

DR. DIMITER N. PETSEV

METHODS OF ANALYSIS IN
CHEMICAL AND NUCLEAR ENGINEERING

ChNE 525 Lecture Notes

WITH ERIC M. BENNER

STUDENTS PRESS

DECEMBER 16, 2014

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Forward

“Not a word of Landau and not a thought of Lifshitz” —Anonymous

This old witticism on the writing of the classic Russian physics texts has held surprisingly close to reality in the process of creating this work of Dr. Petsev’s and mine. Over the past two years, I have had the pleasure of assisting in the teaching of Methods of Analysis in Chemical and Nuclear (and now Biological) Engineering (ChNE 525) at the University of New Mexico. In the Fall of 2012, almost on a whim, I began taking notes of the course in \LaTeX primarily for the excuse of exposing myself to Dr. Petsev’s method of teaching this subject (also for the amusement of doing something ridiculously challenging!). I soon realized the potential value in this clear means of note-taking, as it became my way of helping to give an update of material covered in class whenever a student was unable to attend. Furthermore, the complete set of semester notes was sent out to all students at the end of the course, and I have known several who found the notes useful in studying for their comprehensive examinations.

The result of the work done in 2012 forms the bulk of these notes. These portions primarily sketch the equations used in the class as a complete outline of the material. However, lectures which I have had extra time with reviewing or watching digitally have had the chance to be augmented such that some—or in a few cases a significant quantity of—the material discussed both on the board and orally in the lecture is included in its full essential content in the text. In general, each section is done very much in the style of a lecture with as many of the small steps needed in a strong derivation included to make the mathematical manipulation as easy to follow as possible.

A number of improvements still need to be made to this document. Regretfully, figures tend to be the most difficult to recreate digitally; hence, many of the diagrams that elucidate the problems at hand are not incorporated into the notes at this point in time; those that are, I am certain will be helpful. Few tables or formal citations are included. Many of the macros used in the production of this document are in the process of being superseded by better ones. Finally, it would be especially beneficial to get a thorough transcription of the oral portion of the lectures added in along with the presented equations. As this is very much a work in progress, feel free to give suggestions, comments, and especially corrections about anything in this document.

The primary focus of an advanced course in engineering mathematics is to give the student a strong foundation in the application and analytical solution of ordinary and partial differential equations to engineering and physics problems. Thus, these topics are the central and dominant subject areas described. However, additional topics such as geometric transformations, integral transforms, perturbation theory, and (soon to be added) statistics are also introduced. The student is encouraged to pursue computational methods to enhance their understanding of PDEs and as a complement to analytical methods.

—*Eric M. Benner*, August 25, 2014

UNIT 1

Chapter 7—Vector Calculus

1.1 Lecture 1: August 20, 2012 *Introduction to Fields*

Reading and knowing up through Chapter 5 of the textbook by McQuarrie is prerequisite to the following material.

Fields

- *e.g.* Pressure, Electric, Magnetic, Electrostatic (Potential), *etc...*
- Scalar Field
 - 1 number at a point
 - Electrostatic, Pressure, temperature, concentration
- Vector Field
 - 3 numbers describe point
 - Fluid velocity (magnitude & direction)
 - Electric field

Gradients

- Vector of the direction of greatest change
- Turns scalar into vectors
- Often referred to as “grad”, “del” or the symbol itself as “nabla”
- Expressed in 3D cartesian coordinates as:

$$\nabla = \frac{\partial}{\partial x}\hat{\mathbf{i}} + \frac{\partial}{\partial y}\hat{\mathbf{j}} + \frac{\partial}{\partial z}\hat{\mathbf{k}} \quad (1.1.1)$$

Gradients applied to a vector quantity turns into a tensor.

Contours

Contours are examples of scalar fields. The gradient is normal to the contour of no change. A line of contour is defined by,

$$f(x, y, z) = C.$$

Observe that the gradient is a operator where,

$$\nabla\phi \neq \phi\nabla.$$

A general vector in cartesian coordinates,

$$\mathbf{A} = A_x\hat{\mathbf{i}} + A_y\hat{\mathbf{j}} + A_z\hat{\mathbf{k}}.$$

Operating with the gradient on the vector \mathbf{A} ,

$$\nabla \cdot \mathbf{A} = \hat{\mathbf{i}} \cdot \hat{\mathbf{i}} \frac{\partial A_x}{\partial x} + \hat{\mathbf{j}} \cdot \hat{\mathbf{j}} \frac{\partial A_y}{\partial y} + \hat{\mathbf{k}} \cdot \hat{\mathbf{k}} \frac{\partial A_z}{\partial z} \quad (1.1.2)$$

$$\begin{aligned} &= 1 \frac{\partial A_x}{\partial x} + 1 \frac{\partial A_y}{\partial y} + 1 \frac{\partial A_z}{\partial z} \\ &= \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z} \end{aligned} \quad (1.1.3)$$

This is due to the fact that a unit vector multiplied by itself is simply 1.

The *curl* of a vector (rotation)

$$\nabla \times \mathbf{A} = \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \right) \hat{\mathbf{i}} + \left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} \right) \hat{\mathbf{j}} + \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) \hat{\mathbf{k}} \quad (1.1.4)$$

$$= \begin{vmatrix} \hat{\mathbf{i}} & \hat{\mathbf{j}} & \hat{\mathbf{k}} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{vmatrix}. \quad (1.1.5)$$

Surface Integral

$$\int_S \mathbf{A} \cdot \mathbf{n} dS \equiv \int \mathbf{A} \cdot d\mathbf{S} \quad (1.1.6)$$

only that portion “projected” on the surface normal goes through the surface.

Gauss Divergence Theorem

For the integral over a closed surface we represent by \oint or \oiint .

$$\oiint_S \mathbf{A} \cdot d\mathbf{S} = \int_V \nabla \cdot \mathbf{A} dV \quad (1.1.7)$$

We shall now derive this given that $dV = dx dy dz$ in Cartesian coordinates,

$$\begin{aligned} \int_V \nabla \cdot \mathbf{A} dV &= \int_x \int_y \int_z \left(\frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z} \right) dx dy dz & (1.1.8) \\ &= \int_x \int_y \int_z \frac{\partial A_x}{\partial x} dx dy dz + \int_x \int_y \int_z \frac{\partial A_y}{\partial y} dx dy dz \\ &\quad + \int_x \int_y \int_z \frac{\partial A_z}{\partial z} dx dy dz \end{aligned}$$

Observing that $\int_x \frac{dA_x}{dx} dx = \int dA_x$,

$$\begin{aligned} \int_V \nabla \cdot \mathbf{A} dV &= \int_y \int_z A_x dy dz + \int_x \int_z A_y dx dz + \int_x \int_y A_z dx dy \\ &= \int_y \int_z \mathbf{A} \cdot \mathbf{n}_x dy dz + \int_x \int_z \mathbf{A} \cdot \mathbf{n}_y dx dz + \int_x \int_y \mathbf{A} \cdot \mathbf{n}_z dx dy \end{aligned}$$

Returning to the potential,

$$\int_V \frac{d\phi}{dt} dV = \oint_S \mathbf{A} \cdot \mathbf{n} dS \quad (1.1.9)$$

$$= \int_V \nabla \cdot \mathbf{A} dV \quad (1.1.10)$$

So,

$$\frac{\partial \phi}{\partial t} = \nabla \cdot \mathbf{A} \quad (1.1.11)$$

On a note of Thermodynamic importance. Entropy always increases. 2nd Law of Thermodynamics (expressed without time derivative), $dS \geq 0$.

Laplace operator

The *Laplacian* or Laplace operator is ∇^2 or alternatively represented as Δ .

$$\nabla \cdot \nabla = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (1.1.12)$$

The Laplacian of a scalar field is also a scalar quantity.

$$\lim_{dx \rightarrow 0} \left[\frac{\phi(x) - \frac{1}{2}(\phi(x-dx) + \phi(x+dx))}{dx^2} \right] = \frac{\partial^2 \phi}{\partial x^2} \quad (1.1.13)$$

If $\frac{\partial^2 \phi}{\partial x^2} > 0$ we observe a positive curvature.

Potential Flow

Conservative forces, potential is a conservative force. Note that friction is non-conservative; it has a loss term due to heat. If $\nabla \times \mathbf{b} = 0$ this implies a conservative form (no friction), and is a necessary & sufficient condition for the existence of a potential. We will now demonstrate this.

$$(\nabla \times \mathbf{A})_x = \hat{\mathbf{i}} \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \right) \quad (1.1.14)$$

let $\mathbf{A} = \nabla \phi$, this gives $A_z = \frac{\partial \phi}{\partial z}$, and $A_y = \frac{\partial \phi}{\partial y}$.

$$\begin{aligned} (\nabla \times \mathbf{A})_x &= (\nabla \times \nabla \phi)_x & (1.1.15) \\ &= \hat{\mathbf{i}} \left(\frac{\partial}{\partial y} \left(\frac{\partial \phi}{\partial z} \right) - \frac{\partial}{\partial z} \left(\frac{\partial \phi}{\partial y} \right) \right) \\ &= \hat{\mathbf{i}} \left(\frac{\partial^2 \phi}{\partial y \partial z} - \frac{\partial^2 \phi}{\partial z \partial y} \right) \\ &\equiv 0 & (1.1.16) \end{aligned}$$

The same argument holds for $(\nabla \times \mathbf{A})_y$ and $(\nabla \times \mathbf{A})_z$. Thus, we observe,

$$\nabla \times \nabla \phi \equiv 0 \quad (1.1.17)$$

$$\nabla \cdot \nabla \times \mathbf{A} \equiv 0 \quad (1.1.18)$$

Line Integrals

Line integrals are extremely useful and important for the calculation of thermodynamic and mechanical *work*. $dw = \mathbf{F} \cdot d\mathbf{r}$.

$$\int dw = \int \mathbf{F} \cdot d\mathbf{r} \quad (1.1.19)$$

$$= \int_C F_x dx + \int_C F_y dy + \int_C F_z dz \quad (1.1.20)$$

We know also that

$$\int \mathbf{F} \cdot d\mathbf{r} = \int \mathbf{F} \cdot \frac{d\mathbf{r}}{dt} dt$$

since $\frac{d\mathbf{r}}{dt} dt = d\mathbf{r}$.

Now,

$$\mathbf{F} = \nabla \phi \quad (1.1.21)$$

$$= \frac{\partial \phi}{\partial x} \hat{\mathbf{i}} + \frac{\partial \phi}{\partial y} \hat{\mathbf{j}} + \frac{\partial \phi}{\partial z} \hat{\mathbf{k}} \quad (1.1.22)$$

with $d\mathbf{r} = \hat{\mathbf{i}} dx + \hat{\mathbf{j}} dy + \hat{\mathbf{k}} dz$,

$$\begin{aligned}\int \nabla\phi \cdot d\mathbf{r} &= \int \left(\frac{\partial\phi}{\partial x} \hat{\mathbf{i}} + \frac{\partial\phi}{\partial y} \hat{\mathbf{j}} + \frac{\partial\phi}{\partial z} \hat{\mathbf{k}} \right) \cdot (\hat{\mathbf{i}} dx + \hat{\mathbf{j}} dy + \hat{\mathbf{k}} dz) \\ &= \int \left(\frac{\partial\phi}{\partial x} \hat{\mathbf{i}} \cdot \hat{\mathbf{i}} dx + \frac{\partial\phi}{\partial y} \hat{\mathbf{j}} \cdot \hat{\mathbf{j}} dy + \frac{\partial\phi}{\partial z} \hat{\mathbf{k}} \cdot \hat{\mathbf{k}} dz \right) \\ &= \int \left(\frac{\partial\phi}{\partial x} dx + \frac{\partial\phi}{\partial y} dy + \frac{\partial\phi}{\partial z} dz \right)\end{aligned}\tag{1.1.23}$$

Thus, as a definite integral,

$$\int_a^b \mathbf{F} \cdot d\mathbf{r} = \int_a^b d\phi\tag{1.1.24}$$

$$= \phi(b) - \phi(a)\tag{1.1.25}$$

1.2 Lecture 2: August 22, 2012

Potential Field

Reviewing from last lecture,

$$\int_c \mathbf{F} \cdot d\mathbf{r} = \int_a^b d\phi = \phi(b) - \phi(a) \quad (1.2.1)$$

We see that any path will give the same result if we are in a potential system.

Application to Thermodynamics

$$dU = T dS - p dV$$

where $S \equiv \text{entropy}$. If S is constant you eliminate all paths but one. Then, with $w \equiv \text{work}$,

$$\int dw = - \int p dV \quad (1.2.2)$$

If the path begins and ends at the same point $\oint p dV = 0$, and we see that there is no net work done on the cycle. Potential Forces are always *conservative*.

Example: Newton's Second Law

Note: $d\mathbf{r} = \frac{d\mathbf{r}}{dt} dt$ which may be decided by dt . Also, $\frac{d\mathbf{r}}{dt} = \mathbf{v}$ and $\mathbf{v} \cdot \mathbf{v} = v^2$.

$$m \frac{d^2\mathbf{r}}{dt^2} = \mathbf{F} = -\nabla\phi \quad (1.2.3a)$$

$$m \int \frac{d^2\mathbf{r}}{dt^2} \cdot dt = - \int \nabla\phi dt$$

$$m \int \frac{d^2\mathbf{r}}{dt^2} \cdot \frac{d\mathbf{r}}{dt} dt = - \int \nabla\phi dt$$

$$\frac{m}{2} \int \frac{d}{dt} \left(\frac{d\mathbf{r}}{dt} \cdot \frac{d\mathbf{r}}{dt} \right) dt = - \int \nabla\phi dt$$

$$\frac{m}{2} \int d \left(\frac{d\mathbf{r}}{dt} \right)^2 = \frac{mv^2}{2} + C \quad (1.2.3b)$$

Now for $\mathbf{r} = \mathbf{r}(t)$, a function of time, $d\mathbf{r} = \frac{d\mathbf{r}}{dt} dt$. With $d\mathbf{r} = dx \hat{\mathbf{i}} + dy \hat{\mathbf{j}} + dz \hat{\mathbf{k}}$

$$\begin{aligned} - \int \nabla\phi \cdot d\mathbf{r} &= - \left[\int \frac{\partial\phi}{\partial x} dx + \int \frac{\partial\phi}{\partial y} dy + \int \frac{\partial\phi}{\partial z} dz \right] \\ &= \phi + C_2 \end{aligned} \quad (1.2.4)$$

defining $C = C_1 + C_2$

$$\frac{mv^2}{2} - \phi = C \quad (1.2.5)$$

Thus, we have shown the Energy Conservation Law.

