 2.2, this Green's fx can also be expressed in terms of a basis of functions:

$$\begin{aligned}
\frac{1}{4\pi|x-x'|} &= \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\frac{1}{2\ell+1}\frac{r_<^\ell}{r_>^{\ell+1}}Y_\ell^m(\theta_1,\phi_1)Y_\ell^{m*}(\theta_2,\phi_2) \\
&= \frac{1}{4\pi}\sum_{\ell=0}^{\infty}\frac{r_<^\ell}{r_>^{\ell+1}}P_\ell(\cos\gamma) \\
&= \sum_{m=-\infty}^{\infty}\int_0^\infty \frac{dk}{2\pi^2} I_m(k\rho_<)K_m(k\rho_>)e^{im(\phi_1-\phi_2)}\cos(k(z_1-z_2)).
\end{aligned} \tag{3.15}$$

Here Y_ℓ^m are spherical harmonics properly normalized so that

$$\delta(\cos\theta-\cos\theta')\delta(\phi-\phi') = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} Y_\ell^m(\theta,\phi)Y_\ell^{m*}(\theta',\phi'). \tag{3.16}$$

($Y_\ell^m(\theta,\phi)$ is proportional to the product of associated Legendre polynomial P_ℓ^m and $e^{im\phi}$.) A more compact expression is often preferred over the sum of an infinite basis.

Due to the translation and rotation symmetry, the Green's fx (3.14) is particularly easy to find. Now we show by examples how to compute Green's function in other situations In addition to the expansion of Green's function in terms of a basis of eigenfunctions,

3.0.5 String

As an example, we consider the wave eq. for a string

This discussion can be found in M&W pp. 269-271.

$$\frac{d^2u}{dx^2} + k^2 u = \rho(x), \qquad u(0) = u(L) = 0. \tag{3.17}$$

The goal is to find the Green's function G for this problem (so that $u = \int G\rho$).

First approach

Find normalized eigenfx's

$$u_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right). \tag{3.18}$$

According to (2.24), the Green's fx is

$$G(x, x') = \frac{2}{L} \sum_{n=1}^{\infty} \frac{\sin(n\pi x/L)\sin(n\pi x'/L)}{k^2 - (n\pi/L)^2}. \tag{3.19}$$

Second approach

For $x \neq x'$, we have

$$\frac{d^2G}{dx^2} + k^2 G = 0. \tag{3.20}$$

The boundary condition for G implies that

$$G(x, x') = \begin{cases} a\sin(kx) & (x < x') \\ b\sin(k(x - L)) & (x > x') \end{cases} \tag{3.21}$$

Integrating the diff. eq. from $x' - \epsilon$ to $x' + \epsilon$, we get

$$\left.\frac{dG}{dx}\right|_{x'-\epsilon}^{x'+\epsilon} = 1. \tag{3.22}$$

Integrating again gives

$$G|_{x'-\epsilon}^{x'+\epsilon} = 0. \tag{3.23}$$

These two conditions (that the first derivative of G jumps by 1 at $x = x'$ and G is continuous) fix the values of a and b

For 2nd order diff. op's, the Green's fx. $G(x, x')$ is continuous at $x = x'$, while its first derivative is discontinuous. If $G(x, x')$ is discontinuous at $x = x'$, its first derivative includes a δ-fx., and its second derivative includes δ'.

$$a = \frac{\sin(k(x' - L))}{k\sin(kL)}, \qquad b = \frac{\sin(kx')}{k\sin(kL)}. \tag{3.24}$$

A concise expression of the final answer is

$$G(x, x') = \frac{-1}{k\sin(kL)} \sin(kx_<)\sin(k(L - x_>)), \tag{3.25}$$

where $x_<$ and $x_>$ represent the smaller and larger value of (x, x').

3.0.6 Membrane

What we did for the string can be extended to the membrane. Consider a circular drum

See M&W pp. 271-275.

$$\nabla^2 u + k^2 u = f, \qquad u = 0 \quad \text{when} \quad r = R. \tag{3.26}$$

The Green's fx. satisfies

$$\nabla^2 G + k^2 G = \delta^{(2)}(x - x'). \tag{3.27}$$

For $x \neq x'$, one can solve G by separation of variables

$$G = \begin{cases} \sum_m A_m J_m(kr)\cos(m\theta), & (r < r') \\ \sum_m B_m (J_m(kr)Y_m(kR) - Y_m(kr)J_m(kR))\cos(m\theta). & (r > r'). \end{cases} \tag{3.28}$$

Here we used the BC that $G(r = R, r') = 0$ for $r > r'$, and that $G(r = 0, r')$ should be finite for $r < r'$. The coordinate θ is by definition the angle between x and x'. There is no $\sin(m\theta)$ terms in G because G should be an even fx. of θ.

Similar to the previous case, we integrate the PDE over an infinitesimal region

$$\int \nabla^2 G d^2 x = \oint (\nabla_n G) d\ell = 1. \tag{3.29}$$

The contour of integration should be chosen such that $\nabla_n = \partial_r$ except negligable part of the contour. Then we find

$$\int d\theta r' \left.\frac{\partial G}{\partial r}\right|_{r'-\epsilon}^{r'+\epsilon} = 1, \tag{3.30}$$

which implies that

$$\Delta \frac{\partial G}{\partial r} = \frac{1}{r}\delta(\theta). \tag{3.31}$$

From this discontinuity condition and the continuity of G at $r = r'$, one can solve A_m and B_m

$$A_m = \frac{J_m(kR)Y_m(kr') - J_m(kr')Y_m(kR)}{2\epsilon_m J_m(kR)}, \qquad B_m = -\frac{J_m(kr')}{2\epsilon_m J_m(kR)}, \tag{3.32}$$

where $\epsilon_m = 2$ if $m = 0$ and $\epsilon_m = 1$ if $m > 0$.

3.0.7 Comment on Green's Function

The idea of Green's function can also be applied to sources on the boundary, i.e., inhomogeneous BC's. On the other hand, homogeneous PDE with inhomogeneous BC can be turned into inhomogeneous PDE with homogeneous BC. (Of course the question is whether this change of variable $\phi \to \phi + \phi_0$ really helps you solve the problem.)

Green's function can be used to convert a PDE into an integral eq. For example, the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x)+V(x)\psi(x)=E\psi(x) \tag{3.33}$$

can be rewritten as the integral eq.

$$\psi(x)=\psi_0(x)+\int dyG(x,y)V(y)\psi(y), \tag{3.34}$$

where $G(x,y)$ is the Green's fx for the op. $-(\frac{\hbar^2}{2m}\nabla^2+E)$, and ψ_0, which is analogous to the constant of integration, satisfies

$$-\left(\frac{\hbar^2}{2m}\nabla^2+E\right)\psi_0=0. \tag{3.35}$$

For a weak background potential $V(y)$, an approx. sol. of ψ for an incoming plane wave (scattering of a plane wave by a weak potential) can be derived by iteration. The 0-th order approx. ψ_0 should be chosen to satisfy (3.35). The 1st order correction is then

$$\psi_1(x)=\int dyG(x,y)V(y)\psi_0(y). \tag{3.36}$$

$\psi\simeq\psi_0+\psi_1$ is called the *Born approximation*. A perturbation theory can be constructed by further iterations.

In the above we have focused on elliptic diff. op's. In wave eq's we have hyperbolic diff. op's. Discussions on their Green's fx's will be different because of the difference in how we specify their BC's. We will discuss them later, after we are more familiar with the Fourier transform.

3.0.8 Exercises:

1. Find the Green's fx. satisfying

   $$\nabla^2G(x,x')=\delta(x,x') \tag{3.37}$$

   for d dimensional space. Find also the Green's fx. satisfying

   $$(\nabla^2-m^2)G(x,x')=\delta(x,x') \tag{3.38}$$

   for constant $m\in\mathbb{R}$.

   Hint for Ex.1: Use rotation and translation symmetry. In d dim's $\nabla^2=\frac{1}{r^{d-1}}\partial_r r^{d-1}\partial_r+\cdots$.

2. Find the Green's fx. for $\mathcal{D}=\frac{d}{dx}$ defined for $x\in\mathbb{R}$ with the BC $\lim_{x\to-\infty}\phi(x)=0$.

3. Find the Green's fx. for $\mathcal{D}=\frac{d^2}{dx^2}$ defined for $x\in[0,1]$ with the BC $\phi(0)=\phi(1)=0$. What would you do if the BC is $\phi(0)=a,\phi(1)=b$ for $a,b\neq0$? (We are imaging that we are solving an eq. of the form $\mathcal{D}\phi=\rho$.) Can you find the Green's fx. for the periodic BC?

4. Find the general form of the Green's fx. for the Sturm-Liouville op. $\mathcal{D} = \frac{1}{\mu(x)}\frac{d}{dx}p(x)\frac{d}{dx}$. ($\mathcal{D}G(x,x') = \frac{1}{\mu}\delta(x,x')$.) Assume that $\phi_0(x)$ and $\phi_1(x)$ are solutions to $\mathcal{D}\phi = 0$ and the BC at the two boundaries, respectively.

5. Solve the PDE for $x \in [0,\infty)$ ($\ell > 0$)

$$\left(\frac{d^2}{dx^2} + \frac{2}{x}\frac{d}{dx} - \frac{\ell(\ell+1)}{x^2}\right) G(x,x') = \delta(x-x'), \qquad x' > 0, \qquad (3.39)$$

with the BC $G(0,x') = G(\infty,x') = 0$.

6. For ($x \in (-\infty,\infty), y \in [0,1]$), find the Green's fx. for $\mathcal{D} = \partial_x^2 + \partial_y^2$ and the Dirichlet BC that it vanishes on the boundaries at $y = 0, 1$.