Gauss Law of Electrostatics

Example of a line integral

Gauss law of electrostatics describes the relation between charged particles;

$$\mathbf{E} = \frac{q\mathbf{m}}{4\pi\epsilon_0 r^2}. \quad (1.2.6)$$

For a real medium $\epsilon_0 \rightarrow \epsilon_0\epsilon$, where ϵ is about 8 for room temperature air, and only 1 in a vacuum.

$$\oiint_S \mathbf{E} \cdot \mathbf{n} dS = \frac{q}{\epsilon_0} \quad (1.2.7)$$

Note that $q, 4, \pi, \epsilon_0$, are constants so we will leave them out for now.

$$\oiint_S \frac{m}{r^2} dS = \int_V \nabla \cdot \left(\frac{\mathbf{m}}{r^2} \right) dV \quad (1.2.8)$$

With $\mathbf{r} = (x, y, z)$

$$\nabla \cdot (\mathbf{r}f(r)) = \frac{\partial}{\partial x}(xf(r)) + \frac{\partial}{\partial y}(yf(r)) + \frac{\partial}{\partial z}(zf(r)) \quad (1.2.9)$$

Each of these terms may be simplified similarly as,

$$\begin{aligned} \frac{\partial}{\partial x}(xf(r)) &= f(r) + x \frac{\partial f}{\partial x} \\ &= f(\mathbf{r}) + x \frac{\partial f}{\partial r} \frac{\partial r}{\partial x} \end{aligned}$$

Recall, $r = \sqrt{x^2 + y^2 + z^2}$

$$\begin{aligned} \frac{\partial r}{\partial x} &= \frac{x}{\sqrt{x^2 + y^2 + z^2}} \\ &= \frac{x}{r} \end{aligned} \quad (1.2.10)$$

Thus,

$$\nabla \cdot (\mathbf{r}f(r)) = 3f(r) + r \frac{df}{dr} \quad (1.2.11)$$

Note: $\nabla \cdot \mathbf{r} = 3$, $\mathbf{n} = \frac{\mathbf{r}}{r}$

$$f(r) = r^{n-1}$$

Substituting,

$$\begin{aligned} \nabla \cdot (\mathbf{r} r^{n-1}) &= \nabla \cdot (\mathbf{n} r^n) \\ &= 3r^{n-1} + r \cdot \nabla r^{n-1} \\ &= 3r^{n-1} + (n-1)r^{n-1} \\ &= (n+2)r^{n-1} \\ &= 0 \end{aligned} \quad (1.2.12)$$

Evidently, $n = -2$

$$\int 0 \, d\mathbf{r} = 0$$

Typically, $r = 0$ is the location of the charge.

$$\int_V \nabla \cdot \left(\frac{\mathbf{n}}{r^2} \right) dV = \oiint_S \frac{\mathbf{n}}{r^2} \cdot d\mathbf{S} \quad (1.2.13)$$

$$= \int \frac{\mathbf{n}}{r^2} \cdot d\mathbf{S} + \int \frac{\mathbf{n}}{\nabla ta^2} d\mathbf{S}_2 \quad (1.2.14)$$

Now observe that $d\mathbf{S} = \mathbf{n} dS$, $dS = \nabla ta^2 d\Omega$, $\mathbf{n} \cdot \mathbf{n} = 1$. When you integrate counter-clockwise,

$$\begin{aligned} - \int_{S_2} \frac{\mathbf{n} \cdot \mathbf{n}}{\nabla ta^2} \nabla ta^2 d\Omega &= - \int d\Omega \\ &= 4\pi \end{aligned} \quad (1.2.15)$$

$$\int_V \nabla \cdot \left(\frac{\mathbf{n}}{r^2} \right) dV = \begin{cases} 0 & \text{if } r = 0 \text{ is not included,} \\ -4\pi & \text{if } r = 0 \text{ is included} \end{cases} \quad (1.2.16)$$

$$\oiint_S \mathbf{E} \cdot \mathbf{n} dS = \frac{-4\pi q}{4\pi \epsilon_0} = \frac{-q}{\epsilon_0}$$

Which gives the Poisson Equation result,

$$\boxed{\nabla \cdot \mathbf{E} = \frac{-q}{\epsilon_0}}. \quad (1.2.17)$$

Radial Potential

The potential is $V(r)$. What is the gradient of the function? $\nabla V(r) = ?$ We know $r = \sqrt{x^2 + y^2 + z^2}$.

$$\frac{\partial V(r)}{\partial x} = \frac{dV(r)}{dr} \frac{\partial r}{\partial x} = \frac{x}{r} \frac{dV(r)}{dr} \quad (1.2.18)$$

which additionally gives

$$\begin{aligned} \frac{\partial V(r)}{\partial y} &= \frac{dV(r)}{dr} \frac{\partial r}{\partial y} = \frac{y}{r} \frac{dV(r)}{dr} \\ \frac{\partial V(r)}{\partial z} &= \frac{dV(r)}{dr} \frac{\partial r}{\partial z} = \frac{z}{r} \frac{dV(r)}{dr} \end{aligned}$$

Thus,

$$\begin{aligned} \nabla V(r) &= \left(\frac{x}{r} \hat{\mathbf{i}} + \frac{y}{r} \hat{\mathbf{j}} + \frac{z}{r} \hat{\mathbf{k}} \right) \frac{dV}{dr} \\ &= \frac{\mathbf{r}}{r} \frac{dV}{dr} \\ &= \mathbf{n} \frac{dV}{dr} \end{aligned} \quad (1.2.19)$$

Laplacian of the reciprocal of the radius

Now find $\nabla^2 \frac{1}{r} = ?$

$$\begin{aligned} \nabla^2 \frac{1}{r} &= \nabla \cdot \left(\nabla \frac{1}{r} \right) \\ &= \int \nabla \cdot \left(\frac{\mathbf{n}}{r^2} \right) dV \\ &= \begin{cases} -4\pi & \text{including } r = 0 \\ 0 & \text{excluding } r = 0 \end{cases} \end{aligned} \quad (1.2.20)$$

$$-4\pi \int \delta(\mathbf{r}) dV = \begin{cases} -4\pi & \text{including } r = 0 \\ 0 & \text{excluding } r = 0 \end{cases} \quad (1.2.21)$$

or

$$\nabla^2 \frac{1}{r} = -4\pi \delta(\mathbf{r}) = -4\pi \delta(x) \delta(y) \delta(z) \quad (1.2.22)$$

For this we observe that we have a simple Greens function,

$$G(n) = \frac{1}{-4\pi r} \quad (1.2.23)$$

Green's function method of solving differential equation $\nabla^2 G = \delta(\mathbf{r})$, where

$$F(r) = \int G(r - r') dr' dr \quad (1.2.24)$$

Gradient Transposition

Prove,

$$\int_V \mathbf{A}(\mathbf{r}) \cdot \nabla f(\mathbf{r}) dV = - \int_V f(\mathbf{r}) \nabla \cdot \mathbf{A}(\mathbf{r}) dV \quad (1.2.25)$$

\mathbf{A} , f vanish as $x \rightarrow \infty$

$$\begin{aligned} \int_x \int_y \int_z \left(A_x \frac{\partial f}{\partial x} + A_y \frac{\partial f}{\partial y} + A_z \frac{\partial f}{\partial z} \right) dx dy dz &= \int_y \int_z \left(\int_x A_x \frac{\partial f}{\partial x} dx \right) dy dz \\ &+ \int_x \int_z \left(\int_y A_y \frac{\partial f}{\partial y} dy \right) dx dz \\ &+ \int_x \int_y \left(\int_z A_z \frac{\partial f}{\partial z} dz \right) dx dy \end{aligned}$$

Now, with the first term of the following equation going to zero,

$$\int_x A_x \frac{df}{dx} dx = [A_x f]_{x=-\infty}^{+\infty} - \int_x f \frac{dA_x}{dx} dx. \quad (1.2.26)$$

So the earlier equation now simplifies to

$$= \int_y \int_z \left(\int_x f \frac{\partial A_x}{\partial x} dx \right) dy dz + \int_x \int_z \left(\int_y f \frac{\partial A_y}{\partial y} dy \right) dx dz + \int_x \int_y \left(\int_z f \frac{\partial A_z}{\partial z} dz \right) dx dy$$

which further goes to

$$\begin{aligned} &= - \int_y \int_z \left(\int_x f \frac{\partial A_x}{\partial x} dx \right) dy dz + \int_x \int_z \left(\int_y f \frac{\partial A_y}{\partial y} dy \right) dx dz + \int_x \int_y \left(\int_z f \frac{\partial A_z}{\partial z} dz \right) dx dy \\ &= - \int_x \int_y \int_z f \left(\frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z} \right) dx dy dz \\ &= - \int_x \int_y \int_z f \nabla \cdot \mathbf{A} dx dy dz \\ &= \boxed{- \int_V f(\mathbf{r}) \nabla \cdot \mathbf{A}(\mathbf{r}) dV} \end{aligned} \tag{1.2.27}$$

Green's Theorem

When given $P(x, y)$, $Q(x, y)$, and

$$\oint_c \mathbf{F}(\mathbf{r}) \cdot d\mathbf{r} = \oint [P dx + Q dy]. \tag{1.2.28}$$

Prove,

$$\oint P dx + Q dy = \iint \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y} \right) dx dy. \tag{1.2.29}$$

To be finished next week...

1.3 Lecture 3: August 27, 2012

Notes about class

- TA Office Hour: 11 am Thursdays.
- Homework questions go to Dr. Petsev. Trying to keep the questions and what students know fair and equal.
- TA: for misunderstandings on grading and questions

Greens Theorem, cont.

In an x-y plane with a closed contour. When $P(x, y); Q(x, y)$, given

$$\oint_c \mathbf{F}(\mathbf{r}) \cdot d\mathbf{r} = \oint [P dx + Q dy]. \quad (1.3.1)$$

We want to describe the contour as a function $y(x)$. The following is *Greens theorem*;

$$\oint P dx + Q dy = \iint \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y} \right) dx dy. \quad (1.3.2)$$

We outline the proof below.

$$\iint \frac{\partial Q}{\partial x} dx dy = \int_y \left[\int_x \frac{\partial Q}{\partial x} dx \right] dy \quad (1.3.3)$$

$$\begin{aligned} &= \int_B^D Q(y, x_2(y)) dy - \int_D^B Q(y, x_1(y)) dy \\ &= \int_B^D Q(y, x_2(y)) dy + \int_B^D Q(y, x_1(y)) dy \\ &= \oint Q dy \end{aligned} \quad (1.3.4)$$

Following similar arguments,

$$\begin{aligned} \iint \frac{\partial P}{\partial y} dx dy &= \int_A^C [P(x, y_2(x)) - P(x, y_1(x))] dx \\ &= - \int_A^C P(x, y_2(x)) dx - \int_C^A P(x, y_1(x)) dx \\ &= - \oint P dx \end{aligned} \quad (1.3.5)$$

Stokes Theorem

A similar theorem known as *Stokes theorem*;

$$\oint_C \mathbf{v} \cdot d\mathbf{r} = \iint_S (\nabla \times \mathbf{v}) \cdot \mathbf{n} dS \quad (1.3.6)$$

Tensors and Tensor Algebra

Tensors are a generalization of scalars, vectors, square matrices, etc.

- Scalar: Tensor of order (rank) 0
- Vector: Tensor of order 1

In three-dimensional space we have $\mathbf{a} = (a_1, a_2, a_3)$. Tensors of higher orders exist.

Transforming from coordinates of (x_1, x_2, x_3) to (x'_1, x'_2, x'_3) . These axes correspond by cosines when the two coordinates are arbitrary rotations of each other. So we define a tensor l_{ij} , cosine of the angles between the old axis $(O_i, i = x_1, x_2, x_3)$ and the new one $(O_j, j = x'_1, x'_2, x'_3)$. This gives the transformation to be;

$$x'_j = l_{1j}x_1 + l_{2j}x_2 + l_{3j}x_3 \quad (1.3.7)$$

Transforming back to the original axes,

$$x_i = l_{i1}x'_1 + l_{i2}x'_2 + l_{i3}x'_3 \quad (1.3.8)$$

Rule of repeated indices (Cartesian summation notation):

$$l_{ij}x_i = \sum_i l_{ij}x_i \quad (1.3.9)$$

$$l_{ij}x'_j = \sum_j l_{ij}x'_j \quad (1.3.10)$$

This notation was popularized by Einstein to simplify notation in developing the theory of Relativity. Note that linear algebra and properties of matrices are very pertinent to tensors.

Definition 1 (Vector).

$$a'_j = l_{ij}a_i \quad (1.3.11)$$

Note that there does exist improper rotations because of left-and-right frames of reference. A pseudo vector exists for $\mathbf{a} \times \mathbf{b}$.

Kronecker Delta

$$\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} \quad (1.3.12)$$

This is known as the *unit tensor*. It has the following property

$$\delta_{ij}a_j = \delta_{i1}a_1 + \delta_{i2}a_2 + \delta_{i3}a_3 \quad (1.3.13)$$

Definition 2 (Tensor).

$$A'_{pq} = l_{ip}l_{jq}A_{ij} \equiv \sum_{i=1}^3 \sum_{j=1}^3 l_{ip}l_{jq}A_{ij} \quad (1.3.14)$$

In papers Tensors are often capitalized and bolded, on the whiteboard they are best double-underlined.

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \quad (1.3.15)$$

$$\mathbf{A}' = \mathbf{L}^t \mathbf{A} \mathbf{L} \quad (1.3.16)$$

$$\mathbf{A} = \mathbf{L} \mathbf{A}' \mathbf{L}^t \quad (1.3.17)$$

In the special case of symmetric tensors, $A_{ij} = A_{ji}$. Antisymmetric tensors are defined as $A_{ij} = -A_{ji}$.

We also notice that for the Kronecker Delta,

$$\delta = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (1.3.18)$$

Tensor Product of two vectors

Dyadic Product, inner product

$$\mathbf{a} \cdot \mathbf{b} = a_1 b_1 + a_2 b_2 + a_3 b_3 \quad (1.3.19)$$

Cross Product

$$\mathbf{a} \times \mathbf{b} = \begin{vmatrix} e_1 & e_2 & e_3 \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} \quad (1.3.20)$$

The outer product of two vectors is

$$\mathbf{a} \mathbf{b} = \mathbf{c} \quad (1.3.21)$$

$$c_{ij} = a_i b_j = \begin{pmatrix} a_1 b_1 & a_1 b_2 & a_1 b_3 \\ a_2 b_1 & a_2 b_2 & a_2 b_3 \\ a_3 b_1 & a_3 b_2 & a_3 b_3 \end{pmatrix} \quad (1.3.22)$$

Couchy Stress

Deformation of non-isotropic solid, the stress is

$$\sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix} \quad (1.3.23)$$

$$= \begin{pmatrix} \sigma_{11} & \tau_{12} & \tau_{13} \\ \tau_{21} & \sigma_{22} & \tau_{23} \\ \tau_{31} & \tau_{32} & \sigma_{33} \end{pmatrix} \quad (1.3.24)$$

where the second matrix is expressed for sheer-stress.

For a falling droplet,

$$\mathbf{u} = \frac{\mathbf{f}_g}{6\pi\mu R_P} \quad (1.3.25)$$

This gives rise to the *Oseen tensor*, \mathbf{T} ,

$$\mathbf{u} = \mathbf{T}(\mathbf{r}) \cdot \mathbf{f}_g \quad (1.3.26)$$

Tensor Algebra

1. Addition

$$\mathbf{C} = \mathbf{A} + \mathbf{B} \quad (1.3.27)$$

$$c_{ij} = A_{ij} + B_{ij}$$

2. Multiplication by a Scalar

$$\mathbf{C} = \alpha \mathbf{A} \quad (1.3.28)$$

$$c_{ij} = \alpha A_{ij}$$

3. A tensor may be broken into symmetric and antisymmetric matrices,

$$A_{ij} = \frac{1}{2}(A_{ij} + A_{ji}) + \frac{1}{2}(A_{ij} - A_{ji}) \quad (1.3.29)$$

$$\mathbf{A} = \frac{1}{2}(\mathbf{A} + \mathbf{A}^t) + \frac{1}{2}(\mathbf{A} - \mathbf{A}^t)$$

4. Dot product

$$\mathbf{A} \cdot \mathbf{b} = \mathbf{c} \quad c_i = A_{ij}b_j \quad (1.3.30)$$

$$\mathbf{b} \cdot \mathbf{A} = \mathbf{d} \quad d_i = A_{ij}b_i \quad (1.3.31)$$

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \cdot \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = \begin{pmatrix} A_{11}b_1 + A_{12}b_2 + A_{13}b_3 \\ A_{21}b_1 + A_{22}b_2 + A_{23}b_3 \\ A_{31}b_1 + A_{32}b_2 + A_{33}b_3 \end{pmatrix} \quad (1.3.32)$$

5. Rotation Tensor

$$\mathbf{\Omega} = \begin{pmatrix} 0 & \omega_3 & -\omega_2 \\ -\omega_3 & 0 & \omega_1 \\ \omega_2 & -\omega_1 & 0 \end{pmatrix}, \quad \boldsymbol{\omega} = \begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix} \quad (1.3.33)$$

$$\mathbf{a} \times \boldsymbol{\omega} = \mathbf{\Omega} \cdot \mathbf{a} \quad (1.3.34)$$

$$\boldsymbol{\omega} \times \mathbf{a} = \mathbf{a} \cdot \mathbf{\Omega} \quad (1.3.35)$$

$$(a_1 \quad a_2 \quad a_3) \cdot \begin{pmatrix} \Omega_{11} & \Omega_{12} & \Omega_{13} \\ \Omega_{21} & \Omega_{22} & \Omega_{23} \\ \Omega_{31} & \Omega_{32} & \Omega_{33} \end{pmatrix} = \begin{pmatrix} \Omega_{11}a_1 + \Omega_{12}a_2 + \Omega_{13}a_3 \\ \Omega_{21}a_1 + \Omega_{22}a_2 + \Omega_{23}a_3 \\ \Omega_{31}a_1 + \Omega_{32}a_2 + \Omega_{33}a_3 \end{pmatrix} \quad (1.3.36)$$

1.4 Lecture 4: August 29, 2012

Returning to the operation of rotation of a vector in a plane.

$$\mathbf{a} \times \boldsymbol{\omega} = \boldsymbol{\Omega} \cdot \mathbf{a} \quad (1.4.1)$$

Generally, if

$$\mathbf{c} = \mathbf{A} \cdot \mathbf{b} \quad c_i = A_{ij}b_j \quad (1.4.2)$$

$$\mathbf{c}' = \mathbf{b} \cdot \mathbf{A} \quad c'_j = A_{ij}b_i \quad (1.4.3)$$

$\mathbf{c} \neq \mathbf{c}'$, however for vectors,

$$\mathbf{a} \cdot \mathbf{b} = \mathbf{b} \cdot \mathbf{a} \quad (1.4.4)$$

Similar to the operation known as contraction which we will now discuss.

Contraction

Tensor invariants (for A_{ij})

$$\sum A_{ii} = A_{11} + A_{22} + A_{33} = \text{Tr}(\mathbf{A}) \quad (1.4.5)$$

This is the *trace* of the (formerly $\text{Sp}(\mathbf{A})$ for “Spoor” in German) tensor. Another invariant is the determinant ($\text{set}(\mathbf{A})$)

$$\frac{1}{2} [(\text{Tr } \mathbf{A})^2 - \text{Tr}(\mathbf{A} \mathbf{A})] = A_{11}A_{22} + A_{22}A_{33} + A_{11}A_{33} - A_{12}^2 - A_{23}^2 - A_{13}^2 \quad (1.4.6)$$

Tensor Product

$$\mathbf{A} \otimes \mathbf{B} = \mathbf{C} \quad (1.4.7)$$

$$C_{ijkm} = A_{ij}B_{km} \quad (1.4.8)$$

Double Dot:

$$\mathbf{A} : \mathbf{B} = \sum_i \sum_j A_{ij}B_{ji} \quad (1.4.9)$$

$$= A_{ij}B_{ji} \quad (1.4.10)$$

Levi–Civita introduced the quantity, ε ,

$$\varepsilon_{ijk} = \begin{cases} 0 & \text{if } i = j, j = k, \text{ or } i = k; \\ 1 & \text{if even permutation;} \\ -1 & \text{if odd permutation.} \end{cases} \quad (1.4.11)$$

e.g. $\varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = 1$ and $\varepsilon_{132} = \varepsilon_{213} = \varepsilon_{321} = -1$

This becomes useful for

$$(\mathbf{a} \times \mathbf{b})_k = \varepsilon_{ijk}a_ib_j = \varepsilon_{kij}a_ib_j \quad (1.4.12)$$

If we move from different coordinate systems where the chirality of the axes are changed, this becomes important.

Covariant and Contravariant tensors

These are the same in Cartesian coordinates, but can be different for other curvilinear coordinates.

$$d\mathbf{r} \rightarrow dx_i \quad (i = 1, 2, 3, \dots) \quad (1.4.13)$$

$$d\mathbf{r} \rightarrow dx_i \quad (i = 1, 2, 3, \dots) \quad (1.4.14)$$

Re-written as sums,

$$dx'_i = \sum_j \frac{\partial x'_i}{\partial x_j} dx_j \quad (1.4.15)$$

Comparing with the law of transformation of a vector,

$$a'_i = \sum_j l_{ij} a_j \quad (1.4.16)$$

we observe some important similarity.

Now we see the *contravariant* vector,

$$a'^i = \sum_j \frac{\partial x'_i}{\partial x_j} a^j \quad (1.4.17)$$

Now the gradient,

$$\nabla\phi = \frac{\partial\phi}{\partial x_1} \hat{\mathbf{e}}_1 + \frac{\partial\phi}{\partial x_2} \hat{\mathbf{e}}_2 + \frac{\partial\phi}{\partial x_3} \hat{\mathbf{e}}_3 \quad (1.4.18)$$

So for a different coordinate system the *covariant* is

$$\frac{\partial\phi}{\partial x'^i} = \sum_j \frac{\partial\phi}{\partial x^j} \frac{\partial x^j}{\partial x'^i} \quad (1.4.19)$$

in other words,

$$b'_i = \sum_j \frac{\partial x^j}{\partial x'^i} b_j \quad (1.4.20)$$

In cartesian coordinates we know these are the same because,

$$\frac{\partial x^j}{\partial x'^i} = \frac{\partial x'^i}{\partial x^j} \quad (1.4.21)$$

however we may now do curvilinear coordinates.

UNIT 2

Chapter 8—Curvilinear Coordinates

Useful books on this topic:

- Moon & Spencer, *Field Theory Handbook*, John Zubal (2003)
- Korn & Korn, *Mathematical Handbook*, McGraw–Hill (1968) or Dover (2000)
- Aris, *Vectors, Tensors, and Basic Equations of Fluid Mechanics*, Dover (1990)
- Morse & Feschback, *Methods of Theoretical Physics*, Feschback Publishing (1998)

2.1 Lecture 4 (cont.)

Overview

Polar 2D

Polar coordinates are defined by,

$$x = r \cos(\theta), \quad (2.1.1)$$

$$y = r \sin(\theta). \quad (2.1.2)$$

Observe that

$$r^2 = x^2 + y^2, \quad (2.1.3)$$

and

$$\frac{y}{x} = \tan(\theta). \quad (2.1.4)$$

For the velocity, we will transform the coordinates,

$$\mathbf{v}(t) = \frac{d\mathbf{r}}{dt} = \frac{dx}{dt} \hat{\mathbf{i}} + \frac{dy}{dt} \hat{\mathbf{j}} \quad (2.1.5)$$

$$\frac{d\mathbf{r}}{dt} = \frac{dr}{dt} \hat{\mathbf{e}}_r + r \frac{d\hat{\mathbf{e}}_r}{dr} \quad (2.1.6)$$

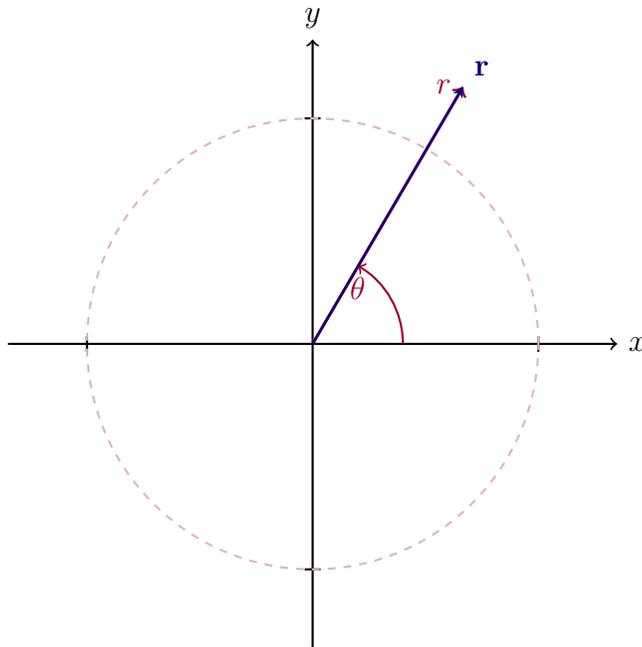


Figure 2.1. Polar Coordinates

$$\mathbf{r} = r\hat{\mathbf{e}}_r \quad (2.1.7)$$

$$\hat{\mathbf{e}}_r = \cos(\theta)\hat{\mathbf{i}} + \sin(\theta)\hat{\mathbf{j}} \quad (2.1.8)$$

Returning to the unit vector in r ,

$$\frac{d\hat{\mathbf{e}}_r}{dr} = \frac{\partial\hat{\mathbf{e}}_r}{\partial\theta} \frac{d\theta}{dr} = \hat{\mathbf{e}}_\theta \quad (2.1.9)$$

$$\frac{\partial\hat{\mathbf{e}}_r}{\partial\theta} = -\sin(\theta)\hat{\mathbf{i}} + \cos(\theta)\hat{\mathbf{j}} \quad (2.1.10)$$

$$\frac{d\hat{\mathbf{e}}_r}{dt} = \frac{\partial\hat{\mathbf{e}}_r}{\partial\theta} \frac{d\theta}{dt} = \hat{\mathbf{e}}_\theta \frac{d\theta}{dt} \quad (2.1.11)$$

For the component velocities,

$$v_r = \frac{dr}{dt} \quad (2.1.12)$$

$$v_\theta = r \frac{d\theta}{dt} \quad (2.1.13)$$

$$\mathbf{v} = v_r\hat{\mathbf{e}}_r + v_\theta\hat{\mathbf{e}}_\theta \quad (2.1.14)$$

The acceleration,

$$\mathbf{a} = \frac{d^2\mathbf{r}}{dt^2} \quad (2.1.15)$$

$$= \frac{d^2r}{dt^2}\hat{\mathbf{e}}_r + \frac{dr}{dt} \frac{d\hat{\mathbf{e}}_r}{dt} + \frac{dr}{dt} \frac{d\theta}{dt} \hat{\mathbf{e}}_\theta + r \frac{d^2\theta}{dt^2} \hat{\mathbf{e}}_\theta + r \frac{d\theta}{dt} \frac{d\hat{\mathbf{e}}_\theta}{dt} \quad (2.1.16)$$

$$\frac{d\hat{\mathbf{e}}_\theta}{d\theta} = \frac{d}{d\theta}(-\sin(\theta)\hat{\mathbf{i}} + \cos(\theta)\hat{\mathbf{j}}) \quad (2.1.17)$$

$$= -\cos(\theta)\hat{\mathbf{i}} - \sin(\theta)\hat{\mathbf{j}} \quad (2.1.18)$$

$$= -(\cos(\theta)\hat{\mathbf{i}} + \sin(\theta)\hat{\mathbf{j}}) \quad (2.1.19)$$

$$= -\hat{\mathbf{e}}_r \quad (2.1.20)$$

Metric Coefficients

$$\frac{\partial \mathbf{r}}{\partial x_i} = \hat{\mathbf{e}}_i \quad (2.1.21)$$

$$\frac{\partial \mathbf{r}}{\partial r} = h_r \hat{\mathbf{e}}_r \quad (2.1.22)$$

$$\frac{\partial \mathbf{r}}{\partial \theta} = h_\theta \hat{\mathbf{e}}_\theta \quad (2.1.23)$$

$$h_r = \left| \frac{\partial \mathbf{r}}{\partial r} \right| \quad (2.1.24)$$

$$h_\theta = \left| \frac{\partial \mathbf{r}}{\partial \theta} \right| \quad (2.1.25)$$

$$h_r = \left[\left(\frac{\partial x}{\partial r} \right)^2 + \left(\frac{\partial y}{\partial r} \right)^2 \right]^{1/2} \quad (2.1.26)$$

$$\begin{aligned} &= \left[\left(\frac{\partial r \cos \theta}{\partial r} \right)^2 + \left(\frac{\partial r \sin \theta}{\partial r} \right)^2 \right]^{1/2} \\ &= [\cos^2(\theta) + \sin^2(\theta)] \\ &= 1 \end{aligned} \quad (2.1.27)$$

$$h_\theta = \left[\left(\frac{\partial x}{\partial \theta} \right)^2 + \left(\frac{\partial y}{\partial \theta} \right)^2 \right]^{1/2} \quad (2.1.28)$$

$$= [r^2 \sin^2(\theta) + r^2 \cos^2(\theta)]^{1/2} \quad (2.1.29)$$

$$= r \quad (2.1.30)$$

So the differential becomes,

$$d\mathbf{r} = \frac{\partial \mathbf{r}}{\partial r} dr + \frac{\partial \mathbf{r}}{\partial \theta} d\theta \quad (2.1.31)$$

$$= h_r dr \hat{\mathbf{e}}_r + h_\theta d\theta \hat{\mathbf{e}}_\theta \quad (2.1.32)$$

$$= dr \hat{\mathbf{e}}_r + r d\theta \hat{\mathbf{e}}_\theta \quad (2.1.33)$$

2.2 Lecture 5: September 5, 2012

Metric coefficients, cont.

Returning to polar coordinates

$$\frac{d\mathbf{r}(t)}{dt} = \frac{dr}{dt}\hat{\mathbf{e}}_r + r\frac{d\hat{\mathbf{e}}_r}{dt} \quad (2.2.1)$$

$$\frac{d\hat{\mathbf{e}}_r}{dt} = \frac{\partial\hat{\mathbf{e}}_r}{\partial\theta}\frac{d\theta}{dt} \quad (2.2.2)$$

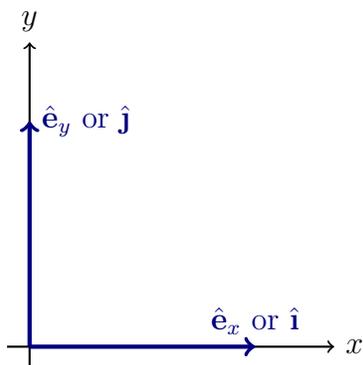


Figure 2.2. Natural unit vectors in Cartesian coordinates

$$\frac{\partial\hat{\mathbf{e}}_y}{\partial y} = 0 \quad (2.2.3)$$

$$\hat{\mathbf{e}}_r = \cos(\theta)\hat{\mathbf{i}} + \sin(\theta)\hat{\mathbf{j}} \quad (2.2.4)$$

$$\hat{\mathbf{e}}_\theta = -\sin(\theta)\hat{\mathbf{i}} + \cos(\theta)\hat{\mathbf{j}} \quad (2.2.5)$$

$$\frac{\partial\hat{\mathbf{e}}_r}{\partial\theta} = -\sin(\theta)\hat{\mathbf{i}} + \cos(\theta)\hat{\mathbf{j}} = \hat{\mathbf{e}}_\theta \quad (2.2.6)$$

This gives that,

$$\hat{\mathbf{e}}_r \cdot \hat{\mathbf{e}}_\theta = 0 \quad (2.2.7)$$

Note that, $\hat{\mathbf{i}} \cdot \hat{\mathbf{i}} = 1$, $\hat{\mathbf{j}} \cdot \hat{\mathbf{j}} = 1$, and $\hat{\mathbf{i}} \cdot \hat{\mathbf{j}} = 0$

Now,

$$\mathbf{b} = b_r\hat{\mathbf{e}}_r + b_\theta\hat{\mathbf{e}}_\theta \quad (2.2.8)$$

$$\mathbf{V} = (v_r, v_\theta) \quad (2.2.9)$$

$$v_r = \frac{dr}{dt}\hat{\mathbf{e}}_r \quad (2.2.10)$$

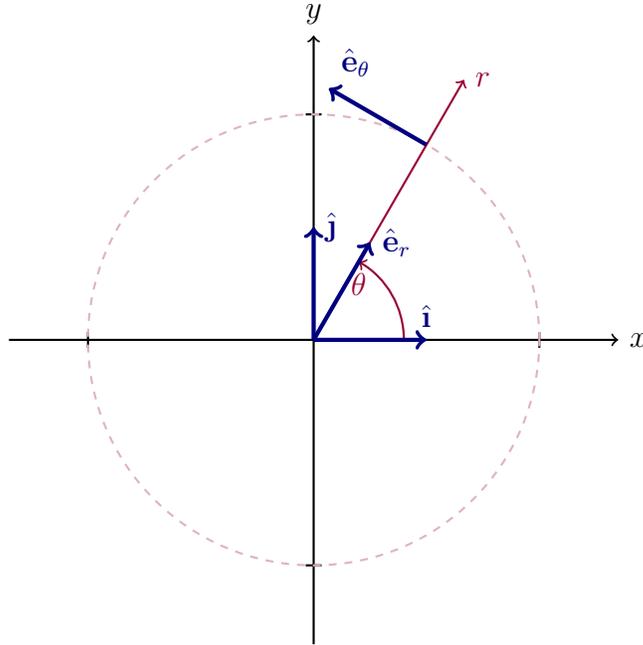


Figure 2.3. Polar coordinates with unit vectors

$$v_\theta = r \frac{d\theta}{dt} \hat{\mathbf{e}}_\theta \quad (2.2.11)$$

$$\mathbf{v} = v_r \hat{\mathbf{e}}_r + v_\theta \hat{\mathbf{e}}_\theta \quad (2.2.12)$$