7. For the 3D space ($x \in \mathbb{R}$, $y \in \mathbb{R}$, $z \in [0,1]$) with periodic boundary condition at $z = 0, 1$, find the Green's fx. for the Laplace op. $\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2$.

Hint for Ex.6: Expand the dependence on y by a complete basis. Use symmetries to argue that G can depend on x only through $|x - x'|$.
Hint for Ex.7: use method of images.

3.0.9 Homework Assignment

1. A&W: Exercise (9.7.3).
2. A&W: Exercise (9.7.9).
3. A&W: Exercises (10.1.12), (10.1.13).
4. A&W: Exercise (10.5.2).
5. A&W: Exercise (10.5.8).

3.1 The Use of Complex Analysis

Analytic continuation is a powerful technique often used in solving PDE's. There are many ways it can be used and it takes experience to use it well. Whenever possible, you may keep in mind the possibility of promoting real variables in your problem to complex variables.

Here we should insert the proof of Liouville theorem using Green's fx.?

Advanced reading: M&W: Sec.8-5 Wiener-Hopf Method pp. 245-253.

Chapter 4

Perturbation Theory

Perturbation theory is very important in physics. A large portion of problems are solved using perturbative appraoches because an exact solution is usually (almost) impossible to find. This is also why (over-)simplified problems are important – more practical problems may be viewed as their perturbations.

When the quantities in a problem are naturally ordered by powers of a scale, perturbation theory can be used to obtain approximate results. If there is a parameter $\epsilon << 1$, we can expand a quantity as

$$\phi = \phi_0 + \epsilon\phi_1 + \epsilon^2\phi_2 + \epsilon^3\phi_3 + \cdots, \qquad \mathcal{O}(\phi_n) = 1. \tag{4.1}$$

Or we can write, using a different definition of variables,

$$\phi = \phi_0 + \phi_1 + \phi_2 + \phi_3 + \cdots, \qquad \mathcal{O}(\phi_n) = \epsilon^n. \tag{4.2}$$

4.1 Elementary Example

Consider the following elementary problem. For given matrix M and colume ρ, we can solve the linear eq.

$$M\phi = \rho \tag{4.3}$$

as

$$\phi = M^{-1}\rho. \tag{4.4}$$

Now suppose we also need to solve another linear eq.

$$(M + \delta M)\phi = \rho, \tag{4.5}$$

where δM is another matrix whose elements are much *smaller* (What this means needs further clarification).

4.2 Formal Expansion

The solution is

$$\begin{aligned}\phi &= (M+\delta M)^{-1}\rho \\ &= \left[(1+\delta M M^{-1})M\right]^{-1}\rho \\ &= M^{-1}\left[1-\delta M M^{-1}+\delta M M^{-1}\delta M M^{-1}-\cdots\right]\rho. \end{aligned} \tag{4.6}$$

The first term is the original solution (4.4). The next term is smaller than the first term, and so on. Naturally, if we denote the n-th term by ϕ_{n-1}, and rewrite (4.6) as

$$\phi = \phi_0 + \phi_1 + \phi_2 + \cdots \tag{4.7}$$

Each term is smaller than the previous terms. The more terms we include, the better the approximation is.

Check that for a matrix A,

$$(1-A)^{-1} = \sum_{n=0}^{\infty} A^n$$

in the sense that formally multiplying $(1-A)$ to the RHS gives 1 (from both left and right). (Here 1 is the unit matrix.) Another way to look at this identity is to diagonalize $A = U^{-1}DU$, if this is possible, so that $(1-A)^{-1} = U^{-1}(1-D)^{-1}U$, where D is diagonal and $(1-D)^{-1}$ is easily defined. From this you can also see that the inverse breaks down if one of the eigenvalues of A is 1.

4.3 2nd Approach

Expecting that the result of ϕ can be organized according to the power of δM appearing in each term in the expansion (4.6), we can rederive the same result in the following way. (This will be the prototype of deriving a perturbation theory.) First we write down (4.7), and remember that ϕ_n is of order $\mathcal{O}(\delta M^n)$. Then we plug it into (4.5) and rearrange the eq. by collecting terms at the same order

$$(M\phi_0 - \rho) + (M\phi_1 + \delta M\phi_0) + (M\phi_2 + \delta M\phi_1) + \cdots = 0. \tag{4.8}$$

To the lowest order approximation, that is, the eq. (4.5) is satisfied up to $\mathcal{O}(\delta M)$ ($(M+\delta M)\phi = \rho + \mathcal{O}(\delta M)$), we just need the first term above $(M\phi_0 - \rho) = 0$ (because all the rest are of order $\mathcal{O}(\delta M)$) and find $\phi_0 = M^{-1}\rho$.

To the next leading order, we want (4.5) to be satisfied up to $\mathcal{O}(\delta M^2)$, and so we need in addition $M\phi_1 + \delta M\phi_0 = 0$, which implies

$$\phi_1 = -M^{-1}\delta M\phi_0 = -M^{-1}\delta M M^{-1}\rho. \tag{4.9}$$

If we repeat the same argument, we reproduce all the terms in (4.6).

4.4 3rd Approach: Iteration

Another way to derive the same result is to rewrite the linear eq. (4.5) as

$$\phi = M^{-1}(\rho - \delta M\phi). \tag{4.10}$$

The reasons why this expression is good for iteration are (1) Only ϕ appears on the LHS. (2) ϕ only appears as a subleading term on the RHS.

This can be used for iteration. For the lowest order approximation, for small δM, we ignore the 2nd term on the RHS, and

$$\phi = M^{-1}\rho. \tag{4.11}$$

Then we plug this back in the RHS of (4.10) and find

$$\phi = M^{-1}(\rho - \delta M M^{-1}\rho). \tag{4.12}$$

Iteration leads to the same result (4.6).

4.5 Perturbation for PDE

Consider the application of perturbation theory to PDE. Consider a differential eq. of the form

$$\mathcal{D}_0\phi(x) = \rho(x). \tag{4.13}$$

Suppose that the solution of this eq. is known to be $\phi_0(x)$. Perturbation theory will be useful if we want to consider a deformation of the diff. eq.

$$\mathcal{D}\phi \equiv (\mathcal{D}_0 + \epsilon\mathcal{D}_1)\phi = \rho. \tag{4.14}$$

To get corrections due to $\mathcal{D}_1$, we plug (4.1) into (4.14), and find that the 0th order eq. is already satisfied. At the first order of ϵ, the diff. eq. implies

$$\mathcal{D}_0\phi_1(x) + \mathcal{D}_1\phi_0(x) = 0, \tag{4.15}$$

which can probably also be solved because ϕ_0 is now given (so the 2nd term is known), and this equation is of the same form as (4.13) (which was assumed to be an easier problem).

At the next order,

$$\mathcal{D}_0\phi_2(x) + \mathcal{D}_1\phi_1(x) = 0. \tag{4.16}$$

Apparently we can repeat this to higher orders of ϵ.

Example: $D_0 = -\frac{d}{dx}$, $\rho = \delta(x - x_0)$. Assume the BC: $\phi(-\infty) = 0$. $\phi_0 = \Theta(x - x_0)$.

Consider the case $\mathcal{D}_1 = f(x)$ for a function $f(x)$ which is "small" in some sense.

$\frac{d}{dx}\phi_1(x) = -f(x)\Theta(x)$ implies $\phi_1(x) = -\Theta(x)\int_0^x dx' f(x')$.

$\phi_2(x) = -\Theta(x)\int_0^x dx' f(x')\phi_1(x') = \Theta(x)\int_0^x dx' \int_0^{x'} dx'' f(x'')$.

4.6 Questions:

1. What is the expression for $\phi_n(x)$ for generic n? (You can assume that $G_0(x, x')$ is known.)

2. What is the expansion of the Green's fx of $\mathcal{D}$? (You can assume that $G_0(x, x')$ is known.)

4.7 Example

The Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x)+V(x)\psi(x)=E\psi(x) \tag{4.17}$$

can be solved approximately by perturbation theory if $V(x)=V_0(x)+V_1(x)$ where $V_1(x)$ is very "small" and $V_0(x)$ is a "familiar" potential, such as a constant or the potential for SHO.

If the operator $\left[-\frac{\hbar^2}{2m}\nabla^2\psi(x)+V_0(x)\right]$ has a discrete spectrum, please refer to Sec. 4.8. It this op. has a continuous spectrum, we can ask the question: For given E, how is $\psi(x)$ changed when $V(x)$ is slightly deformed from $V_0(x)$ to $V_0(x)+V_1(x)$?

When we say something is "small" or " big" we are always comparing it with something else. (Only pure numbers without units can be "small" or " big" without further justification.) Ususally the derivation of perturbation theory will tell you necessary assumptions corresponding to what you meant by "small" or "big", while a good physical intuition will also help.

4.8 Perturbation for Eigenvalue Problems

Suppose that the eigenvalue problem

$$\mathcal{D}_0\phi=\lambda\phi \tag{4.18}$$

can be solved and a complete basis of eigenfunctions $\{\phi_n^{(0)}\}$ and their eigenvalues $\{\lambda_n^{(0)}\}$ are known. Now if we want to solve the eigenvalue problem for another operator

$$\mathcal{D}\simeq\mathcal{D}_0+\epsilon\mathcal{D}_1, \tag{4.19}$$

we can use the perturbation theory. The idea is the same. Plugging

$$\phi=\phi_n^{(0)}+\epsilon\phi_n^{(1)}+\cdots, \qquad \lambda=\lambda_n^{(0)}+\epsilon\lambda_n^{(1)}+\cdots \tag{4.20}$$

into

$$(\mathcal{D}_0+\epsilon\mathcal{D}_1)\phi=\lambda\phi, \tag{4.21}$$

we find

$$\mathcal{D}_0\phi_n^{(0)}=\lambda_n^{(0)}\phi_n^{(0)}, \tag{4.22}$$

$$\mathcal{D}_0\phi_n^{(1)}=-\mathcal{D}_1\phi_n^{(0)}+\lambda_n^{(0)}\phi_n^{(1)}+\lambda_n^{(1)}\phi_n^{(0)}, \tag{4.23}$$

$$\vdots$$

The 1st eq. is trivial because that is just how we have defined $\phi_n^{(0)}$ and $\lambda_n^{(0)}$. The 2nd eq. is nontrivial, but since we already have a complete basis $\{\phi_n^{(0)}\}$, we can expand $\phi_n^{(1)}$ in the basis

$$\phi_n^{(1)}=\sum_{m\neq n}a_{nm}\phi_m^{(0)}. \tag{4.24}$$

Note that we have skipped $\phi_n^{(0)}$ in the sum, because that term should be combined with the 0-th order term. (We have not yet tried to normalized ϕ_n.)