Acceleration,

$$\mathbf{a} = \frac{d^2 \mathbf{r}}{dt^2} \quad (2.2.13)$$

$$= \frac{d\mathbf{v}}{dt} \quad (2.2.14)$$

$$= \frac{d^2 r}{dt^2} \hat{\mathbf{e}}_r + \frac{dr}{dt} \frac{d\hat{\mathbf{e}}_r}{dt} + \frac{dr}{dt} \frac{d\theta}{dt} \hat{\mathbf{e}}_\theta + r \frac{d^2 \theta}{dt^2} \hat{\mathbf{e}}_\theta + r \frac{d\theta}{dt} \frac{d\hat{\mathbf{e}}_\theta}{dt} \quad (2.2.15)$$

$$\frac{d\hat{\mathbf{e}}_\theta}{dt} = \frac{d\theta}{dt} \frac{d\hat{\mathbf{e}}_\theta}{dt} \quad (2.2.16)$$

$$\frac{d\hat{\mathbf{e}}_\theta}{d\theta} = \frac{d}{d\theta} (-\sin(\theta)\hat{\mathbf{i}} + \cos(\theta)\hat{\mathbf{j}}) = -\cos(\theta)\hat{\mathbf{i}} - \sin(\theta)\hat{\mathbf{j}} = -(\cos(\theta)\hat{\mathbf{i}} + \sin(\theta)\hat{\mathbf{j}}) = -\hat{\mathbf{e}}_r \quad (2.2.17)$$

$$\mathbf{r}(t) = \left[\frac{d^2 r}{dt^2} - r \left(\frac{d\theta}{dt} \right)^2 \right] \hat{\mathbf{e}}_r \quad (2.2.18)$$

Metric coefficients—Generalization

Cartesian, $\frac{\partial \mathbf{r}}{\partial x_i} = \hat{\mathbf{e}}_i$

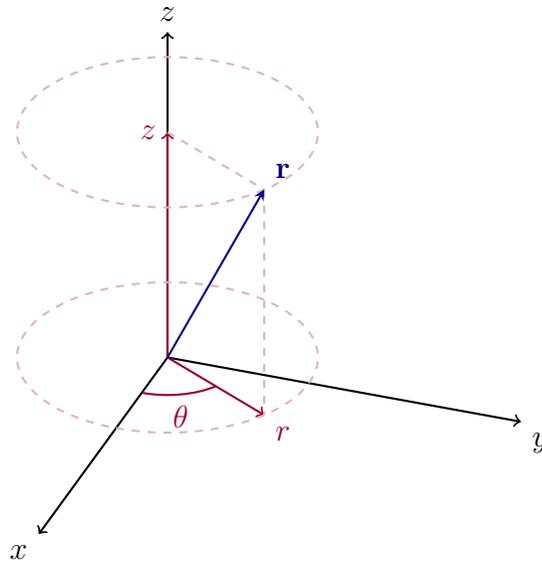


Figure 2.4. Cylindrical Coordinates

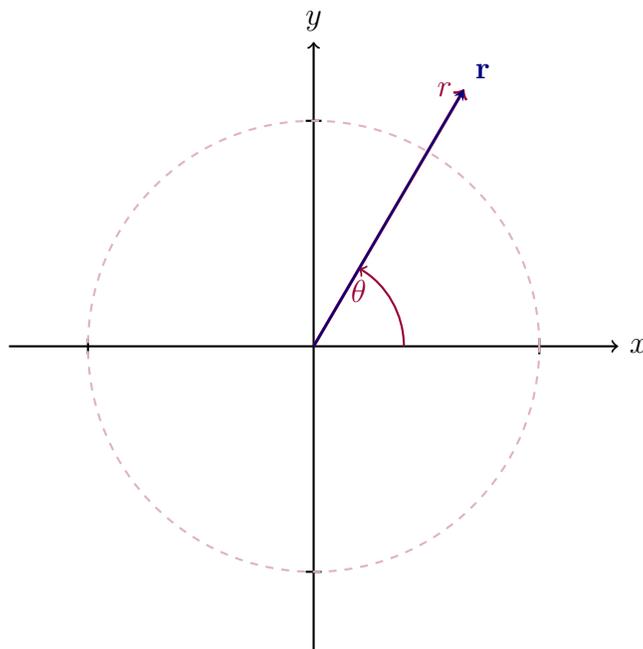


Figure 2.5. Polar Coordinates

$$\mathbf{r} = r \cos(\theta)\hat{\mathbf{i}} + r \sin(\theta)\hat{\mathbf{j}} \quad (2.2.19)$$

$$\frac{d\mathbf{r}}{dr} = \cos(\theta)\hat{\mathbf{i}} + \sin(\theta)\hat{\mathbf{j}} = \hat{\mathbf{e}}_r \quad (2.2.20)$$

$$\frac{d\mathbf{r}}{d\theta} = -r \sin(\theta)\hat{\mathbf{i}} + r \cos(\theta)\hat{\mathbf{j}} = r\hat{\mathbf{e}}_\theta \quad (2.2.21)$$

In cartesian coordinates, the velocity is,

$$\mathbf{v} = x \hat{\mathbf{i}} + y \hat{\mathbf{j}} \quad (2.2.22)$$

$$\frac{d\mathbf{r}}{dx} = \hat{\mathbf{i}}, \quad \frac{d\mathbf{r}}{dy} = \hat{\mathbf{j}} \quad (2.2.23)$$

For the Cartesian case the metric coefficients are always 1.

In Polar Coordinates,

$$h_r \hat{\mathbf{e}}_r = \frac{\partial \mathbf{r}}{\partial r}, \quad h_\theta = \frac{\partial \mathbf{r}}{\partial \theta} \quad (2.2.24)$$

$$h_r = \left[\left(\frac{\partial x}{\partial r} \right)^2 + \left(\frac{\partial y}{\partial r} \right)^2 \right]^{1/2} \quad (2.2.25)$$

$$\begin{aligned} &= \left[\left(\frac{\partial r \cos(\theta)}{\partial r} \right)^2 + \left(\frac{\partial r \sin(\theta)}{\partial r} \right)^2 \right]^{1/2} \\ &= [\cos^2 \theta + \sin^2 \theta]^{1/2} \\ &= 1 \end{aligned} \quad (2.2.26)$$

$$h_\theta = \left[\left(\frac{\partial x}{\partial \theta} \right)^2 + \left(\frac{\partial y}{\partial \theta} \right)^2 \right]^{1/2} \quad (2.2.27)$$

$$\begin{aligned} &= \left[\left(\frac{\partial r \cos(\theta)}{\partial \theta} \right)^2 + \left(\frac{\partial r \sin(\theta)}{\partial \theta} \right)^2 \right]^{1/2} \\ &= [r^2 \sin^2 \theta + r^2 \cos^2 \theta]^{1/2} \\ &= r \end{aligned} \quad (2.2.28)$$

Thus, in polar coordinates, $h_r = 1$ and $h_\theta = r$.

$$ds^2 = d\mathbf{r} \cdot d\mathbf{r} \quad (2.2.29)$$

$$d\mathbf{r} = h_r dr \hat{\mathbf{e}}_r + h_\theta d\theta \hat{\mathbf{e}}_\theta \quad (2.2.30)$$

$$ds^2 = h_r^2 dr^2 + h_\theta^2 d\theta^2 \quad (2.2.31)$$

$$h_r^2 = \left(\frac{\partial x}{\partial r}\right)^2 + \left(\frac{\partial y}{\partial r}\right)^2 \quad (2.2.32)$$

Operators,

$$\nabla^2, \quad \nabla, \quad \nabla \cdot, \quad \nabla \times$$

For $f(\mathbf{r})$,

$$df = \nabla f \cdot d\mathbf{r} = \text{Gradient } f \cdot d\mathbf{r} \quad (2.2.33)$$

The gradient is

$$\nabla f = (\nabla f)_r \hat{\mathbf{e}}_r + (\nabla f)_\theta \hat{\mathbf{e}}_\theta \quad (2.2.34)$$

$$df = [(\nabla f)_r \hat{\mathbf{e}}_r + (\nabla f)_\theta \hat{\mathbf{e}}_\theta] \cdot [\hat{\mathbf{e}}_r dr + r d\theta \hat{\mathbf{e}}_\theta] \quad (2.2.35)$$

Noticing, $\mathbf{r} \cdot \mathbf{r} = 1$ $\hat{\mathbf{e}}_r \cdot \hat{\mathbf{e}}_\theta = 0$.

$$df = (\nabla f)_r dr + (\nabla f)_\theta d\theta \quad (2.2.36)$$

$$= \frac{\partial f}{\partial r} dr + \frac{\partial f}{\partial \theta} d\theta \quad (2.2.37)$$

because $(\nabla f)_r = \frac{\partial f}{\partial r}$, and $r(\nabla f)_\theta = \frac{\partial f}{\partial \theta}$,

$$\nabla f = \frac{\partial f}{\partial r} \hat{\mathbf{e}}_r + \frac{1}{r} \frac{\partial f}{\partial \theta} \hat{\mathbf{e}}_\theta \quad (2.2.38)$$

In general we see,

$$\nabla = \frac{\hat{\mathbf{e}}_1}{h_1} \frac{\partial}{\partial x_1} + \frac{\hat{\mathbf{e}}_2}{h_2} \frac{\partial}{\partial x_2} + \dots \quad (2.2.39)$$

$$\nabla = \hat{\mathbf{i}} \frac{\partial}{\partial x} + \hat{\mathbf{j}} \frac{\partial}{\partial y} + \hat{\mathbf{k}} \frac{\partial}{\partial z} \quad (2.2.40)$$

$$\nabla \mathbf{A} = \hat{\mathbf{i}} \frac{\partial A_x}{\partial x} + \hat{\mathbf{j}} \frac{\partial A_y}{\partial y} + \hat{\mathbf{k}} \frac{\partial A_z}{\partial z} \quad (2.2.41)$$

For the Divergence, $\nabla \cdot \mathbf{u}$,

$$\mathbf{u} = u_r \hat{\mathbf{e}}_r + u_\theta \hat{\mathbf{e}}_\theta \quad (2.2.42)$$

$$\begin{aligned} \nabla \cdot \mathbf{u} &= \left(\frac{\partial}{\partial r} \hat{\mathbf{e}}_r + \frac{\hat{\mathbf{e}}_\theta}{r} \frac{\partial}{\partial \theta} \right) \cdot (u_r \hat{\mathbf{e}}_r + u_\theta \hat{\mathbf{e}}_\theta) \\ &= \hat{\mathbf{e}}_r \hat{\mathbf{e}}_r \frac{\partial u_r}{\partial r} + \hat{\mathbf{e}}_r u_r \frac{\partial \hat{\mathbf{e}}_r}{\partial r} + \hat{\mathbf{e}}_r u_\theta \frac{\partial \hat{\mathbf{e}}_\theta}{\partial r} + \hat{\mathbf{e}}_r \cdot \hat{\mathbf{e}}_\theta \frac{\partial u_\theta}{\partial r} \\ &\quad + \frac{\hat{\mathbf{e}}_\theta \cdot \hat{\mathbf{e}}_r}{r} \frac{\partial u_r}{\partial \theta} + \frac{\hat{\mathbf{e}}_\theta}{r} u_r \frac{\partial \hat{\mathbf{e}}_r}{\partial \theta} + \frac{\hat{\mathbf{e}} \cdot \hat{\mathbf{e}}_\theta}{r} \frac{\partial u_\theta}{\partial \theta} + \frac{\hat{\mathbf{e}}_\theta}{r} u_\theta \frac{\partial \hat{\mathbf{e}}_\theta}{\partial \theta} \end{aligned} \quad (2.2.43)$$

Recall, $\frac{\partial \hat{e}_r}{\partial \theta} = \hat{e}_\theta$ and $\frac{\partial \hat{e}_\theta}{\partial r} = -\hat{e}_r$

$$\nabla \cdot \mathbf{u} = \frac{\partial u_r}{\partial r} + \frac{u_r}{r} + \frac{1}{r} \frac{\partial u_\theta}{\partial \theta} - \frac{u_\theta}{r} \quad (2.2.44)$$

$$\nabla \cdot \mathbf{u} = \frac{\partial u_r}{\partial r} + \frac{u_r}{r} + \frac{1}{r} \frac{\partial u_\theta}{\partial \theta} \quad (2.2.45)$$

$$\nabla f = \frac{\partial f}{\partial r} \hat{e}_r + \frac{\hat{e}_\theta}{r} \frac{\partial f}{\partial \theta} \quad (2.2.46)$$

or

$$\nabla = \frac{\partial}{\partial r} \hat{e}_r + \frac{\hat{e}_\theta}{r} \frac{\partial}{\partial \theta} \quad (2.2.47)$$

The Laplacian is,

$$\nabla^2 = \nabla \cdot \nabla = \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} \quad (2.2.48)$$

and we know that there is no curl operator in only two dimensions.

Cylindrical coordinates

$$x = r \cos(\theta), \quad y = r \sin(\theta), \quad z = z \quad (2.2.49)$$

This gives,

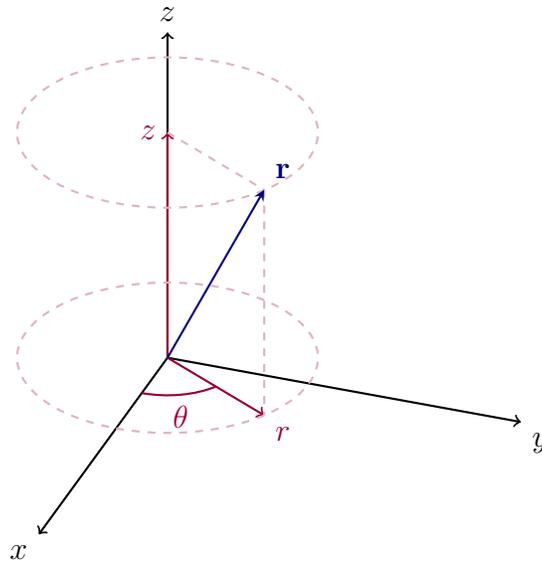


Figure 2.6. Cylindrical Coordinates

$$r^2 = x^2 + y^2, \quad (2.2.50a)$$

$$\theta = \arctan\left(\frac{y}{x}\right), \quad (2.2.50b)$$

$$z = z \quad (2.2.50c)$$

Unit Vectors

$$\hat{\mathbf{e}}_r = \frac{\partial \mathbf{r} / \partial r}{|\partial \mathbf{r} / \partial r|} \quad (2.2.51)$$

$$\hat{\mathbf{e}}_\theta = \frac{\partial \mathbf{r} / \partial \theta}{|\partial \mathbf{r} / \partial \theta|} \quad (2.2.52)$$

$$\hat{\mathbf{e}}_z = \frac{\partial \mathbf{r} / \partial z}{|\partial \mathbf{r} / \partial z|} \quad (2.2.53)$$

$$R^2 = x^2 + y^2 + z^2. \quad (2.2.54)$$

$$\nabla = \frac{\hat{\mathbf{e}}_r}{h_r} \frac{\partial}{\partial r} + \frac{\hat{\mathbf{e}}_\theta}{h_\theta} \frac{\partial}{\partial \theta} + \frac{\hat{\mathbf{e}}_z}{h_z} \frac{\partial}{\partial z} \quad (2.2.55)$$

$$h_r = \left[\left(\frac{\partial x}{\partial r} \right)^2 + \left(\frac{\partial y}{\partial r} \right)^2 + \left(\frac{\partial z}{\partial r} \right)^2 \right]^{1/2} = 1 \quad (2.2.56)$$

$$h_\theta = \left[\left(\frac{\partial x}{\partial \theta} \right)^2 + \left(\frac{\partial y}{\partial \theta} \right)^2 + \left(\frac{\partial z}{\partial \theta} \right)^2 \right]^{1/2} = r \quad (2.2.57)$$

$$h_z = \left[\left(\frac{\partial x}{\partial z} \right)^2 + \left(\frac{\partial y}{\partial z} \right)^2 + \left(\frac{\partial z}{\partial z} \right)^2 \right]^{1/2} = 1 \quad (2.2.58)$$

$$\nabla = \frac{\partial}{\partial r} \hat{\mathbf{e}}_r + \frac{\hat{\mathbf{e}}_\theta}{r} \frac{\partial}{\partial \theta} + \hat{\mathbf{e}}_z \frac{\partial}{\partial z} \quad (2.2.59)$$

$$\hat{\mathbf{e}}_i \times \hat{\mathbf{e}}_i = 0 \quad (2.2.60)$$

$$\nabla \times \mathbf{a} = \begin{vmatrix} \hat{\mathbf{e}}_r & \hat{\mathbf{e}}_\theta & \hat{\mathbf{e}}_z \\ \frac{\partial}{\partial r} & \frac{1}{r} \frac{\partial}{\partial \theta} & \frac{\partial}{\partial z} \\ a_r & a_\theta & a_z \end{vmatrix} \quad (2.2.61)$$

General Approach to Orthogonal Curvilinear Coordinates

$$x = x(u_1, u_2, u_3) \quad (2.2.62a)$$

$$y = y(u_1, u_2, u_3) \quad (2.2.62b)$$

$$z = z(u_1, u_2, u_3) \quad (2.2.62c)$$

An arbitrary position in space can be written by.

$$\mathbf{r} = x(u_1, u_2, u_3) \hat{\mathbf{i}} + y(u_1, u_2, u_3) \hat{\mathbf{j}} + z(u_1, u_2, u_3) \hat{\mathbf{k}} \quad (2.2.63)$$

A general differential volume element is defined by;

$$dV = dx dy dz \left(\hat{\mathbf{i}} \cdot \left(\hat{\mathbf{j}} \times \hat{\mathbf{k}} \right) \right) \quad (2.2.64)$$

Unit Vectors

$$\hat{\mathbf{e}}_i = \frac{\partial \mathbf{r} / \partial u_i}{|\partial \mathbf{r} / \partial u_i|} \quad (2.2.65)$$

$$= \frac{1}{h_i} \frac{\partial \mathbf{r}}{\partial u_i} \quad (2.2.66)$$

$$h_i = \left[\left(\frac{\partial x}{\partial u_i} \right)^2 + \left(\frac{\partial y}{\partial u_i} \right)^2 + \left(\frac{\partial z}{\partial u_i} \right)^2 \right]^{1/2} \quad (2.2.67)$$

$$dx \, dy \, dz = |J| \, du_1 \, du_2 \, du_3 \quad (2.2.68)$$

2.3 Lecture 6: September 10, 2012

Review of Metric Coefficients

Previously we introduced the *metric coefficients*. Their number is dependent on the dimensions of space and their value is dependent on the geometry of the coordinate system. We define a three-dimensional metric coefficient,

$$h_i = \left[\left(\frac{\partial x}{\partial r_i} \right)^2 + \left(\frac{\partial y}{\partial r_i} \right)^2 + \left(\frac{\partial z}{\partial r_i} \right)^2 \right]^{1/2}. \quad (2.3.1)$$

The differential distance is

$$d\mathbf{r} = h_1 du_1 + h_2 du_2 + h_3 du_3, \quad (2.3.2)$$

where u_i are the variables of the new coordinate system.

Generalized Differential Operators

The common differential operators may now be expressed in terms of the general coordinate variables. The gradient,

$$\nabla = \frac{1}{h_1} \frac{\partial}{\partial u_1} \hat{\mathbf{e}}_1 + \frac{1}{h_2} \frac{\partial}{\partial u_2} \hat{\mathbf{e}}_2 + \frac{1}{h_3} \frac{\partial}{\partial u_3} \hat{\mathbf{e}}_3. \quad (2.3.3a)$$

The divergence,

$$\nabla \cdot \mathbf{v} = \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial u_1} (h_2 h_3 v_1) + \frac{\partial}{\partial u_2} (h_1 h_3 v_2) + \frac{\partial}{\partial u_3} (h_1 h_2 v_3) \right]. \quad (2.3.3b)$$

Finally, the Laplace operator,

$$\nabla^2 f = \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial u_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial f}{\partial u_1} \right) + \frac{\partial}{\partial u_2} \left(\frac{h_1 h_3}{h_2} \frac{\partial f}{\partial u_2} \right) + \frac{\partial}{\partial u_3} \left(\frac{h_1 h_2}{h_3} \frac{\partial f}{\partial u_3} \right) \right]. \quad (2.3.3c)$$

The steps required in problems involving change of coordinates are

- Select coordinate system,
- Define the necessary differential operators
- Write the new differential equation
- Solve the equation
- (Revert to original coordinates)

Some examples of unusual, but helpful, coordinate systems include the biconical and the bipolar coordinate systems. More common coordinate systems are Cartesian, cylindrical, and spherical geometries. The definition of spherical coordinates,

$$z = r \cos \theta, \quad (2.3.4a)$$

$$x = r \sin \theta \cos \phi, \quad (2.3.4b)$$

$$y = r \sin \theta \sin \phi. \quad (2.3.4c)$$

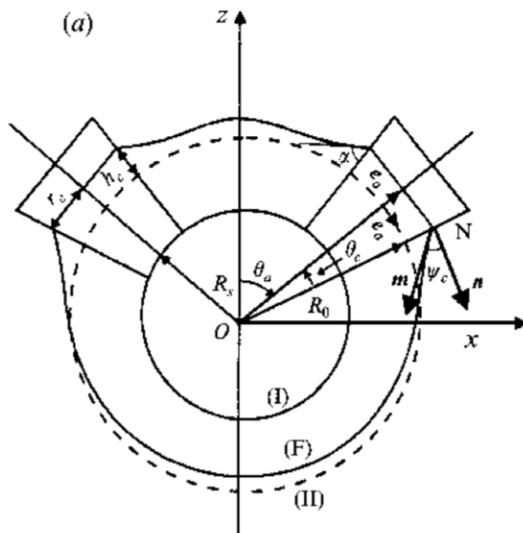


Figure 2.7. Biconical Coordinates

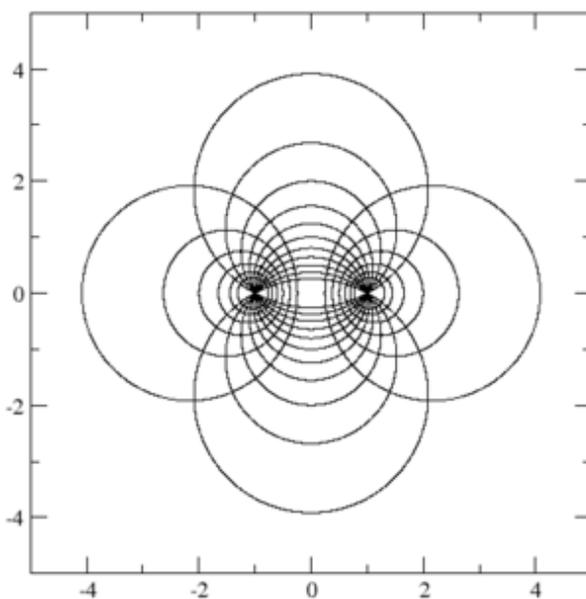


Figure 2.8. Bi-polar Coordinates

Four Dimensional Spherical Coordinates

To understand the stability of orbitals in n -dimensional spaces, we will discuss the four-dimensional spherical coordinate system. We will develop the metric coefficients from the

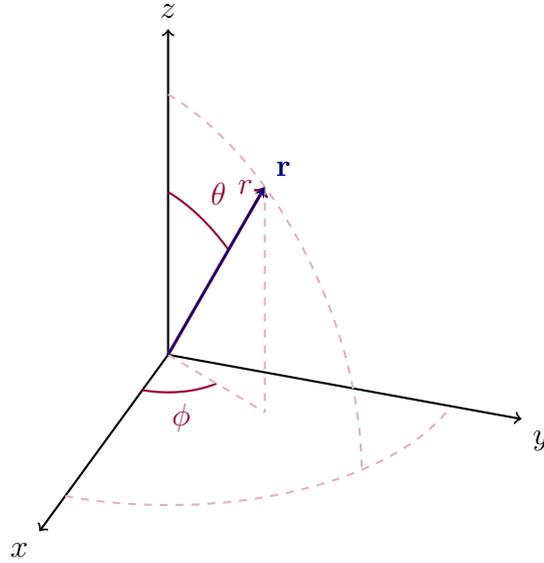


Figure 2.9. Spherical Coordinates

definition of the coordinate variables:

$$x_1 = r \cos \theta, \tag{2.3.5a}$$

$$x_2 = r \sin \theta \cos \phi, \tag{2.3.5b}$$

$$x_3 = r \sin \theta \sin \phi \cos \psi, \tag{2.3.5c}$$

$$x_4 = r \sin \theta \sin \phi \sin \psi. \tag{2.3.5d}$$

Metric Coefficients

Let's find the metric coefficients of our four-dimensional system; h_1, h_2, h_3, h_4 or $h_r, h_\theta, h_\phi, h_\psi$. In the radial direction,

$$h_r = \left[\left(\frac{\partial x_1}{\partial r} \right)^2 + \left(\frac{\partial x_2}{\partial r} \right)^2 + \left(\frac{\partial x_3}{\partial r} \right)^2 + \left(\frac{\partial x_4}{\partial r} \right)^2 \right]^{1/2}, \tag{2.3.6a}$$

$$= [\cos^2 \theta + \sin^2 \theta \cos^2 \phi + \sin^2 \theta \sin^2 \phi \cos^2 \psi + \sin^2 \theta \sin^2 \phi \sin^2 \psi]^{1/2},$$

$$= \boxed{1}. \tag{2.3.6b}$$

In the altitudinal angular direction,

$$h_\theta = \left[\left(\frac{\partial x_1}{\partial \theta} \right)^2 + \left(\frac{\partial x_2}{\partial \theta} \right)^2 + \left(\frac{\partial x_3}{\partial \theta} \right)^2 + \left(\frac{\partial x_4}{\partial \theta} \right)^2 \right]^{1/2}, \tag{2.3.7a}$$

$$= [r^2 \sin^2 \theta + r^2 \cos^2 \theta \cos^2 \phi + r^2 \cos^2 \theta \sin^2 \phi \cos^2 \psi + r^2 \cos^2 \theta \sin^2 \phi \sin^2 \psi]^{1/2},$$

$$= r [\sin^2 \theta + \cos^2 \theta \cos^2 \phi + \cos^2 \theta \sin^2 \phi \cos^2 \psi + \cos^2 \theta \sin^2 \phi \sin^2 \psi]^{1/2},$$

$$= \boxed{r}. \tag{2.3.7b}$$

In the azimuthal angular direction,

$$h_\phi = \left[\left(\frac{\partial x_1}{\partial \phi} \right)^2 + \left(\frac{\partial x_2}{\partial \phi} \right)^2 + \left(\frac{\partial x_3}{\partial \phi} \right)^2 + \left(\frac{\partial x_4}{\partial \phi} \right)^2 \right]^{1/2}, \quad (2.3.8a)$$

$$\begin{aligned} &= [0 + r^2 \sin^2 \theta \sin^2 \phi + r^2 \sin^2 \theta \cos^2 \phi \cos^2 \psi + r^2 \sin^2 \theta \cos^2 \phi \sin^2 \psi]^{1/2}, \\ &= r [\sin^2 \theta \sin^2 \phi + \sin^2 \theta \cos^2 \phi \cos^2 \psi + \sin^2 \theta \cos^2 \phi \sin^2 \psi]^{1/2}, \\ &= \boxed{r \sin \theta}. \end{aligned} \quad (2.3.8b)$$

In the second azimuthal angular direction,

$$h_\psi = \left[\left(\frac{\partial x_1}{\partial \psi} \right)^2 + \left(\frac{\partial x_2}{\partial \psi} \right)^2 + \left(\frac{\partial x_3}{\partial \psi} \right)^2 + \left(\frac{\partial x_4}{\partial \psi} \right)^2 \right]^{1/2}, \quad (2.3.9a)$$

$$\begin{aligned} &= [0 + 0 + r^2 \sin^2 \theta \sin^2 \phi \sin^2 \psi + r^2 \sin^2 \theta \sin^2 \phi \cos^2 \psi]^{1/2}, \\ &= r [\sin^2 \theta \sin^2 \phi \sin^2 \psi + \sin^2 \theta \sin^2 \phi \cos^2 \psi]^{1/2}, \\ &= \boxed{r \sin \theta \sin \phi}. \end{aligned} \quad (2.3.9b)$$

Thus, we have found all the metric coefficients for a 4D spherical coordinate system.

Moving on to other useful operators, the total differential is,

$$d\mathbf{s} = h_r dr \hat{\mathbf{e}}_r + h_\theta d\theta \hat{\mathbf{e}}_\theta + h_\phi d\phi \hat{\mathbf{e}}_\phi + h_\psi d\psi \hat{\mathbf{e}}_\psi, \quad (2.3.10)$$

where

$$\hat{\mathbf{e}}_r = \frac{1}{h_r} \left(\frac{\partial \mathbf{s}}{\partial r} \right) = \frac{\partial \mathbf{s}}{\partial r}, \quad (2.3.11a)$$

$$\hat{\mathbf{e}}_\theta = \frac{1}{h_\theta} \left(\frac{\partial \mathbf{s}}{\partial \theta} \right) = \frac{1}{r} \frac{\partial \mathbf{s}}{\partial \theta}, \quad (2.3.11b)$$

$$\hat{\mathbf{e}}_\phi = \frac{1}{h_\phi} \left(\frac{\partial \mathbf{s}}{\partial \phi} \right) = \frac{1}{r \sin \theta} \frac{\partial \mathbf{s}}{\partial \phi}, \quad (2.3.11c)$$

$$\hat{\mathbf{e}}_\psi = \frac{1}{h_\psi} \left(\frac{\partial \mathbf{s}}{\partial \psi} \right) = \frac{1}{r \sin \theta \sin \phi} \frac{\partial \mathbf{s}}{\partial \psi}. \quad (2.3.11d)$$

Substituting the values of the metric coefficients, the differential length of a line is,

$$d\mathbf{s} = dr \hat{\mathbf{e}}_r + r d\theta \hat{\mathbf{e}}_\theta + r \sin \theta d\phi \hat{\mathbf{e}}_\phi + r \sin \theta \sin \phi d\psi \hat{\mathbf{e}}_\psi. \quad (2.3.12)$$

The total line length is

$$\mathbf{s} = r \cos \theta \hat{\mathbf{i}} + r \sin \theta \cos \phi \hat{\mathbf{j}} + r \sin \theta \sin \phi \cos \psi \hat{\mathbf{k}} + r \sin \theta \sin \phi \sin \psi \hat{\mathbf{l}}. \quad (2.3.13)$$

We may also sketch out all the differentials of the different unit vectors as shown in the table. Note that some of the expressions are rearranged and that two of the items are expressions of two unit vectors (these have been split using the dot product, note $\hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_i = 1$ while $\hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j = 0$).