The standard thing to do now is to take the inner product of (4.23) with an eigenfunction $\phi_k^{(0)}$. If we take the inner product with $\phi_n^{(0)}$, (4.23) gives

$$0 = -\langle \phi_n^{(0)} | \mathcal{D}_1 | \phi_n^{(0)} \rangle + 0 + \lambda_n^{(1)} \langle \phi_n^{(0)} | \phi_n^{(0)} \rangle. \tag{4.25}$$

which gives the first order correction to the eigenvalue

$$\lambda_n^{(1)} = \frac{\langle \phi_n^{(0)} | \mathcal{D}_1 | \phi_n^{(0)} \rangle}{\langle \phi_n^{(0)} | \phi_n^{(0)} \rangle}. \tag{4.26}$$

If we take the inner product with $\phi_m^{(0)}$ for $m \neq n$, (4.23) gives

$$a_{nm} = \frac{\langle \phi_m^{(0)} | \mathcal{D}_1 | \phi_n^{(0)} \rangle}{\lambda_n^{(0)} - \lambda_m^{(0)}}, \tag{4.28}$$

where we assume that $\phi_m^{(0)}$ is normalized.

Therefore, the 1st order eq. (4.23) gives the 1st order correction to both the eigenvalue and eigenvector. One can continue the same kind of analysis to higher orders of ϵ.

The 2nd order correction to the eigenvalue is

$$\lambda_n^{(2)} = \sum_{m \neq n} \frac{Q_{mn} Q_{nm}}{\lambda_n^{(0)} - \lambda_m^{(0)}}, \tag{4.27}$$

where $Q_{nm} = \langle \phi_n^{(0)} | \mathcal{D}_1 | \phi_m^{(0)} \rangle$, assuming that $\phi_m^{(0)}$'s are normalized.

4.9 Question

What are the 2nd order corrections to the eigenvalue and eigenfunction?

4.10 Perturbation for Nonlinear PDE

Consider the nonlinear PDE

$$(\nabla^2 + k^2)\phi(x) + g\phi^2(x) = \rho(x). \tag{4.29}$$

If $g = 0$, this eq. is linear and solvable for standard BC's. For small g, we can solve this eq. perturbatively.

Let

$$\phi = \phi_0 + \phi_1 + \cdots. \tag{4.30}$$

To the lowest order, the eq. is linear

$$(\nabla^2 + k^2)\phi_0(x) = \rho(x). \tag{4.31}$$

The 1st order correction of the eq. is

$$(\nabla^2 + k^2)\phi_1(x) = -g\phi_0^2(x). \tag{4.32}$$

This can be easily solved if the Green's function of $(\nabla^2 + k^2)$ is known for the given BC.

You can try to find the 2nd order corrections yourself.

4.11 WKB

The Schrödinger eq.

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right)\psi(t,x) = i\hbar\partial_t\psi(t,x) \tag{4.33}$$

should agree with classical mechanics when $\hbar \to 0$. The WKB (Wentzel, Kramers and Brillouin) method, or *semiclassical approximation*, is the perturbation theory corresponding to the expansion of $\hbar$.

$\hbar$ is (comparatively) small if the phenomenon is not too different from what is described by classical mechanics. $\hbar$ is the parameter of quantum correction.

We can write the wave function in the form

$$\psi(t,x) = A(t,x)e^{i\theta(t,x)}, \tag{4.34}$$

where A and θ are both real. The first crucial question to ask is: what are the orders of A and θ? In other words, what are m and n in $A = \mathcal{O}(\hbar^m)$ and $\theta = \mathcal{O}(\hbar^n)$? This is important because A and θ will both appear in the Schrödinger eq., and to divide the Schrödinger eq. into eqs at different orders, we need to know at least the relative order of magnitude between A and θ $(m-n)$.

Physically, A gives the density $\rho = |A|^2$, so it should be of order 1 $(m = 0)$. What is the classical interpretation of θ? For the simplest case $V = 0$, $\theta = \frac{i}{\hbar}(p\cdot x - Et)$, where $p\cdot x - Et$ is the action. So we propose that $\theta = \mathcal{O}(\hbar^{-1})$ $(n = -1)$. It is thus natural to rename θ as $S/\hbar$ and

$$\psi(t,x) = A(t,x)e^{iS(t,x)/\hbar}. \tag{4.35}$$

We can expand A and S as

$$A = A_0 + \hbar A_1 + \hbar^2 A_2 + \cdots, \qquad S = S_0 + \hbar S_1 + \hbar^2 S_2 + \cdots. \tag{4.36}$$

4.11.1 Equations and Solutions

Plugging these into the Schrödinger eq., we get

$$-\frac{\hbar^2}{2m}\left(\nabla^2 A + \frac{2i}{\hbar}\nabla A\cdot\nabla S - \frac{1}{\hbar^2}A(\nabla S)^2 + \frac{i}{\hbar}A\nabla^2 S\right) + VA = i\hbar\left(\partial_t A + \frac{i}{\hbar}A\partial_t S\right). \tag{4.37}$$

At the 0th order, we find

$$\frac{1}{2m}(\nabla S)^2 + V + \partial_t S = 0, \tag{4.38}$$

assuming that $A \neq 0$. (Solution of this eq. should be denoted S_0.) For a state with given energy, the solution is of the form

$$S = W(x) - Et. \tag{4.39}$$

For 1D, its solution is

$$S = W(x) - Et,$$

where $W(x) = \pm\int^x dx'\sqrt{2m(E - V(x'))}$.

At the 1st order, the Schrödinger eq. gives

$$\frac{1}{2m}\left(2\nabla A\cdot\nabla S + A\nabla^2 S\right) + \partial_t A = 0. \tag{4.40}$$

Multiplying A to it and denoting $\rho = A^2$, this can be rewritten as the continuity eq.

$$\frac{1}{m}\nabla\cdot(\rho\nabla S) + \partial_t\rho = 0. \tag{4.41}$$

For a stationary state, ρ is time-independent, so

$$\rho\nabla W = \text{constant}.$$

In 1D, we find

$$A = \frac{\text{constant}}{|E - V(x)|^{1/4}}$$

4.11.2 Patching Solutions

Consider the 1 dimensional case in more detail. In this case, A blows up when $E = V(x)$, and WKB breaks down. In the neighborhood of the point x_0 where $E = V(x_0)$, we can use the approximation

$$V(x) \simeq E + \frac{dV}{dx}(x_0)(x - x_0), \tag{4.42}$$

and then ψ can be solved from the Schrödinger equation without using WKB.

For a generic problem where $E = V(x)$ holds for a number of points, we divide the space into several regions. In each region, we can either use WKB, or we can use the approx. (4.42). For each region, the solution of the wave fx. is not totally fixed until the BC's are given, and the BC's should be chosen to impose the continuity of the wave fx.

Another way to deal with the problem at $E = V(x_0)$ is to analytically continuate x into the complex plane and circumvent the point x_0.

4.11.3 Question

What is the solution of the Schrödinger eq.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \frac{dV}{dx}(x_0)(x - x_0)\psi(x) = 0, \tag{4.43}$$

which is valid in the neighborhood of $x = x_0$. ($E = V(x_0)$.)

It is a Bessel fx. of order $\pm 1/3$.

4.12 WKB in general

Forgetting QM, what we did for WKB for 1 dimensional problems was that we started with a diff. eq. of the form

$$\frac{d^2y}{dx^2} + f(x)y = 0. \tag{4.44}$$

Then the solution of y for constant f suggests the substitution

$$y = e^{i\phi(x)}. \tag{4.45}$$

The diff. eq. becomes

$$-(\phi'(x))^2 + i\phi'' + f = 0. \tag{4.46}$$

Now if we assume that ϕ'' is small, this eq. has the approximate solutions

$$\phi' = \pm\sqrt{f} \Rightarrow \phi(x) = \pm\int^x dx'\sqrt{f(x')}. \tag{4.47}$$

This approximation is good if

$$|\phi''(x)| \simeq \frac{1}{2}\left|\frac{f'}{\sqrt{f}}\right| << |f|. \tag{4.48}$$

While $\sqrt{f}$ is roughly the inverse of wavelength, this condition means that the change of f in one wavelength is much smaller than $|f|$.

By iteration, we find from (4.46) the next order correction

$$(\phi')^2 = i\phi'' + f \simeq \pm\frac{i}{2}\frac{f'}{\sqrt{f}} + f, \tag{4.49}$$

which implies that

$$\phi' \simeq \pm\sqrt{f} + \frac{i}{4}\frac{f'}{f}. \tag{4.50}$$

Thus

$$\phi(x) \sim \pm\int^x dx'\sqrt{f(x')} + \frac{i}{4}\log f, \tag{4.51}$$

and so

$$y(x) \simeq \frac{1}{f^{1/4}(x)}\left(c_+ e^{i\int^x\sqrt{f(x')}dx'} + c_- e^{-i\int^x\sqrt{f(x')}dx'}\right). \tag{4.52}$$

Note that this is an example of the cases where 1st order corrections are not less important than the 0th order term.

4.13 Homework Assignment

1. Find the the solution ϕ to the linear eq.

$$M\phi = \rho \tag{4.53}$$

where

$$M = \begin{pmatrix} 1 & \epsilon \\ -\epsilon & -1 \end{pmatrix}, \qquad \rho = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{4.54}$$

up to terms of order $\mathcal{O}(\epsilon^2)$.

2. (a) Find the Green's fx. defined by

$$\left(\frac{d^2}{dx^2} + m^2\right)G(x, x') = \delta(x - x'). \tag{4.55}$$

Use Fourier transform to compute, and let $m \to m + i\epsilon$ ($\epsilon > 0$) to fix the ambiguity.

(b) Find the lowest order correction to the solution

$$\phi(x) = e^{imx} \tag{4.56}$$

for the diff. eq.

$$\left(\frac{d^2}{dx^2} + m^2 + \alpha(\Theta(x+1) - \Theta(x-1))\right)\phi(x) = 0 \tag{4.57}$$

for small α.

3. Find the lowest frequency of oscillation of a string of length L, tension T, and mass per unit length ρ_0 if a mass m is fastened to the string a distance $L/4$ from one end. The wave eq. is

$$\frac{\partial^2 y}{\partial x^2} - \frac{\rho}{T}\frac{\partial^2 y}{\partial t^2} = 0, \tag{4.58}$$

where

$$\rho = \rho_0 + m\delta(x - L/4). \tag{4.59}$$

The string is fixed at both ends (Dirichlet BC). Find the answer to the 1st order correction, and find the condition on m for this to be a good approximation.

4. For $\epsilon << 1$, let

$$M = \begin{pmatrix} 2+\epsilon & 1-\epsilon \\ 1-\epsilon & 2+2\epsilon \end{pmatrix}. \tag{4.60}$$

(a) Find eigenvectors and eigenvalues at the 0th order.

(b) Find corrections at the 1st order and 2nd order.

(c) Find the exact result and compare.

5. Find λ, the lowest eigenvalue of the diff. eq.

$$\nabla^2\phi(r,\theta) + \lambda(1+\alpha r^2)\phi(r,\theta) = 0, \tag{4.61}$$

defined for the disk $r < R$ in polar coordinates, to first order for $\alpha << 1$. (The BC is $\phi(R,\theta) = 0$.)

4.14 Exercises

1. Find the lowest eigenvalue of the diff. eq.

$$\phi''(x) + a\phi'(x) + k^2\phi(x) = 0, \tag{4.62}$$

with the boundary condition

$$\phi(0) = \phi(1) = 0, \tag{4.63}$$

for small a up to terms of order a^3. (We want to keep terms of order a^2.)

2. In this section we have only showed the 1st order corrections explicitly. Work out the general formula for 2nd order corrections.

3. Repeat what we did in Sec. 4.8 for the case when the eigenvalue problem is deformed from

$$\mathcal{D}_0\phi = \lambda\phi \tag{4.64}$$

to

$$\mathcal{D}_0\phi = \lambda(1 + \mathcal{D}_1)\phi. \tag{4.65}$$

Chapter 5

Integral Equations

5.1 Introduction

Read A&W Chapter 16 Integral Equations.

Usually a differential equation comes with some BC's in order to uniquely fix the solution. One can "integrate" the diff. eq. to rewrite the eq. as an integral eq. As integration introduces constants of integration, the BC's are automatically encoded into the integral eq. Sometimes this is a preferred form of eq. to solve.

As an example, consider the scattering of a charged particle off a fixed potential $V(x)$. The Schrödinger eq. for the charge with energy E is

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(x)\psi = E\phi(x). \tag{5.1}$$

If the potential $V(x)$ is weak, it is natural to rewrite the wave fx in the form

$$\psi(x) = \psi_0(x) + \psi_1(x), \tag{5.2}$$

where $\psi_0(x)$ is the plan wave representing the incoming particle, and so it is a solution of the eq. with $V = 0$. (That is, $\psi_0(x)$ is a plane wave with energy E.) Note that here $\psi_1(x)$ is defined as $\psi(x) - \psi_0(x)$ without approximation, rather than the 1st order correction to ψ.

Now the Schrödinger eq. can be written as

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - E\right)\psi_1(x) = -V(x)(\psi_0 + \psi_1). \tag{5.3}$$

This can be integrated (using the Green's fx) to give

$$\psi_1(x) = \rho(x) - \int dx' G(x, x')V(x')\psi_1(x'), \tag{5.4}$$

where $\rho(x)$ is a given fx. defined by

$$\rho(x) \equiv \int dx' G(x, x')V(x')\phi_0(x'). \tag{5.5}$$

The Schrödinger eq. (5.1) (together with the specification of the incoming wave fx.) is thus equivalent to the integral eq. (5.4) of $\psi_1(x)$, which should satisfy the BC that $\psi_1(x) \to 0$ for $x \to \pm\infty$.

Sometimes the problem naturally appears as an integral eq. In those cases one might want to "differentiate" the integral eq. to rewrite it as a diff. eq.

For example, the integral eq.

$$u(x) = x + \int_0^x dy\, xyu(y) \tag{5.6}$$

can be turned into a diff. eq. easy to solve:

$$f'(x) = x^2(1 + f(x)), \tag{5.7}$$

where $f(x)$ is define by

$$f(x) = \int_0^x yu(y)dy \tag{5.8}$$

and thus $u(x) = f'(x)/x$.

Apart from rewriting the integral eq. as a diff. eq., the integral eq. can also be solved perturbatively, or iteratively.

5.2 Neumann Series

The integral eq.

$$\phi(x) = \rho(x) + \lambda \int dx'\, K(x, x')\phi(x'), \tag{5.9}$$

can be iterated to give the solution

$$\phi(x) = \rho(x)+\lambda \int dx'\, K(x, x')\rho(x')+\lambda^2 \int\int dx'\, dx''\, K(x, x'')K(x'', x')\rho(x')+\cdots . \tag{5.10}$$

The expansion makes some sense if K is small in some sense. This is called the Neumann series.

If we apply the Neumann series to the example above (5.4), the lowest order correction is called Born approximation.

Apparently, if K coincides with the Green's fx for an op. $\mathcal{D}$, the integral eq. above is equivalent to a diff. eq.

$$(\mathcal{D} - \lambda)\phi(x) = \mathcal{D}\rho(x) \tag{5.11}$$

plus suitable BC.

5.3 Homework Assignment

1. Solve the integral eq.

$$f(x) = x + \lambda \int_0^1 y(x + y)f(y)dy \tag{5.12}$$

(a) by Neumann series (to all orders).

(b) by first proving that $f(x)$ is of the form $f(x) = ax + b$ for some constants a, b, and then solving for a, b.

Hint: Let

$$A = \int_0^1 yf(y)dy,$$

$$B = \int_0^1 y^2 f(y)dy.$$

2. (a) Use the Neumann series to solve the integral eq.

$$\phi(x) = 1 - 2\int_0^x t\phi(t)dt. \tag{5.13}$$

(b) Solve the same eq. by first turning it into a differential eq.

5.4 Exercises

1. Solve for $f(x)$

$$f(x) = e^x + \lambda \int_{-\infty}^x dy e^{x+y} f(y). \tag{5.14}$$

Try Neumann series to all orders.

2. Solve for $f(x)$

$$f(x) = e^x + \lambda \int_0^x dy e^y f(y). \tag{5.15}$$

3. Find all eigenvalues λ for

$$f(x) = \lambda \int_0^1 dy(1 + xy) f(y). \tag{5.16}$$

Chapter 6

Calculus of Variations

Read A&W Chapter 17 Calculus of Variations.

The calculus of variations is needed for the Lagrangian formulation of a physical system. Canonically, a physical system can be described in terms of the Lagrangian formulation and/or the Hamiltonian formulation. For fundamental physics, the Lagrangian formulation has the advantage of showing symmetries of the theory more manifestly than the Hamiltonian formulation. While the latter is more amenable to the operator formulation of QM, the former is more readily used in the path integral formulation. Although most physical systems admit both formulations, it is convenient to be familiar with both and use the formulation more convenient for the problem at hand.

6.1 Euler-Lagrange Equation

To minimize the *action* S, or any quantity of the form

$$S[y] = \int_{t_0}^{t_1} dt L(y, \dot{y}), \tag{6.1}$$

$S[y]$ is called a *functional*. It maps a function to a number, i.e., it is a function of a function. In constrast, $F(y(t)) \equiv y(t)^2$ is not a functional because it maps a function to a function, not to a number. $S[y] \equiv \int dt y^2(t)\delta(t) = y(0)^2$ and $S[y] = \int dt(\dot{y}^2 + y^2)$ are examples of functional.

we variate S with respect to $y(t)$ and demand $y(t)$ to be such that $\delta S = 0$ against infinitesimal variations of $y(t)$. This is analogous to the problem of minimizing a function $f(x_i)$. The function is minimized when $\partial_i f = 0$, or equivalently when $\delta f(x_i) = 0$ for generic infinitesimal δx_i. We can imagine that the functions $y(x_i)$ defined on the interval $[t_0, t_1]$ can be approximated for all practical purposes by a function on a lattice $\{t_0, t_0 + \Delta, \cdots, t_1 - \Delta, t_1\}$. ($\Delta = \frac{t_1 - t_0}{N}$ for large N.) We can label the values of y at the n-th point by y_n ($y_n = y(t_n)$). Then S is simply a function with $N - 1$ variables. (There are $N + 1$ points on the lattice, but there should be two BC's: $\delta y_0 = \delta y_{N+1} = 0$.) S is minimized at $\{y_i = y_i^{(0)}\}$ if $\frac{\partial}{\partial y_i} S[y^{(0)}] = 0$. This means that $\partial S = 0$ at $y = y^{(0)}$, or more precisely

$$\delta S[y^{(0)}] \equiv S[y^{(0)} + \delta y] - S[y^{(0)}] = 0 + \mathcal{O}(\delta y^2). \tag{6.2}$$

In the limit $N \to \infty$, $\delta y = \{\delta y_i\}_{i=1}^{N-1}$ corresponds to a generic infinitesimal variation of the function $y(t)$.