Table 2.1. Four dimensional spherical coordinates: vector and variable relations

$\frac{\partial \hat{e}_j}{\partial x_i}$	$\hat{e}_j : \hat{e}_r$	\hat{e}_θ	\hat{e}_ϕ	\hat{e}_ψ
$i : r$	$\frac{d\hat{e}_r}{dr} = \mathbf{0}$	$\frac{d\hat{e}_\theta}{dr} = \mathbf{0}$	$\frac{d\hat{e}_\phi}{dr} = \mathbf{0}$	$\frac{d\hat{e}_\psi}{dr} = \mathbf{0}$
θ	$\frac{d\hat{e}_r}{d\theta} = \hat{e}_\theta$	$\frac{d\hat{e}_\theta}{d\theta} = -\hat{e}_r$	$\frac{d\hat{e}_\phi}{d\theta} = \mathbf{0}$	$\frac{d\hat{e}_\psi}{d\theta} = \mathbf{0}$
ϕ	$\frac{d\hat{e}_r}{d\phi} = \hat{e}_\phi \sin \theta$ or: $\frac{1}{\sin \theta} \frac{d\hat{e}_r}{d\phi} = \hat{e}_\phi$	$\frac{d\hat{e}_\theta}{d\phi} = \hat{e}_\phi \cos \theta$ or: $\frac{1}{\cos \theta} \frac{d\hat{e}_\theta}{d\phi} = \hat{e}_\phi$	$\frac{d\hat{e}_\phi}{d\phi} \cdot \hat{e}_r = -\sin \theta$ $\frac{d\hat{e}_\phi}{d\phi} \cdot \hat{e}_\theta = \cos \theta$	$\frac{d\hat{e}_\psi}{d\phi} = \mathbf{0}$
ψ	$\frac{d\hat{e}_r}{d\psi} = \hat{e}_\psi \sin \theta \sin \phi$ or: $\frac{1}{\sin \theta \sin \phi} \frac{d\hat{e}_r}{d\psi} = \hat{e}_\psi$	$\frac{d\hat{e}_\theta}{d\psi} = \hat{e}_\psi \cos \theta \sin \phi$ or: $\frac{1}{\cos \theta \sin \phi} \frac{d\hat{e}_\theta}{d\psi} = \hat{e}_\psi$	$\frac{d\hat{e}_\phi}{d\psi} = \hat{e}_\psi \cos \phi$ or: $\frac{1}{\cos \phi} \frac{d\hat{e}_\phi}{d\psi} = \hat{e}_\psi$	$\frac{d\hat{e}_\psi}{d\psi} \cdot \hat{e}_r = -\sin \theta \sin \phi$ $\frac{d\hat{e}_\psi}{d\psi} \cdot \hat{e}_\phi = -\cos \phi$

Differential Operators

We want to convert the operators from the 4D cartesian space into the 4D spherical space, or

$$f(x_1, x_2, x_3, x_4) \rightarrow f(r, \theta, \phi, \psi). \quad (2.3.14)$$

We begin with the gradient operator;

$$\nabla f = \frac{1}{h_r} \frac{\partial f}{\partial r} \hat{e}_r + \frac{1}{h_\theta} \frac{\partial f}{\partial \theta} \hat{e}_\theta + \frac{1}{h_\phi} \frac{\partial f}{\partial \phi} \hat{e}_\phi + \frac{1}{h_\psi} \frac{\partial f}{\partial \psi} \hat{e}_\psi, \quad (2.3.15)$$

$$= \frac{\partial f}{\partial r} \hat{e}_r + \frac{1}{r} \frac{\partial f}{\partial \theta} \hat{e}_\theta + \frac{1}{r \sin \theta} \frac{\partial f}{\partial \phi} \hat{e}_\phi + \frac{1}{r \sin \theta \sin \phi} \frac{\partial f}{\partial \psi} \hat{e}_\psi. \quad (2.3.16)$$

Thus, the essential gradient is

$$\nabla = \frac{\partial}{\partial r} + \frac{1}{r} \frac{\partial}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} + \frac{1}{r \sin \theta \sin \phi} \frac{\partial}{\partial \psi} \quad (2.3.17)$$

We may define a general vector function A ,

$$\mathbf{A}(r, \theta, \phi, \psi) = A_r \hat{e}_r + A_\theta \hat{e}_\theta + A_\phi \hat{e}_\phi + A_\psi \hat{e}_\psi. \quad (2.3.18)$$

The divergence operator on A becomes,

$$\begin{aligned} \nabla \cdot \mathbf{A} &= \frac{1}{h_r h_\theta h_\phi h_\psi} \left[\frac{\partial}{\partial r} (h_\theta h_\phi h_\psi A_r) + \frac{\partial}{\partial \theta} (h_r h_\phi h_\psi A_\theta) + \frac{\partial}{\partial \phi} (h_r h_\theta h_\psi A_\phi) + \frac{\partial}{\partial \psi} (h_r h_\theta h_\phi A_\psi) \right] \\ &= \frac{1}{r^3 \sin^2 \theta \sin \phi} \left[\frac{\partial}{\partial r} (r^3 \sin^2 \theta \sin \phi A_r) + \frac{\partial}{\partial \theta} (r^2 \sin^2 \theta \sin \phi A_\theta) \right. \\ &\quad \left. + \frac{\partial}{\partial \phi} (r^2 \sin \theta \sin \phi A_\phi) + \frac{\partial}{\partial \psi} (r^2 \sin \theta A_\psi) \right] \\ &= \frac{1}{r^3} \frac{\partial r^3 A_r}{\partial r} + \frac{1}{r \sin^2 \theta} \frac{\partial}{\partial \theta} (\sin^2 \theta A_\theta) + \frac{1}{r \sin \theta \sin \phi} \frac{\partial}{\partial \phi} (\sin \phi A_\phi) + \frac{1}{r \sin \theta \sin \phi} \frac{\partial A_\psi}{\partial \psi} \end{aligned} \quad (2.3.19)$$

The Laplacian operator

$$\begin{aligned} \nabla^2 f &= \nabla \cdot \nabla f, & (2.3.20a) \\ &= \frac{1}{h_r h_\theta h_\phi h_\psi} \left[\frac{\partial}{\partial r} \left(\frac{h_\theta h_\phi h_\psi}{h_r} \frac{\partial f}{\partial r} \right) + \frac{\partial}{\partial \theta} \left(\frac{h_r h_\phi h_\psi}{h_\theta} \frac{\partial f}{\partial \theta} \right) + \frac{\partial}{\partial \phi} \left(\frac{h_r h_\theta h_\psi}{h_\phi} \frac{\partial f}{\partial \phi} \right) + \frac{\partial}{\partial \psi} \left(\frac{h_r h_\theta h_\phi}{h_\psi} \frac{\partial f}{\partial \psi} \right) \right], & (2.3.20b) \\ &= \frac{1}{r^3 \sin^2 \theta \sin \phi} \left[\frac{\partial}{\partial r} \left(r^3 \sin^2 \theta \sin \phi \frac{\partial f}{\partial r} \right) + \frac{\partial}{\partial \theta} \left(r \sin^2 \theta \sin \phi \frac{\partial f}{\partial \theta} \right) + \frac{\partial}{\partial \phi} \left(r \sin \phi \frac{\partial f}{\partial \phi} \right) + \frac{\partial}{\partial \psi} \left(\frac{r}{\sin \phi} \frac{\partial f}{\partial \psi} \right) \right], & (2.3.20c) \\ &= \frac{1}{r^3} \frac{\partial}{\partial r} \left(r^3 \frac{\partial f}{\partial r} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial}{\partial \theta} \left(\sin^2 \theta \frac{\partial f}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta \sin \phi} \frac{\partial}{\partial \phi} \left(\sin \phi \frac{\partial f}{\partial \phi} \right) + \frac{1}{r^2 \sin^2 \theta \sin^2 \phi} \frac{\partial^2 f}{\partial \psi^2}. & (2.3.20d) \end{aligned}$$

Orbitals in a General Dimensional Space

From the laplacian expression, the potential in the radial direction in 4D is

$$\nabla_r f = \frac{1}{r^3} \frac{\partial}{\partial r} \left(r^3 \frac{\partial f}{\partial r} \right). \quad (2.3.21)$$

In 3D

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial f}{\partial r} \right) = 0, \quad (2.3.22)$$

which gives a solution of $f \sim \frac{1}{r}$. In 2D

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial f}{\partial r} \right) = 0. \quad (2.3.23)$$

In 1D

$$\frac{1}{r^0} \frac{\partial}{\partial r} \left(r^0 \frac{\partial f}{\partial r} \right) = 0. \quad (2.3.24)$$

There are no 4D orbits. However, orbits are mathematically possible in 3D and 2D.

Volume of 4D sphere

The differential hyper-surface of a 4D sphere at $r = R$,

$$dV_3 = R^3 \sin^2 \theta \sin \phi d\theta d\phi d\psi. \quad (2.3.25)$$

The differential volume in 4D is

$$dV_4 = r^3 \sin^2 \theta \sin \phi dr d\theta d\phi d\psi. \quad (2.3.26)$$

We note that the *solid angle* in 4D is $\sin^2 \theta \sin \phi \, d\theta \, d\phi \, d\psi$. If we now integrate over the solid angle, we get something different from 4π as in 3D;

$$\int_0^\pi \sin^2 \theta \, d\theta \int_0^\pi \sin \phi \, d\phi \int_0^{2\pi} d\psi = \frac{\pi}{2} \int_0^\pi \sin \phi \, d\phi \int_0^{2\pi} d\psi, \quad (2.3.27a)$$

$$= \pi \int_0^{2\pi} d\psi, \quad (2.3.27b)$$

$$= 2\pi^2. \quad (2.3.27c)$$

Finally, considering the elementary integral, $\int_0^R r^3 \, dr = \frac{1}{4}r^4$, the total volume of a hypersphere is

$$V_4 = \frac{\pi^2 R^4}{2}. \quad (2.3.28)$$

UNIT 3

Chapter 11—Differential Equations

3.1 Lecture 7: September 12, 2012

Suggested reading: pgs. 516–524.

1. ODE and PDE
2. Order 1st, 2nd, . . . , nth
3. Linear and Nonlinear. *e.g.* $y \frac{d^n y}{dx^n}$
4. Homogeneous and Nonhomogeneous
5. Degree—Power of the highest order derivative, *e.g.* $\frac{d^n y}{dx^n} \left(\frac{d^n y}{dx^n} \right)^2$
6. Constant Coefficients and Variable Coefficients

Linear First Order ODEs

The general form of a (non-homogeneous, variable coefficient) linear first order ordinary differential equation.

$$\frac{dy}{dx} + P(x)y = q(x) \tag{3.1.1}$$

Normally we keep an equation in the following form,

$$A(x) \frac{dy}{dx} + B(x)y = C(x) \tag{3.1.2}$$

because we may divide by $A(x)$, so that we get the previous equation where $P(x) = B(x)/A(x)$ and $q(x) = C(x)/A(x)$.

Integrating Factors

$$dy + [P(x)y + q(x)] dx = 0 \quad \times \quad \mu(x) \quad (3.1.3)$$

$$\mu(x) dy + [\mu(x)P(x)y + \mu(x)q(x)] dx = 0 \quad (3.1.4)$$

because we have a total differential,

$$\frac{\partial^2 F}{\partial x \partial y} = \frac{\partial^2 F}{\partial y \partial x} \quad (3.1.5)$$

$$dF = \frac{\partial F}{\partial x} dx + \frac{\partial F}{\partial y} dy = 0 \quad (3.1.6)$$

$$\frac{\partial \mu}{\partial x} = \frac{\partial}{\partial y}(\mu p(x)y - \mu x q(x)) = \mu p(x) \quad (3.1.7)$$

$$\frac{\partial \mu(x)q(x)}{\partial y} \equiv 0 \quad (3.1.8)$$

$$\frac{\partial \mu}{\partial x} = \mu(x)p(x) \quad (3.1.9)$$

$$\mu(x) = e^{\int p(x)dx} = \text{Integrating Factor} \quad (3.1.10)$$

$$\frac{dy}{dx} + P(x)y = q(x) \quad (3.1.11)$$

$$e^{\int p(x)dx} \frac{dy(x)}{dy} + p(x)e^{\int p(x)dx} y(x) = e^{\int p(x)dx} q(x) \quad (3.1.12)$$

$$\frac{d}{dx} \left(y e^{\int p(x)dx} \right) = e^{\int p(x)dx} q(x) \quad (3.1.13)$$

Now,

$$y e^{\int p(x)dx} = \int q(x) e^{\int p(x)dx} q(x) dx + C \quad (3.1.14)$$

$$y = e^{-\int p(x)dx} \int q(x) e^{\int p(x)dx} q(x) dx + C e^{-\int p(x)dx} \quad (3.1.15)$$

where the second term in the solution is the solution to the homogeneous equation.

The solution of an inhomogeneous ODE is unique up to an arbitrary multiple of the solution of the homogeneous ODE.

Example

$$\frac{dy}{dx} + \left(\frac{2x+1}{x}\right)y = e^{-2x} \quad (3.1.16)$$

where $p(x) = \left(\frac{2x+1}{x}\right)$ and $q(x) = e^{-2x}$. So,

$$e^{\int p(x)dx} = e^{\int \frac{2x+1}{x} dx} = e^{2x - \ln|x|} = xe^{2x} \quad (3.1.17)$$

$$\frac{d}{dx}(xe^{2x}y) = x \quad (3.1.18)$$

$$xe^{2x}y = \frac{x^2}{2} + C \quad (3.1.19)$$

$$y = \frac{1}{2}xe^{-2x} + \frac{C}{2}e^{-2x} \quad (3.1.20)$$

Bernoulli Equation

$$\frac{dy}{dx} + P(x)y = q(x)y^n \quad (3.1.21)$$

for $n \neq 0$

$$\frac{dy}{dx} + P(x)y = q(x) \quad (3.1.22)$$

Which we have done above. If $n = 1$,

$$\frac{dy}{dx} + P(x)y = q(x)y \quad (3.1.23)$$

which rearranges to a homogeneous equation. For If $n = 2, 3, \dots$ the solution can be solved by substituting $u = y^{1-n}$, and we get,

$$\frac{du}{dx} + (1-n)P(x)u = (1-n)q(x) \quad (3.1.24)$$

Homogeneous Linear Differential Equations with Constant Coefficients

In general (with non constant coefficients),

$$a_n(x)\frac{d^n y}{dx^n} + a_{n-1}(x)\frac{d^{n-1}y}{dx^{n-1}} + \dots + a_1(x)\frac{dy}{dx} + a_0(x)y(x) = f(x) \quad (3.1.25)$$

with constant coefficients, we simply have,

$$a_n\frac{d^n y}{dx^n} + a_{n-1}\frac{d^{n-1}y}{dx^{n-1}} + \dots + a_1\frac{dy}{dx} + a_0y(x) = b \quad (3.1.26)$$

For a linear system $\mathcal{L}y = 0$

- if $y(x)$ is a solution, so is $Cy(x)$
- if $y_1(x)$ is some solution and $y_2(x)$ is another solution then $c_1y_1(x) + c_2y_2(x)$.
- generally there are n linearly independent solutions to the equation, *e.g.* our solution becomes $y = \sum_{i=1}^n c_i y_i(x)$

We know whether the solutions are linearly independent by the Wronski Determinant, or simply *wronskian*. For $f_i(x), i = 1, 2, \dots, n$,

$$\sum_{i=1}^n c_i y_i(x) = 0 \quad (3.1.27)$$

our linear system is expressed,

$$\begin{pmatrix} f_1 & f_2 & \cdots & f_n \\ f'_1 & f'_2 & \cdots & f'_n \\ \vdots & \vdots & & \vdots \\ f_1^{(n-1)} & f_2^{(n-1)} & \cdots & f_n^{(n-1)} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} = 0 \quad (3.1.28)$$

$$d[w] = 0 \quad (3.1.29)$$

2nd Order Differential Equation

$$a_2 \frac{d^2 y}{dx^2} + a_1 \frac{dy}{dx} + a_0 y(x) = 0 \quad (3.1.30)$$

Form $y = e^{\alpha x}$ and substitute

$$a_2 \alpha^2 e^{\alpha x} + a_1 \alpha e^{\alpha x} + a_0 e^{\alpha x} = 0 \quad (3.1.31)$$

$$a_2 \alpha^2 + a_1 \alpha + a_0 = 0 \quad (3.1.32)$$

$$\alpha_1 = - \left(\frac{a_1 + (a_1^2 - 4a_0 a_2)^{1/2}}{2a_2} \right) \quad (3.1.33)$$

$$\alpha_2 = \frac{a_1 - (a_1^2 - 4a_0 a_2)^{1/2}}{2a_2} \quad (3.1.34)$$

$$y = C_1 e^{\alpha_1 x} + C_2 e^{\alpha_2 x} \quad (3.1.35)$$

Non-homogeneous ODEs

For a linear, nonhomogeneous system,

$$\mathcal{L}y = f(x)$$

Overview

1. Method of undetermined coefficients The solution is then,

$$y = y_c + y_p \quad (3.1.36)$$

This requires guessing the solution form of the particular solution of the right hand side. See textbook for further details.