To consider this variation of a fx., we generalized the Taylor expansion of a function

$$f(x+\delta x) = f(x) + \delta x_i \partial_i f(x) + \cdots \tag{6.3}$$

to

$$L(y+\delta y, \dot{y} + \frac{d}{dt}\delta y) = L(y,\dot{y}) + \delta y \frac{\partial L}{\partial y} + \left(\frac{d}{dt}\delta y\right)\frac{\partial L}{\partial \dot{y}} + \cdots . \tag{6.4}$$

The variation of the action is then

$$\begin{aligned} \delta S[y] &\simeq \int_{t_0}^{t_1} dt \left[\delta y \frac{\partial L}{\partial y} + \left(\frac{d}{dt}\delta y\right)\frac{\partial L}{\partial \dot{y}}\right] \\ &= \int_{t_0}^{t_1} dt \left[\delta y \frac{\partial L}{\partial y} + \frac{d}{dt}\left(\delta y \frac{\partial L}{\partial \dot{y}}\right) - \delta y \frac{d}{dt}\frac{\partial L}{\partial \dot{y}}\right] \\ &= \left[\delta y \frac{\partial L}{\partial \dot{y}}\right]_{t_0}^{t_1} + \int_{t_0}^{t_1} dt \left[\delta y \left(\frac{\partial L}{\partial y} - \frac{d}{dt}\frac{\partial L}{\partial \dot{y}}\right)\right]. \end{aligned} \tag{6.5}$$

In order for S to be minimized at $y = y_0(t)$, we need $\delta S[y_0] = 0$. This can be satisfied only if both the first and the second terms vanish

$$\left[\delta y \frac{\partial L}{\partial \dot{y}}\right]_{t_0}^{t_1} = 0, \qquad \frac{\partial L}{\partial y} - \frac{d}{dt}\frac{\partial L}{\partial \dot{y}} = 0. \tag{6.6}$$

If S is an action and t is time, the 1st term vanishes because we always assume that $\delta y(t_0) = \delta y(t_1) = 0$ as part of the definition of the *least action principle*. (It is also called the *Hamilton's principle*.) In other cases, the problem should specify the BC of y such that the first term vanishes. The 2nd eq. is called the *Euler-Lagrange equation*.

For example, $\delta y(t) = \sum_n a_n \sin(n\pi \frac{t-t_0}{t_1-t_0})$, and the variation of $y(t)$ is the same as varying a_n's.

Depending on the specific problem, there can be many advantages to use the action to specify a physical system. The formulation starting with the action is called the *Lagrangian formulation*. (The integrand L is called the em Lagrangian.) The formulation starting with the Hamiltonian (how to define energy in terms of coordinates and momenta) is called the *Hamiltonian formulation*.

For more details about the connection between the two formulations and discussions about their validity, see my notes on QM3, also available at the webpage for Appl. Math. 4.

6.1.1 Newtonian Mechanics

The action of a Newtonian particle with potential energy $V(x)$ is

$$S = \int dt L, \qquad L = \frac{1}{2}m\dot{x}^2 - V(x). \tag{6.7}$$

That is, Lagrangian equals the kinetic energy minus the potential energy.

Example: brachistochrone

Let A and B be two points in a vertical plane, with A higher than B. Along what curve connecting A and B will a particle slide (without friction) from A (starting at rest) to B in the shortest time?

"Brachistochrone" is Greek for "shortest time".

we want to minimize

$$T = \int dt, \tag{6.8}$$

where

$$dt = \frac{ds}{v} = \frac{\sqrt{1+y'^2}dx}{\sqrt{2gy}}. \tag{6.9}$$

Here $ds = \sqrt{dx^2+dy^2} = \sqrt{1+y'^2}dx$ is the distance, and $v = \sqrt{2gy}$ is the velocity gained by reducing the potential energy. So we want to minimize

$$T = \int_0^{x_0} dx \sqrt{\frac{1+y'^2}{2gy}}. \tag{6.10}$$

The Euler-Lagrange eq. derived from minimizing T can be solved and the solution is

$$x = A(\phi - \sin\phi), \qquad y = A(1-\cos\phi). \tag{6.11}$$

6.1.2 Geodesic

In Riemannian geometry, a manifold can be equipped with the notion of distance by assigning the distance between two infinitesimally separated points to be given by

$$ds^2 = g_{ij}(x)dx^i dx^j, \tag{6.12}$$

where dx^i is the coordinate difference of the two points. The tensor $g_ij(x)$ is called the " metric".

A change of coordinate will change how the metric looks, but the notion of "distance" is independent of the choice of coordinate system.

For two given points A and B on the manifold with metric $g_{ij}(x)$, the geodesic (the shortest path) connecting them should minimize

$$S = \int ds = \int \sqrt{g_{ij}(x)dx^i dx^j} = \int d\tau \sqrt{g_{ij}\frac{dx^i}{d\tau}\frac{dx^j}{d\tau}}, \tag{6.13}$$

where τ is an arbitrary parametrization of the path. The derivation of the Euler-Lagrange eq. (the geodesic eq.) is left as an exercise.

6.1.3 Generalizations

When there are more than one variables and higher than first derivatives, the derivation of Eular-Lagrange eq. is straightforward. For the integral

$$S = \int dt L(x_i, \dot{x}_i, \ddot{x}_i, \cdots), \tag{6.14}$$

there is an Euler-Lagrange equation for each x_i derived by varying δx_i. S is minimized when all Euler-Lagrange eq's are simultaneously satisfied. This is analogous to what we do to minimize a multi-variable fx.

6.2 Lagrange Multiplier

Often it is convenient to use redundent variables, that is, variables with constraints. For example, a point on a circle can be specified by the Cartesian coordinates (x, y) or the angular coordinate θ. The difference is that (x, y) is constrained by $x^2 + y^2 = R^2$, while $\theta = \theta_0$ and $\theta = \theta_0 + 2\pi$ represent the same point.

When we express a fx. in terms of variables with constraints, we can not minimize it by demanding that its derivatives vanishe for all derivatives with respect to all variables. We can either choose to use only variables without constraints, or we can use the trick of Lagrange multipliers. The trick of Lagrange multiplier is this: to minimize the fx. $f(x_a)$ with the constraints $\{g_i(x_a) = 0\}$, we can just minimize the fx.

$$F(x_a, \lambda_i) \equiv f(x_a) + \lambda_i g_i(x_a) \tag{6.15}$$

In addition to the constraints $g_i = 0$, the EL eqs are $\partial_a f(x) + \lambda_i \partial_a g(x) = 0$.

as if all variables x_a, λ_i are free of constraints.

6.2.1 Example

The fx. to be minimized is $f = x$ for the Cartesian coord. on the circle of radius $R = 1$. It is wrong to demand that $\frac{df}{dx} = 0$, which is impossible. The trick is to consider $F = f + \lambda(x^2 + y^2 - 1)$, where λ is called the "Lagrange multiplier". F is a fx. of x, y, λ. Now we can demand that all derivatives of F vanish

The same trick works when the variables are fx's. In that case the Lagrange multipliers are also fx's.

$$\partial_x F = 1 + 2\lambda x = 0, \qquad \partial_y F = 2\lambda y = 0, \qquad \partial_\lambda F = x^2 + y^2 - 1 = 0. \tag{6.16}$$

The EL eq. for the Lagrange multiplier is just the constraint. The other two EL eq's are different from $\frac{df}{dx} = 0$, and are the correct conditions to minimize f. We can solve the EL eq's by

$$x = -\frac{1}{2\lambda}, \quad y = 0, \quad x = \pm 1. \tag{6.17}$$

(So in the end we find $\lambda = \mp 1/2$ but we don't really care about the value of the Lagrange multiplier.)

Another way to find the same result is to use the angular variable $f = \cos\theta$ and so it is extremized at $\theta = 0, \pi$.

Let us consider this problem in a slightly more general setting. Suppose we want to minimize $f(x, y)$ with the constraint $g(x, y) = 0$. To get some intuition, one can imagine that we draw curves along which $f(x, y)$ is constant on the $x - y$ plane. These curves would be the equipotential surfaces if $f(x, y)$ is a potential, so we will call them equipotential curves of f. Now we also draw the curve satisfying $g(x, y) = 0$. To minimize $f(x, y)$ with the constraint

$g(x,y)=0$ is to look for minimal values of f along the curve of $g=0$. When we reach a local extremum of f along the curve of $g=0$, the value of f will hardly change when we walk an infinitesimal distance along the curve of $g=0$. Therefore, the extremal value of f will happen at a point where the tangent of the curve of $g=0$ is parallel to the tangent of the equipotential curve of f passing through that point. In equations,

$$\partial_x f(x,y)=\lambda\partial_x g(x,y), \qquad \partial_y f(x,y)=\lambda\partial_y g(x,y). \tag{6.18}$$

Actually these eq's say that the gradient (which is the normal to the tangent) of f is parallet to the gradient of g.

6.2.2 Example

What is the EOM for a point mass constrained to a frictionless circle? The action for a point mass in flat space is

$$S_0=\int dt\frac{1}{2}m(\dot{x}^2+\dot{y}^2). \tag{6.19}$$

The constraint is

$$x^2+y^2=R^2. \tag{6.20}$$

So the action for the particle on a circle should be

$$S=S_0+\int dt\lambda(t)(x^2(t)+y^2(t)-R^2). \tag{6.21}$$

Check that the EOM's derived from varying $x(t), y(t), \lambda(t)$ this action is equivalent to the action

$$S'=\int dt\frac{1}{2}mR^2\dot{\theta}^2(t), \tag{6.22}$$

which is written in terms of the variable θ that solves the constraint (i.e. the constraint is solved by $x=R\cos\theta, y=R\sin\theta$).

Check that $\lambda(t)$ is proportional to the normal force exerted on the point mass to keep it on the circle.

Now we generalize the problem to the motion of a point mass constrained by a generic condition $g(x,y)=0$. The track that constrains the point mass will exert force on the point mass to keep it on the track. The difference between a constraint and a potential is that the force due to a potential $V(x,y)$ is $-\nabla V$, while the force due to a constraining track depends on the motion of the point mass. On the other hand, we know that motion along the track is not obstructed, and thus the force due to the track must be perpendicular to the tangent of the track. The force is thus parallel to the gradient of g, i.e., the force is

$$\lambda(\partial_x g(x,y),\partial_y g(x,y)) \tag{6.23}$$

for some $\lambda\in\mathbb{R}$. The EOMs are therefore

$$m\ddot{x}=\lambda\partial_x g(x,y), \qquad m\ddot{y}=\lambda\partial_y g(x,y). \tag{6.24}$$

The magnitude of the normal force, or the magnitude of λ, should be exactly what is needed to keep the point mass on the track. That is, the EOMs above together with the constraint

$$g(x, y) = 0 \tag{6.25}$$

should determine x, y, λ altogether. This is exactly what we get by using the Lagrange multiplier.

6.3 Eigenvalue Problems

A&W: Exercise 17.7.6

Check that the EL eq. for minimizing

$$\int_a^b dx \left[p \left(\frac{d}{dx}\phi(x) \right)^2 + q(x)\phi^2(x) \right] \tag{6.26}$$

with the constraint

$$\int_a^b dx \rho(x)\phi^2(x) = 1 \tag{6.27}$$

is the eigenvalue eq.

$$\mathcal{D}\phi(x) = \lambda(x)\phi(x), \tag{6.28}$$

where $\lambda(x)$ is the Lagrange multiplier, for the Sturm-Liouville op.

$$\mathcal{D} = \frac{1}{\rho(x)} \left[-\frac{d}{dx} p(x) \frac{d}{dx} + q(x) \right]. \tag{6.29}$$

On the other hand, to minimize (6.26) with the constraint (6.27) is the same as minimizing

$$K \equiv \frac{\int dx [p(x)\phi'^2(x) + q(x)\phi^2(x)]}{\int dx \rho(x)\phi^2(x)}. \tag{6.30}$$

While the numerator of K is the same as (6.26), the effect of the constraint (6.27) is the same as that of the denominator of K, that is, to exclude the influence on (6.26) due to scaling $\phi(x)$.

Plugging an eigenfx. $\phi_n(x)$ into K, and using the BC for the eigenfx., we find that the minimal values of K are the eigenvalues of $\mathcal{D}$.

If we know the eigenfx. ϕ_0 for the lowest eigenvalue λ_0 to a first order approximation, one can check that the estimation of λ_0 by K is good up to 2nd order approx. Hence K is useful for estimating the lowest eigenvalue of an op.

See A&W p. 1073 for the proof.

6.3.1 Example

For the eigenvalue problem

$$\frac{d^2}{dx^2}u(x) + \lambda u(x) = 0, \tag{6.31}$$

with the BC

$$u(0) = u(1) = 0, \tag{6.32}$$

we know that the exact value of the lowest eigenvalue is

$$\lambda_0 = \pi^2. \tag{6.33}$$

If we use a polynomial satisfying the BC

$$u(x) = x(1-x) \tag{6.34}$$

(there is no need to normalize it), we find that

$$\lambda_0 \leq K = 10, \tag{6.35}$$

which is a good approx. of $\pi^2 \simeq 9.87$. ($\Delta\lambda_0 \simeq 1.3\%$.)

6.4 Homework Assignment

1. For a uniform string of length L hanging from two supports at the same height, by minimizing the potential energy of the string, find the eq. determining the shape of the string, and the vertical distance from the supports and the lowest point on the string.

2. Find the minimum of the function

   $$f(x) = x^2 + 2y^2 + 3z^2 + 2xy + 2xz \tag{6.36}$$

   subject to the constraint

   $$x^2 + y^2 + z^2 = 1. \tag{6.37}$$

3. Estimate the lowest freq. of a circular drum head of radius a. (Use the trial fx. of the form $u(r) = 1 - ar$.) Compare it with the exact result.

6.5 Exercises:

- Find the minimal and maximal values of the fx. $f(x) = ax + by + cz$ with the constraint $x^2 + y^2 + z^2 = 1$.

- An object of mass m is in the 2 dimensional force field

  $$\vec{F}(\vec{r}) = \frac{GMm}{r^2}\hat{r}. \tag{6.38}$$

  Curves along which the mass falls between given points in the shortest time are solutions of a differential eq. of the form

  $$\frac{dr}{d\theta} = f(r). \tag{6.39}$$

  Find the fx. $f(r)$.

- Estimate the lowest eigenvalue of the op.

$$\mathcal{D} = -\frac{d^2}{dx^2} + V(x), \qquad V(x) = \omega^2 x^2, \tag{6.40}$$

defined on the real line $x \in \mathbb{R}$. The BC's to be satisfied by the eigenfx's ϕ are

$$\phi(\pm\infty) = 0. \tag{6.41}$$

Use trial fx's of the form $e^{-\frac{a}{2}x^2}$ to estimate the lowest eigenvalue.

K is now a fx. of a. Determine a by $\frac{dK}{da} = 0$.

Chapter 7

Differential Geometry

Chapter 8

Groups

8.1 Definition and Examples

A set of elements $G = \{g_a\}$ equipped with a product $\cdot$ is a group if the following conditions are met:

- For any $g_a, g_b \in G$, $g_a \cdot g_b \in G$. (Closure of the algebra.)
- For any $g_a, g_b, g_c \in G$, $(g_a \cdot g_b) \cdot g_c = g_a \cdot (g_b \cdot g_c)$. (Associativity of the algebra)
- There is an element $e \in G$ such that $e \cdot g_a = g_a \cdot e = g_a$ for all $g_a \in G$. (Existence of identity.)
- For each $g_a \in G$, there is a $g_b \in G$ so that $g_b \cdot g_a = g_a \cdot g_b = e$, and we will denote $g_b = g_a^{-1}$. (Existence of inverse.)

8.1.1 Example: $U(1)$ and $SO(2)$

The set of rotations of a 2 dimensional flat space is a group. In terms of the Cartesian coordinates x, y, a rotation is labelled by an angle $\theta \in [0, 2\pi)$

$$\begin{pmatrix} x \\ y \end{pmatrix} \to \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}. \tag{8.1}$$

This group, whose elements have a 1-1 matching with these 2×2 matrices, is called $SO(2)$. It is also defined as the group of 2×2 matrices which satisfy the following properties

- All entries are real.
- Its determinant is 1.
- Its transpose is its inverse.

If we consider $n \times n$ matrices with these properties, they form the group denoted by $SO(n)$. $SO(n > 2)$ are non-Abelian while $SO(2)$ is Abelian.

In terms of a complex coordinate $z = x + iy$, a rotation corresponds to a phase $e^{i\theta}$ ($z \to e^{i\theta} z$). The set of phases $\{e^{i\theta}\}$ is the group denoted by $U(1)$.

The notion of a group can be abstract (e.g. " the group of rotations of an n-dimensional flat space", or, say, $G = \{a, b\}$). The product of group elements can be induced from its definition (e.g. two rotations of the flat space is equivalent to a certain rotation) or assigned abstractly by hand (e.g. $aa = a, ab = b, ba = b, bb = a$).

Very often we use the algebra of matrix multiplication to realize the algebra of a group. That is, for every element $g_a \in G$, there is a corresponding matrix $M(g_a)$ such that

$$M(g_a)M(g_b) = M(g_a \cdot g_b). \tag{8.2}$$

We say that $M(g)$ is a *representation* of G. Representations related to each other by the conjugation of a nonsingular matrix S

$$M'(g) = SM(g)S^{-1} \tag{8.3}$$

are said to be *equivalent*.

If we have two representations of G (or even two copies of the same rep.), we can construct a new representation

$$M(g) = \begin{pmatrix} M_1(g) & 0 \\ 0 & M_2(g) \end{pmatrix}. \tag{8.4}$$

A rep. that is equivalent to a rep. like M is called *reducible*, otherwise it is *irreducible*. If we would like to study *all* rep's of a group G, we only need to study all irreducible representations.

Another way to construct new rep's out of old ones is to take a product (the previous operation is called a "sum")

$$M(g)_{(ia)(jb)} = (M_1(g))_{ij}(M_2(g))_{ab}. \tag{8.5}$$

If some elements in a group do not commute, i.e., $g_1 \cdot g_2 \neq g_2 \cdot g_1$, the group is *non-Abelian*. Otherwise it is *Abelian*.

$U(n)$ is the group of $n \times n$ matrices which are unitary, i.e., its Hermitian conjugate is its inverse. This implies that the determinant of a $U(n)$ matrix is either 1 or -1. If we also demand that the determinant is 1, the group is called $SU(n)$.

Check that if M_1, M_2 are rep's, M is also a rep.

8.1.2 Example: Z_n

The group Z_n can be defined as $Z_n = \{e, a, a^2, \cdots, a^{n-1}\}$ where the rule of multiplication is just $a^n = e$ and those implies by the criteria of a group. The algebra of Z_n also agrees with the algebra of addition modulo n, as well as the algebra of multiplication generated by $e^{2\pi i/n}$ (i.e. $e \to 1$ and $a \to e^{2\pi i/n}$).