2. Method of Variation of Parameters

3. Integral Transforms Works best for constant coefficients

4. Eigenfunction expansions

5. Green Functions Good for variable coefficients. The Green functions are well tabulated.

Method of Undetermined Coefficients

First, Solve $Ly = 0$ to get the homogeneous solution

$$y_c = C_1y_1 + C_2y_2 + \cdots + C_ny_n \quad (3.1.37)$$

which is also known as the complimentary solution. Then find the particular solution,

$$y_p \rightarrow \text{particular solution.} \quad (3.1.38)$$

Method of Variation of Parameters

The method of variation of parameters works with variable coefficients, so for a general form second-order ODE, we have,

$$a_2(x)y''(x) + a_1(x)y'(x) + a_0(x)y(x) = f(x). \quad (3.1.39)$$

It also has no limitations on the form of $f(x)$. A minus with the method is that it requires one known particular solution.

$$y(x) = C_1y_1(x) + C_2y_2(x). \quad (3.1.40)$$

$$y(x) = u_1(x)y_1(x) + u_2(x)y_2(x). \quad (3.1.41)$$

3.2 Lecture 8: September 17, 2012

Method of Variation of Parameters

1. Works for non-homogeneous equations
2. Variable Coefficients

$$y''(x) + P(x)y'(x) + Q(x)y = f(x) \quad (3.2.1)$$

For homogeneous systems $f(x) = 0$ and the solution is of the form of,

$$y = C_1y_1(x) + C_2y_2(x) \quad (3.2.2)$$

The Wronskian determinant,

$$W = \begin{vmatrix} y_1 & y_2 \\ y_1' & y_2' \end{vmatrix} \quad (3.2.3)$$

$$W = y_1y_2' - y_1'y_2 \quad (3.2.4)$$

$$\begin{aligned} W' &= \frac{d}{dx}(y_1y_2' - y_1'y_2) \\ &= y_1'y_2' + y_1y_2'' - y_1''y_2 - y_1'y_2' \\ &= y_1y_2'' - y_1''y_2 \end{aligned} \quad (3.2.5)$$

with

$$y''(x) = -P(x)y'(x) - Q(x)y \quad (3.2.6)$$

we get that the Wronskian derivative is,

$$W' = y_1[-P(x)y_2'(x) - Q(x)y_2] - y_2[-P(x)y_1'(x) - Q(x)y_1] \quad (3.2.7)$$

$$\begin{aligned} &= -P(x)y_2'(x)y_1 + P(x)y_1'(x)y_2 \\ &= -P(x)(y_2'(x)y_1 - y_1'(x)y_2) \\ &= -P(x)W \end{aligned} \quad (3.2.8)$$

This first order equation is therefore solved by,

$$W = W_0e^{-\int P(x)dx}. \quad (3.2.9)$$

$$\frac{y_1y_2' - y_1'y_2}{y_1^2} = \frac{W}{y_1^2} = \frac{1}{y_1^2} \quad (3.2.10)$$

for $P(x) = 0$. Also,

$$\left(\frac{y_2}{y_1}\right)' = \frac{W}{y_1^2} = \frac{1}{y_1^2}. \quad (3.2.11)$$

Therefore we find the second solution

$$y_2 = y_1(x) \int \frac{W}{y_1^2(x)} dx \quad (3.2.12)$$

The solution of a homogeneous system is simply

$$y = C_1 y_1(x) + C_2 y_2(x) \quad (3.2.13)$$

However for a non homogeneous system, we need

$$y = u_1(x)y_1(x) + u_2(x)y_2(x) \quad (3.2.14)$$

Plugging this into the general equation, $y''(x) + P(x)y'(x) + Q(x)y = f(x)$, we get

$$u_1(y_1'' + Py_1' + Qy_1) + u_2(y_2'' + Py_2' + Qy_2) + (u_1'y_1' + u_2'y_2') + (u_1'y_1 + u_2'y_2) + P(u_1'y_1 + u_2'y_2) = f(x) \quad (3.2.15)$$

The first two terms are solutions to the homogeneous equations, so they are simply zero.

$$(u_1'y_1' + u_2'y_2') + (u_1'y_1 + u_2'y_2) + P(u_1'y_1 + u_2'y_2) = f(x) \quad (3.2.16)$$

We must obtain u_1 and u_2 . This gives rise to two requirements,

1. $u_1 y_1 + u_2 y_2$ is a solution
2. $u_1' y_1 + u_2' y_2 = 0$

This gives system along with,

$$u_1' y_1' + u_2' y_2' = f(x) \quad (3.2.17)$$

$$u_1' y_1 + u_2' y_2 = 0 \quad (3.2.18)$$

We know then,

$$u_1' = \frac{-y_2 f(x)}{W} \quad (3.2.19)$$

$$u_1 = - \int \frac{-y_2 f(x)}{W} dx + C_1 \quad (3.2.20)$$

$$u_2' = \frac{y_1 f(x)}{W} \quad (3.2.21)$$

$$u_2 = \int \frac{-y_1 f(x)}{W} dx + C_2 \quad (3.2.22)$$

Where the C 's are found from the boundary conditions

To Solve—In Review

1. Determine particular solution
2. Find $|W|$ where, $W = e^{\int P(x)dx}$, note that if $P(x) = 0$, $W = 1$
3. Find the second solution $y_2 = y_1 \int \frac{W}{y_1^2} dx$
4. Write the solution in the form $u = u_1(x)y_1(x) + u_2(x)y_2(x)$
5. Find u_1 and u_2 .

$$u_1 = - \int \frac{-y_2 f(x)}{W} dx + C_1$$

$$u_2 = \int \frac{-y_1 f(x)}{W} dx + C_2$$

6. Find C_1 and C_2 from the boundary conditions corresponding to the problem.

Example: Capillary electrostatics

Electrostatic problem within a small capillary .

$$\frac{d^2 y}{dx^2} - \cosh(\Psi_0)y = \frac{d\Psi_0}{dx} \quad (3.2.23)$$

where

$$\Psi_0 = 2 \ln \left[\frac{1 + te^{-x}}{1 - te^{-x}} \right]. \quad (3.2.24)$$

As general background,

$$\nabla^2 \Psi = \kappa^2 \sinh(\Psi) \quad (3.2.25)$$

In cylindrical coordinates,

$$\frac{d^2 \Psi}{dr^2} + \frac{1}{r} \frac{d\Psi}{dr} = \kappa^2 \sinh(\Psi)$$

In Cartesian coordinates,

$$\frac{d^2 \Psi}{dx^2} = \kappa^2 \sinh(\Psi)$$

We know that there is a particular solution,

$$y_1 = \frac{4te^x}{t^2 - e^{2x}} = f(x) \quad (3.2.26)$$

so we may use the Wronskian to find the second solution.

$$y_1 y_2' - y_1' y_2 = 1 = W \quad (3.2.27)$$

$$y_2 = \frac{4te^x}{t^2 - e^{2x}} \int \left(\frac{t^2 - e^{2x}}{4te^x} \right)^2 dx \quad (3.2.28)$$

$$= \frac{e^{3x} - e^{-x}t^4 - 4e^xt^2x}{8(t^3 - e^{2xt})} \quad (3.2.29)$$

This gives our solution to the homogeneous equation.

For the other solutions $C_1y_1 + C_2y_2$, we set

$$u_1(x)y_1(x) + u_2(x)y_2(x) \quad (3.2.30)$$

$$u_1 = - \int \frac{-y_2 f(x)}{W} dx + C_1 \quad (3.2.31)$$

$$= \frac{1}{2} \left(x + \frac{2t^2x}{e^{2x} - t^2} \right) + C_1 \quad (3.2.32)$$

$$u_2 = \int \frac{-y_1 f(x)}{W} dx + C_2 \quad (3.2.33)$$

$$= \int \left(\frac{d\Psi_0}{dx} \right)^2 dx + C_1 \quad (3.2.34)$$

$$= \frac{8t^2}{e^{2x} - t^2} + C_2 \quad (3.2.35)$$

Now we can use the boundary conditions, where $y(x=0) = 0$ and $y(x \rightarrow \infty) = 0$ or we get two equations for the two unknowns, C_1 and C_2 .

$$u_1(0)y_1(0) + u_2(0)y_2(0) = 0 \quad (3.2.36)$$

$$u_1(\infty)y_1(\infty) + u_2(\infty)y_2(\infty) = 0 \quad (3.2.37)$$

Method of Green's Functions

Example: electrostatic problems

Laplace equation works within a vacuum,

$$\nabla^2 \Psi = 0 \quad (3.2.38)$$

For charged systems we need the Poisson equation, which includes the charge density as a continuous function ($\epsilon_r \sim 80$ for water).

$$\nabla^2 \Psi = -\frac{\rho}{\epsilon_0} \quad (3.2.39)$$

$$\Psi = \frac{1}{4\pi\epsilon_0} \sum_i \frac{q_i}{r_i} \quad (3.2.40)$$

The force is given by,

$$\mathbf{F} = \frac{q_1 q_2}{4\pi\epsilon_0 r^2} \mathbf{n} \quad (3.2.41)$$

We may now approximate the sum by an integral to give the continuum approximation.

$$\Psi(\mathbf{r}_1) = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} dV \quad (3.2.42)$$

Where $dV_2 = d\mathbf{r}_2$. Now, $\rho(\mathbf{r}) \rightarrow \delta(\mathbf{r}) \rightarrow$ for a single point charge.

The physical equation of true distribution is

$$\nabla^2 \Psi = -\frac{\rho}{\epsilon_0} \quad (3.2.43)$$

but,

$$\nabla^2 G = -\delta(\mathbf{r}_1 - \mathbf{r}_2) \quad (3.2.44)$$

where G is the Green's function.

Green's Theorem,

$$\int (\Psi \nabla^2 G - G \nabla^2 \Psi) dV_2 = \int (\Psi \nabla G - G \nabla \Psi) \cdot d\mathbf{S} \quad (3.2.45)$$

The right hand side is simply 0 for surrounding boundaries/surfaces that are very far from r_2 and the integrand that drops of proportionally to $1/r^2$ or faster. This simplifies us to,

$$\begin{aligned} \int \Psi \nabla^2 G dV_1 &= \int G \nabla^2 \Psi dV_2 \\ \int \Psi(\mathbf{r}_2) \delta(r_1 - r_2) &= \int G(\mathbf{r}_1, \mathbf{r}_2) \rho(r_2) dV_2 \end{aligned}$$

This gives,

$$\Psi(\mathbf{r}) = \int G(\mathbf{r}_1, \mathbf{r}_2) \rho(r_2) dV_2 \quad (3.2.46)$$

3.3 Lecture 9: September 19, 2012

Resources for Greens functions,

- Polyanin, *Handbook of Linear Partial Differential Equations*, Chapman-Hall (2001)
- Korn and Korn, *Mathematical Handbook*, Dover (2000)

Greens Functions, cont.

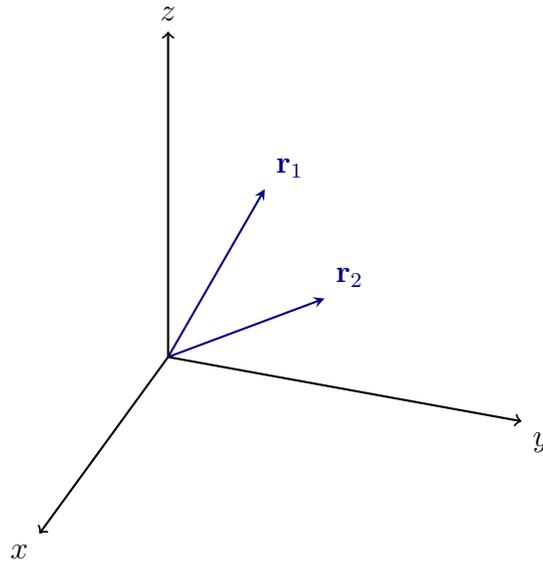


Figure 3.1. Variation of interaction of two particles in three dimensions

$$\Psi(\mathbf{r}_1) = \frac{1}{\epsilon_0} \int G(\mathbf{r}_1, \mathbf{r}_2) \rho(\mathbf{r}_2) dV_2 \quad (3.3.1)$$

where, $dV_2 = d\mathbf{r}_2$,

$$\int \nabla^2 \left(\frac{1}{r} \right) dV = \int \nabla \left(\frac{\mathbf{n}}{r^2} \right) dV = \begin{cases} -4\pi \\ 0 \end{cases} \quad (3.3.2)$$

with $\nabla^2 \left(\frac{1}{r} \right) = \nabla \left(\frac{\mathbf{n}}{r^2} \right)$.

$$\frac{1}{4\pi} \int \nabla^2 \left(\frac{1}{r} \right) dV = - \int \delta(\mathbf{r}) dV \quad (3.3.3)$$

$$\nabla^2 \left(\frac{1}{r} \right) = -4\pi \delta(\mathbf{r}) \quad (3.3.4)$$

In this case now the Greens function is simply $\frac{1}{4\pi r}$.

For,

$$\nabla^2 \Psi = -\frac{\rho}{\epsilon_0} \quad (3.3.5)$$

gives a Greens function of

$$G(\mathbf{r}_1, \mathbf{r}_2) = \frac{-1}{4\pi|\mathbf{r}_1 - \mathbf{r}_2|} \tag{3.3.6}$$

$$\mathcal{L}y(\mathbf{r}_1) = -f(\mathbf{r}_1) \tag{3.3.7}$$

$$\mathcal{L}G(\mathbf{r}_1, \mathbf{r}_2) = -\delta(\mathbf{r}_1 - \mathbf{r}_2) \tag{3.3.8}$$

$$y(\mathbf{r}_1) = \int G(\mathbf{r}_1, \mathbf{r}_2)f(\mathbf{r}_2) d\mathbf{r}_2 \tag{3.3.9}$$

$$\int \nabla^2 G dV_2 = \int \nabla G \cdot d\mathbf{s}_2 = -1 \tag{3.3.10}$$

in two dimensions $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$

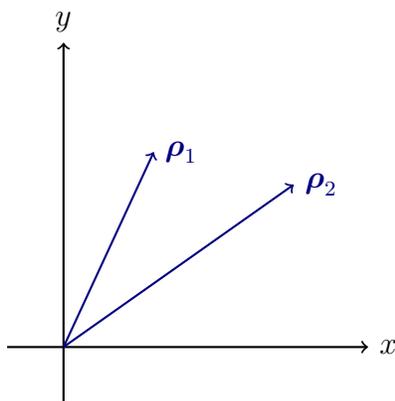


Figure 3.2. Two dimensional case

$$\frac{\partial G(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2)}{\partial \rho_{12}} = \frac{-1}{2\pi} \frac{1}{|\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2|} \tag{3.3.11}$$

In 3D

$$\frac{\partial G(\mathbf{r}_1, \mathbf{r}_2)}{\partial r_{12}} = \frac{-1}{4\pi} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|^2} \tag{3.3.12}$$

For the solutions, 3D $\sim \frac{1}{r}$ and 2D $\sim \ln(\rho)$. In 2D,

$$G(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2) = \frac{-1}{2\pi} \ln(\rho_{12}) \tag{3.3.13}$$

$$\nabla^2 F = -f(\rho) \tag{3.3.14}$$

$$F(\rho_1) = \frac{1}{2\pi} \int \ln |\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2| f(\rho_2) d\boldsymbol{\rho}_2 \tag{3.3.15}$$

in 1D there is no green function for the laplacian, $\frac{d^2 F}{dx^2} = -f(x)$.