Z_2 is also the group of flipping a coin. We can use 1×1 matrices to realize Z_2 as $M(e) = 1, M(a) = -1$. This is a 1 dimensional realization of the group Z_2. Z_2 also has a 2 dimensional realization as

$$M(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad M(a) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{8.6}$$

The groups Z_n is quite different from $SO(m)$ or $SU(m)$ in that the former have a finite number of elements, while the latter have infinitely many elements.

8.2 Lie Group and Lie Algebra

Lie groups are groups which have continuous parameters to label elements in the group. For example, $SO(n)$ and $SU(n)$ are Lie groups. Due to the fact that parameters can take continuous values, we can define differentiation with respect to these parameters. What we get in the end from differentiation of Lie groups are Lie algebras.

Obviously Lie groups are not finite groups.

8.2.1 Example $SU(2)$

The group $SU(2)$ is the most important example of Lie groups. It can be defined as the group of 2×2 unitary matrices with their determinant equal to 1

$$U(\alpha, \beta) = \begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix}, \qquad |\alpha|^2 + |\beta|^2 = 1, \qquad \alpha, \beta \in \mathbb{C}. \tag{8.7}$$

It takes 2 complex parameters α, β satisfying a constraint, or equivalently, 3 continuous real parameters to parametrize elements in the group. For example, we can define 3 real parameters θ, ϕ, φ by

$$\alpha = \cos\theta e^{i\phi}, \qquad \beta = \sin\theta e^{i\varphi}. \tag{8.8}$$

Or, we can define 3 real parameters a_1, a_2, a_3 by

$$U(a_1, a_2, a_3) = e^{i\sum_{i=1}^{3} a_i \sigma_i}, \tag{8.9}$$

where σ_i are Pauli matrices

$$\sigma_1 = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{8.10}$$

This is also a natural way to parametrize elements in $SU(2)$ because $\sum_i a_i\sigma_i$ is the most general traceless Hermitian 2×2 matrices, so that its exponential is the most general unitary 2×2 matrices with unit determinant.

There is some advantage to this parametrization of $SU(2)$ because we will take the differentiation and exponentials are easier when it comes to differentiation. We differentiate $U(a_i)$ with respect to a_i and evaluate at the identity of the group, which is the point parametrized by $a_1 = a_2 = a_3 = 0$. We get

$$\frac{\partial}{\partial a_i} U(a_1, a_2, a_3)\bigg|_{a_1=a_2=a_3=0} = i\sigma_i. \tag{8.11}$$

The algebra of the Pauli matrices

$$[\sigma_i, \sigma_j] = i\epsilon_{ijk}\sigma_k \tag{8.12}$$

is then the Lie algebra of $SU(2)$, denoted by $su(2)$.

Conceivably if we had started with a different parametrization of the group, we might get a slightly different result. But they should be related by a linear transformation

$$\sigma_i' = A_{ij}\sigma_j \tag{8.13}$$

for some constant A_{ij}. Therefore the commutators in $su(2)$ may look different in a different basis.

Since there are 3 independent parameters for $SU(2)$, there will always be 3 linearly independent elements in $su(2)$.

8.2.2 Example $SO(3)$

What is the Lie algebra for the Lie group $SO(3)$? $SO(3)$, the group of 3D rotations, has 3 degrees of freedom. We can rotate around the x, y or z-axis. Using Cartesian coordinates for a vector in 3 dim Euclidean space, a rotation around the z-axis corresponds to the matrix

$$M_3(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{8.14}$$

For an infinitesimal rotation around the $z4$-axis, the change of a 3-vector is

$$\delta x = M_3(\theta)x - x \simeq i\theta\lambda_3 x, \tag{8.15}$$

where

$$\lambda_3 = \begin{pmatrix} 0 & i & 0 \\ -i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{8.16}$$

This is the Lie algebra generator corresponding to an infinitesimal rotation around the z-axis. Now we can write down the Lie algebra generators for rotations around the x and y-axes by permutation of directions. It is straightforward to check that the Lie algebra of $SO(3)$ is the same as that of $SU(2)$

$$[\lambda_i, \lambda_j] = i\epsilon_{ijk}\lambda_k \tag{8.17}$$

up to a scaling, so these two Lie algebras are equivalent.

This algebra is very important in physics. It is the algebra of angular momentum operators. The Lie algebra $so(3)$ is the same algebra that angular momentum operators satisfy in QM, regardless of the details of the physical system. However, for a different physical system, the angular momentum op. may be in a different rep. of $so(3)$.

The fact that $su(2)$ and $so(3)$ are the same also have significant physical consequences. While representations of $SO(3)$ only admits integral spin (spin = eigenvalue of the matrices $M(\tau_i)$), representations of $SU(2)$

8.2.3 Lie Algebra

For every continuous symmetry of a physical theory or a physical model, e.g. the translation symmetry or rotation symmetry of 3D space,

- It is a Lie group G, and has a Lie algebra. (G is $\mathbb{R}^3$ or $SO(3)$ for translation and rotation symmetry.)
- There are corresponding conserved charges (due to Noether's theorem). (E.g. momentum, angular momentum.)
- The commutators of the conserved charge operators in QM are the same as the Lie algebra.

In general, a Lie algebra is a linear space $\{\sum_a \alpha_a \tau_a\}$, where τ_a's are the generators/basis, equipped with the algebra defined by the brackets

$$[\tau_a, \tau_b] = i f_{abc} \tau_c, \tag{8.18}$$

where the constants f_{abc} are called structure constants. The structure constants are antisymmetric

$$[\tau_a, \tau_b] = -[\tau_b, \tau_a], \tag{8.19}$$

These two properties are automatic if we recall that the bracket comes from the commutator.

and they satisfying the Jacobi identity

$$[\tau_a, [\tau_b, \tau_c]] + [\tau_b, [\tau_c, \tau_a]] + [\tau_c, [\tau_a, \tau_b]] = 0. \tag{8.20}$$

The Lie algebra is related to a Lie group through exponentiation

$$g = e^{i\alpha_a \tau_a}. \tag{8.21}$$

More than one Lie groups can correspond to the same Lie algebra. Check that $SU(2)$ and $SO(3)$ have the same Lie algebra.

A representation of a Lie algebra realizes the bracket by commutators of matrices

$$[M(\tau_a), M(\tau_b)] \equiv M(\tau_a)M(\tau_b) - M(\tau_a)M(\tau_b) = i f_{abc} M(\tau_c). \tag{8.22}$$

Apparently they go hand in hand with representations of the corresponding group

$$M(g) = e^{i\alpha_a M(\tau_a)} \tag{8.23}$$

unless there are more than one groups for the same Lie algebra.

8.3 Exercises:

- Which of the following are groups? (1) A group of people. (2) Coordinate transformations $x \to x+a$ with any $a \in \mathbb{R}$. (3) Coord. transfs. $x \to x+n$ with $n \in \mathbb{Z}$. (4) Coord. transfs. $x \to x + a$ with $a > 0$.

- Derive the Lie algebra for the group G which consists of 2×2 matrices of the form

$$\begin{pmatrix} 1 & a \\ 0 & 1 \end{pmatrix}, \qquad a \in \mathbb{R}. \tag{8.24}$$

- Derive the Lie algebra for the group G which consists of rotations and translations of the 2 dimensional Euclidean space.

8.4 Isometry

Symmetry is one the most important subject in physics. There are several types of symmetries. *All symmetries are groups.*

The symmetry of a space is called its *isometry*. For instance, Poincare group is the isometry of Minkowski space. Here we consider two examples of spaces with large isometries.

Symmetry of a theory, symmetry of a configuration or a state; global symmetry, gauge symmetry, ···

8.4.1 Example: $\mathbb{R}^2$

Consider the example of 2 dimensional Euclidean space. This space has the rotation symmetry and translation symmetry. Functions on this space is transformed under rotation and translation as

$$f(x,y) \to f(x',y') = f(\cos\theta x - \sin\theta y + x_0, \sin\theta x + \cos\theta y + y_0). \tag{8.25}$$

They form a representation of the isometry group.

Let us choose the Fourier basis

$$\psi_{\vec{k}} = e^{i(k_x x + k_y y)} \tag{8.26}$$

for fx's on $\mathbb{R}^2$. Under an isometry transformation,

$$\psi_{\vec{k}} \to e^{i(k_x x_0 + k_y y_0)} \psi_{\vec{k}_R}, \tag{8.27}$$

where $\vec{k}_R$ represents the result of rotating $\vec{k}$.

First, focusing on the group of translations, each Fourier mode is by itself a rep. for which a translation by (x_0, y_0) is represented by a phase factor (1×1 matrix)

$$e^{i(k_x x_0 + k_y y_0)}. \tag{8.28}$$

The Fourier modes are also the eigenfx's of the translation op's

$$p_x = -i\partial_x, \qquad p_y = -i\partial_y. \tag{8.29}$$

The translation op's generate translations on fx's

$$f(x,y) \to f(x + x_0, y + y_0) = e^{i(x_0 p_x + y_0 p_y)} f(x,y). \tag{8.30}$$

The infinitesimal version is

$$\delta f(x,y) = i(x_0 p_x + y_0 p_y) f(x,y). \tag{8.31}$$

Therefore, p_x and p_y are Lie algebra generators corresponding to translations.

Including rotations, the set of Fourier modes with the same wave number $|\vec{k}|$ is a rep. of the group of rotation and translation. The generator of rotation is

$$J = -i(x\partial_y - y\partial_x). \tag{8.32}$$

8.4.2 Example: S^2

Consider the Schrödinger eq. for a particle in a spherically symmetric potential

$$\left(-\nabla^2 + V(r)\right)\Psi(r,\theta,\phi) = E\Psi(r,\theta,\phi). \tag{8.33}$$

Here the Laplace op. for 3D Euclidean space is

$$\nabla^2 = \partial_r^2 + \frac{1}{r^2}\nabla_{S^2}^2. \tag{8.34}$$

We have learned before that the eigenvalues of

$$\nabla_{S^2}^2 = \frac{1}{\sin\theta}\partial_\theta \sin\theta \partial_\theta + \frac{1}{\sin^2\theta}\partial_\phi^2 \tag{8.35}$$

are $-\ell(\ell+1)$ for $\ell = 0, 1, 2, \cdots$.

The eigenfx's of $\nabla_{S^2}^2$ are the spherical harmonics $Y_{\ell m}(\theta,\phi)$:

$Y_{\ell m} = \pm\mathcal{N}_{\ell m} P_\ell^{|m|}(\cos\theta) e^{im\phi}$,

where $\mathcal{N}_{\ell m}^2 = \frac{(2\ell+1)}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}$ is chosen such that $Y_{\ell m}$ is an orthonormal basis

$\int d\cos\theta d\phi Y_{\ell m}^\dagger Y_{\ell' m'} = \delta_{\ell\ell'}\delta_{mm'}$.

The sign $\pm$ is chosen to be $(-1)^m$ for $m \geq 0$, $+1$ for $m < 0$.

By separation of variables, we can decompose the Schrödinger eq. into

$$-\nabla_{S^2}^2 \psi(\theta,\phi) = \ell(\ell+1)\psi(\theta,\phi) \tag{8.36}$$

and

$$\left(-\partial_r^2 - \frac{1}{r^2}\ell(\ell+1) + V(r)\right) R(r) = ER(r) \tag{8.37}$$

for the ansatz $\Psi(r,\theta,\phi) = R(r)\psi(\theta,\phi)$. From now on we will focus our attention on $\psi(\theta,\phi)$, a fx. defined on S^2. The radial part depends on the potential $V(r)$ and is irrelevant to the $SO(3)$ symmetry of S^2.

Note that, by the definition of $\nabla_{S^2}^2$ (8.34) (without looking at the complicated expression in (8.35)) it should be clear that it is invariant under 3D rotations, since ∇^2 and r are both invariant. On the other hand, eigenfx's of $\nabla_{S^2}^2$ will in general change under rotations. This means that, for an eigenvalue of $\nabla_{S^2}^2$ and its corresponding eigenfx, we can rotate it and obtain another eigenfx with the same eigenvalue. That is, the set of eigenfx's with the same eigenvalue constitute a representation of the group $SO(3)$.

Let us first consider functions in $\mathbb{R}^3$. In the end we can set $x^2+y^2+z^2 = 1$ and reinterpret them as functions on S^2. In terms of the Cartesian coordinates,

it is easy to see that the following sets of functions form representations of $SO(3)$

$$\{1\} \tag{8.38}$$

$$\{x, y, z\} \tag{8.39}$$

$$\{x^2, xy, xz, y^2, yz, z^2\} \tag{8.40}$$

$$\vdots \tag{8.41}$$

In general, since $SO(3)$ is a linear map on the Cartesian coordinates, any set of fx's generated by monomials $\{x^{i_1} \cdots x^{i_n}\}$ of a fixed order n is a rep. of $SO(3)$. However, they are not irreducible except for $n = 0, 1$. In the above, while the first two rep's are irreducible, the 3rd rep. is not, because the element $x^2 + y^2 + z^2$ is invariant under $SO(3)$ rotations, and so it must be a trivial rep. by itself. Eliminating this element from the rep., we get

$$\{Y^{ij} \equiv x^i x^j - \frac{1}{3}\delta^{ij} x^2\} \qquad (x^2 \equiv \sum_k x_k^2), \tag{8.42}$$

which is an irreducible rep. Note that not all elements in this set are linearly independent, because $Y^{ii} = 0$.

We will use "irrep" as the abbreviation of "irreducible representation".

Similarly, from the rep. $\{x^i x^j x^k\}$, we can project out elements like $x^2 x^i$, which transform in exactly the same way as $\{x^i\}$ by themselves, and get an irrep.

$$\{Y^{ijk} \equiv x^i x^j x^k - a x^2(\delta^{ij} x^k + \delta^{jk} x^i + \delta^{ki} x^j)\}. \tag{8.43}$$

The constant a here should be determined by demanding that $Y^{iij} = 0$, because Y^{iij} will transform like x^j by themselves. (So $a = \frac{1}{5}$.) After eliminating those elements which form their own reps, we get irreps.

Therefore we see that we get a basis of functions which is organized by listing fxs in the same irrep together. Setting

$$x = \sin\theta\cos\phi, \quad y = \sin\theta\sin\phi, \quad z = \cos\theta, \tag{8.44}$$

this basis is reduced to a basis of fxs on S^2.

Although the Cartesian coordinate system has its obvious advantage of maintaining the symmetry among the 3 variables, sometimes we would like to use a different coordinate system

$$w = x + iy = \sin\theta e^{i\phi}, \quad \bar{w} = x - iy = \sin\theta e^{-i\phi}, \quad z = \cos\theta, \tag{8.45}$$

which has the advantage that rotations around the z-axis are realized in a simpler way.

In terms of the new coord. system, the irrep. $\{x^i x^j - \frac{1}{3}x^2\delta^{ij}\}$ is written as

$$\{w^2, \bar{w}^2, wz, \bar{w}z, z^2 - \frac{1}{3}(w\bar{w} + z^2)\}. \tag{8.46}$$

In terms of θ, ϕ, these fxs on S^2 are the same as the spherical harmonics $\{Y_{2m}\}_{m=-2}^2$ (up to normalization factors). We list here some of the spherical harmonics for comparison:

Question: Why are fx's in the same irrep's also eigenfx's?

$$Y_{00} = \tfrac{1}{\sqrt{4\pi}},$$
$$Y_{1\pm1} = \mp\sqrt{\tfrac{3}{8\pi}}\sin\theta e^{\pm i\phi}, \qquad Y_{10} = \sqrt{\tfrac{3}{4\pi}}\cos\theta,$$
$$Y_{2\pm2} = \sqrt{\tfrac{15}{32\pi}}\sin^2\theta e^{\pm 2i\phi}, \qquad Y_{2\pm1} = \mp\sqrt{\tfrac{15}{8\pi}}\sin\theta\cos\theta e^{\pm i\phi}, \qquad Y_{20} = \sqrt{\tfrac{5}{16\pi}}(3\cos^2\theta - 1).$$

In the above, we constructed irrep's of $SO(3)$ by fx's on S^2, and these fx's are identified with eigenfx's of the Laplace op. $\nabla^2_{S^2}$ on S^2.

From the action of $SO(3)$ on fx's on S^2, one can deduce the action of $so(3)$ on these fx's. Consider a rotation along the z-axis, for example. A rotation by the angle ϕ_0 corresponds to

$$\phi \to \phi + \phi_0. \tag{8.47}$$

Its action on a fx. is

$$f(\theta, \phi) \to f(\theta, \phi + \phi_0) = e^{\phi_0 \partial_\phi} f(\theta, \phi). \tag{8.48}$$

An infinitesimal rotation $\theta_0 \ll 1$ along the z-axis is generated by the diff. op.

$$J_z \equiv -i\partial_\phi \tag{8.49}$$

in the sense that

$$\delta f(\theta, \phi) = i\theta_0 J_z f(\theta, \phi). \tag{8.50}$$

The spherical harmonics $Y_{\ell m}$ have eigenvalue m for J_z. If the fx's here are wave fx's, J is the angular momentum op.

In terms of Cartesian coordinates,

$$J_z = -i(x\partial_y - y\partial_x). \tag{8.51}$$

Apparently, the complete angular momentum op., which is a 3-vector, can be written as

$$J_i = -i\epsilon_{ijk} x^j \partial_k. \tag{8.52}$$

One can check that, when acting on fx's on S^2, the Laplace op. on S^2 is equivalent to

$$\nabla^2_{S^2} = J_1^2 + J_2^2 + J_3^2. \tag{8.53}$$

The Lie algebra of $SO(3)$ can be derived from (8.52)

$$[J_i, J_j] = i\epsilon_{ijk} J_k. \tag{8.54}$$

This relation is independent of the rep. We can use this algebraic relation to show universal properties of rep's. For example, an irrep. corresponding to a

given ℓ, e.g. $\{Y_{\ell m}\}_{m=-\ell}^{\ell}$, has elements with eigenvalues $m = -\ell, \cdots \ell$ of J_z at intervals of 1. We can derive this property from the algebraic relation (8.54) as follows. Let

$$J_\pm = J_1 \pm iJ_2. \tag{8.55}$$

Then (8.54) is equivalent to

$$[J_\pm, J_z] = \mp J_z, \qquad [J_+, J_-] = 2J_z. \tag{8.56}$$

It follows that, if a fx f_m has eigenvalue m for J_z, i.e.

$$J_z f_m = m f_m, \tag{8.57}$$

then $(J_\pm f_m)$, which is another fx., has the eigenvalue $m \pm 1$ for J_z (unless $J_\pm f_m = 0$) because

$$J_z(J_\pm f_m) = (J_\pm J_z + [J_z, J_\pm])f_m = (m \pm 1)(J_\pm f_m). \tag{8.58}$$

This is why it is useful to extract the algebraic structure of Lie algebra from specific problems.

In this example, we demonstrated the connection between partial differential eqs, geometry, group theory and Lie algebra. In both physics and mathematics, problems with different appearances may turn out to be closely connected. A good comprehension of a topic often demands understanding of several seemingly independent subjects. As promising young investigators, you are encouraged to learn as much as possible, as a preparation for uncovering previously unknown deep connections among concepts and phenomena.

********** END **********