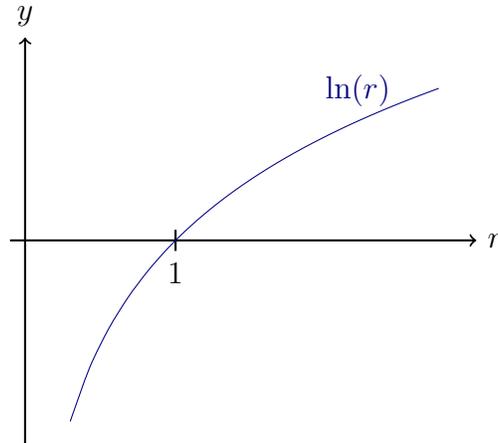


Figure 3.3. Behavior of 3D solution nearing the singularity at zero

Example: Schrodinger's Equation and Quantum Mechanics

One of the most important equations of all time and a foundational one to quantum mechanics is the *Schrodinger equation*,

$$-\frac{\hbar}{2m}\nabla^2\Psi(\mathbf{r}) + k^2\Psi(\mathbf{r}) = -f(\mathbf{r}) \quad (3.3.16)$$

The simplified form is known as the *Helmholtz equation*. Note

$$k^2 = \frac{2mE}{\hbar^2} \quad (3.3.17)$$

$$f(\mathbf{r}) = -\frac{2m}{\hbar^2}V(r)\Psi(r) \quad (3.3.18)$$

The Born approximation,

$$\Psi(\mathbf{r}_1) = -\int \frac{2m}{\hbar^2}V(\mathbf{r}_2)\Psi(\mathbf{r}_2)G(\mathbf{r}_1, \mathbf{r}_2)dV_2 \quad (3.3.19)$$

$$\Psi \sim e^{ik_0\mathbf{r}} \quad (3.3.20)$$

From the literature, we know that the the Greens function of,

$$\nabla^2G + k^2G = -\delta(\mathbf{r}_1 - \mathbf{r}_2) \quad (3.3.21)$$

is

$$G(\mathbf{r}_1, \mathbf{r}_2) = \frac{e^{i\mathbf{k}\cdot|\mathbf{r}_1-\mathbf{r}_2|}}{4\pi|\mathbf{r}_1 - \mathbf{r}_2|}. \quad (3.3.22)$$

Substituting,

$$\Psi(\mathbf{r}_1) = -\int \frac{2m}{\hbar^2}V(\mathbf{r}_2)\frac{e^{i\mathbf{k}\cdot|\mathbf{r}_1-\mathbf{r}_2|}}{4\pi|\mathbf{r}_1 - \mathbf{r}_2|}dV_2 \quad (3.3.23)$$

note that the integral equation is much more stable numerically than the differential equation.

Brownian Motion and Stochastic Equations

Einstien's Method

$$\langle x^2 \rangle = 2Dt \tag{3.3.24}$$

$$\langle x \rangle = 0 \tag{3.3.25}$$

$$\langle mv^2 \rangle = \kappa T \tag{3.3.26}$$

Langevin's Method

Langevin accelerated the development of *stochastic differential equations*. From Newton we know,

$$m\mathbf{a} = \sum_i \mathbf{F}_i \tag{3.3.27}$$

$$m \frac{d^2x}{dt^2} = -\beta \frac{dv}{dt} + fx \tag{3.3.28}$$

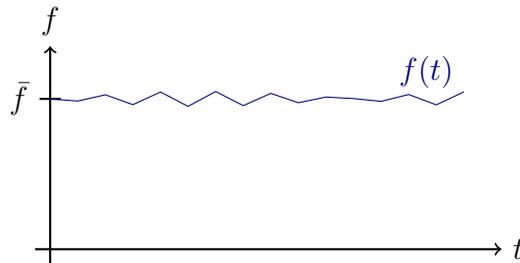


Figure 3.4. Brownian motion of a particle force over time

$$\langle x \rangle \rightarrow \langle x^2 \rangle \tag{3.3.29}$$

$$\frac{1}{2} \frac{d^2x^2}{dt^2} = \frac{d}{dt} \left(2x \frac{dx}{dt} \right) = 2x \frac{d^2x}{dt^2} + \left(\frac{dx}{dt} \right)^2 \tag{3.3.30}$$

$$x \frac{d^2x}{dt^2} = \frac{1}{2} \frac{d^2x^2}{dt^2} - \left(\frac{dx}{dt} \right)^2 \tag{3.3.31}$$

$$mx \frac{d^2x}{dt^2} = -\beta x \frac{dx}{dt} + fx \tag{3.3.32}$$

$$\frac{m}{2} \frac{d^2x^2}{dt^2} - m \left(\frac{dx}{dt} \right)^2 = -\frac{\beta}{2} \frac{dx^2}{dt} + fx \tag{3.3.33}$$

$$\frac{m}{2} \frac{d^2 x^2}{dt^2} - mv^2 = -\frac{\beta}{2} \frac{dx^2}{dt} + fx \quad (3.3.34)$$

with, $\langle mv^2 \rangle = kT$,

$$\frac{m}{2} \frac{d^2 \langle x^2 \rangle}{dt^2} - kT = -\frac{\beta}{2} \frac{d \langle x^2 \rangle}{dt} + fx \quad (3.3.35)$$

Introducing $y = \frac{d \langle x^2 \rangle}{dt}$, we have the first-order ODE,

$$\frac{dy}{dt} = -\frac{\beta}{m} \left(y - \frac{2kt}{\beta} \right) \quad (3.3.36)$$

$$\frac{d}{dt} \left(y - \frac{2kt}{\beta} \right) = -\frac{\beta}{m} \left(y - \frac{2kt}{\beta} \right) \quad (3.3.37)$$

$$\int \frac{d \left(y - \frac{2kt}{\beta} \right)}{\left(y - \frac{2kt}{\beta} \right)} = -\frac{\beta}{m} \int dt \quad (3.3.38)$$

gives the solution,

$$y - \frac{2kt}{\beta} = C e^{-\frac{\beta}{m}t} \quad (3.3.39)$$

Langevin found that the timescale is $\tau_{\text{ch}} \sim 1 \times 10^{-8}$ s, thus the exponential is mostly

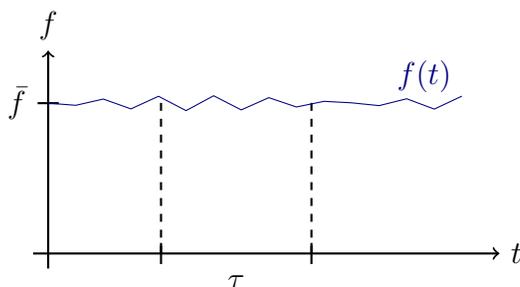


Figure 3.5. Range of time over which observation is taking place

negligible.

$$\frac{d \langle x^2 \rangle}{dt} = \frac{2kT}{\beta} \quad (3.3.40)$$

$$\langle x^2 \rangle = \frac{2kT}{\beta} t \quad (3.3.41)$$

$$\langle x^2 \rangle = 2Dt \quad (3.3.42)$$

where $D = \frac{kT}{6\pi\eta R}$

Evolution of the particle velocity analyzed by Ornstein and Uhlenbeck.

$$m \frac{dv}{dt} = -\beta v + f(t) \quad (3.3.43)$$

$$\frac{dv}{dt} = -\gamma v + R(t) \quad (3.3.44)$$

where $\gamma = \beta/m$, and $R(t) = f(t)/m$. Making an assumption that $\langle R(t) \rangle = 0$, and $\langle R(t_1)R(t_2) \rangle = 2\mathcal{D} \delta(t_1 - t_2)$. One may also use

$$\langle R_1(t_1)R_2(t_2) \rangle = 2\mathcal{D}\delta_{ij} \delta(t_1 - t_2)$$

$$v = v_0 e^{-\gamma(t-t_0)} + e^{-\gamma(t-t_0)} \int_{t_0}^t e^{\gamma(t'-t_0)} R(t') dt' \quad (3.3.45)$$

$$\langle v \rangle = v_0 e^{-\gamma(t-t_0)} \quad (3.3.46)$$

shifting our integral notation, *e.g.* $\int f(t) dt = \int dt f(t)$

$$\langle v(t_0)v(t) \rangle = v_0^2 e^{-2\gamma(t-t_0)} + e^{-2\gamma(t-t_0)} \int_{t_0}^t dt' \int_{t_0}^t dt'' e^{2\gamma(t-t_0)} \langle R(t')R(t'') \rangle \quad (3.3.47)$$

where $\langle R(t')R(t'') \rangle = 2\mathcal{D} \delta(t' - t'')$.

$$\int_{t_0}^t dt' \int_{t_0}^t dt'' e^{2\gamma(t-t_0)} 2\mathcal{D} \delta(t' - t'') = 2\mathcal{D} \int_{t_0}^t dt' e^{2\gamma(t'-t_0)} \quad (3.3.48)$$

3.4 Lecture 10: September 24, 2012

Example: Langevin Equation, cont.

Returning to the Langevin Equation,

$$\frac{dv}{dt} = -\gamma v + R(t) \quad (3.4.1)$$

$R(t) \rightarrow$ Random term. 1. $\langle R(t) \rangle = 0$ 2. $\langle R(t_1)R(t_1) \rangle = 2\mathcal{D} \delta(t_1 - t_2)$

$$v(t) = v_0 e^{-\gamma(t-t_0)} + e^{-\gamma(t-t_0)} \int_{t_0}^t e^{\gamma(t'-t_0)} R(t') dt' \quad (3.4.2)$$

$$\frac{mv_0^2}{2} = \frac{kT}{2} \rightarrow v_0^2 = \frac{kT}{m}$$

$$\langle v(t_0)v(t) \rangle = \langle v(t)^2 \rangle \quad (3.4.3)$$

$$= v_0^2 e^{-2\gamma(t-t_0)} + e^{2\gamma(t-t_0)} \int_{t_0}^t dt' \int_{t_0}^t dt'' e^{\gamma(t-t_0)-\gamma t_0} \langle R(t')R(t'') \rangle_{v_0} \quad (3.4.4)$$

$$\int_{t_0}^t dt' \int_{t_0}^t dt'' e^{2\gamma(t-t_0)} 2\mathcal{D} \delta(t' - t'') = 2\mathcal{D} \int_{t_0}^t dt' e^{2\gamma(t'-t_0)} \quad (3.4.5)$$

it is a rule that,

$$\int f(t' + t'') \delta(t'') dt'' = f(2t') \quad (3.4.6)$$

$$\frac{2\mathcal{D}}{\gamma} e^{-2\gamma(t-t_0)} (e^{2\gamma(t-t_0)} - 1) = \frac{\mathcal{D}}{\gamma} (1 - e^{-2\gamma(t-t_0)}) \quad (3.4.7)$$

$$\langle v^2 \rangle = v_0^2 e^{-2\gamma(t-t_0)} + \frac{\mathcal{D}}{\gamma} (1 - e^{-2\gamma(t-t_0)}) \quad (3.4.8)$$

where second term is the Green's function.

To reach equilibrium, we take $t_0 \ll t$,

$$\langle v^2 \rangle = \frac{\mathcal{D}}{\gamma} \quad (3.4.9)$$

This provides us with an understanding of \mathcal{D} ;

$$\frac{kT}{m} = \frac{\mathcal{D}}{\gamma} \quad (3.4.10)$$

for velocity,

$$\mathcal{D} = \frac{kT\gamma}{m} \quad (3.4.11)$$

for configurational,

$$\mathcal{D} = \frac{kT}{\beta} \quad (3.4.12)$$

UNIT 4

Chapter 12—Series Solutions of Differential Equations

4.1 Lecture 10, cont.

Series solutions

Looking at a second order ODE,

$$a_2(x) \frac{d^2y}{dx^2} + a_1(x) \frac{dy}{dx} + a_3(x)y(x) = 0 \quad (4.1.1)$$

$$y(x) = \sum_{n=0}^{\infty} C_n x^n \quad (4.1.2)$$

which is a *power series method*.

Power Series

Simplification of the Helmholtz equation ($y''(x) + \kappa^2 y(x) = 0$)

$$y''(x) + y(x) = 0 \quad (4.1.3)$$

Differentiating, our solution must be,

$$\sum_{n=0}^{\infty} n(n-1)C_n x^{n-2} + \sum_{n=0}^{\infty} C_n x^n = 0 \quad (4.1.4)$$

$n = 0$ or $n = 1$.

$$\sum_{n=2}^{\infty} n(n-1)C_n x^{n-2} \quad (4.1.5)$$

for $n = 2$, we get, $2C_2$. With $n = 3$ we see $6a_3x$, $n = 4 \rightarrow 12C_4x^2$, $n = 5 \rightarrow 20C_5x^3$, etc. We can replace for $n \rightarrow n + 2$ in our equation.

$$\sum_{n=0}^{\infty} [(n+2)(n+1)C_{n+2} + C_n] x^n = 0 \quad (4.1.6)$$

This quickly shows a recursive relation where,

$$C_{n+2} = -\frac{C_n}{(n+2)(n+1)} \quad (4.1.7)$$

Even terms give

$$c_2 = \frac{-c_0}{2 \cdot 1}$$

$$c_4 = \frac{-c_2}{4 \cdot 3} = \frac{c_0}{4 \cdot 3 \cdot 2 \cdot 1} = \frac{c_0}{4!}$$

$$c_{2n} = \frac{(-1)^n}{(2n)!} c_0, \quad n = 0, 1, 2, \dots \quad (4.1.8)$$

Odd terms give,

$$c_3 = \frac{-c_1}{3 \cdot 2}$$

$$c_5 = \frac{c_1}{5!}$$

$$c_{2n+1} = \frac{(-1)^n}{(2n+1)!} c_1, \quad n = 0, 1, 2, \dots \quad (4.1.9)$$

We get our c_0 and c_1 from the boundary conditions. Again the even becomes,

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} x^{2n} = \cos(x) \quad (4.1.10)$$

the odd becomes,

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} x^{2n+1} = \sin(x) \quad (4.1.11)$$

Returning now to our original equation,

$$y''(x) + y(x) = 0 \quad (4.1.12)$$

from Euler,

$$y(x) = e^{\alpha x} \quad (4.1.13)$$

substituting the form into the equation,

$$\alpha^2 e^{\alpha x} + e^{\alpha x} = 0 \quad (4.1.14)$$

which simplifies to the characteristic equation,

$$\alpha^2 + 1 = 0 \quad (4.1.15)$$

and we know that $\alpha \pm \sqrt{-1} = \pm i$.

$$y(x) = C_A e^{ix} + C_B e^{-ix} \quad (4.1.16)$$

From Euler's Equation (Identity),

$$e^{ix} = \cos(x) + i \sin(x) \quad e^{-ix} = -\cos(x) + i \sin(x) \quad (4.1.17)$$

$$C_A [\cos(x) + i \sin(x)] + C_B [-\cos(x) + i \sin(x)] = (C_A + C_B) \cos(x) + i(C_A - C_B) \sin(x) \quad (4.1.18)$$

Ordinary and Singular Points

$$A(x) \frac{d^2 y}{dx^2} + P(x) \frac{dy}{dx} + Q(x)y(x) = 0 \quad (4.1.19)$$

$$\frac{d^2 y}{dx^2} + p(x) \frac{dy}{dx} + q(x)y(x) = 0 \quad (4.1.20)$$

From a Theorem, we know that x_0 is oral.

to deal with a singularity,

$$y(x) = C_1 \sum_{n=0}^{\infty} a_n (x - x_0)^n + C_2 \sum_{n=0}^{\infty} b_n (x - x_0)^n \quad (4.1.21)$$

as an example:

$$(1 - x^2)y''(x) - 6xy' - 4xy = 0 \quad (4.1.22)$$

So our $p(x) = -\frac{6x}{1-x^2}$, and $q(x) = \frac{-4}{1-x^2}$

$$p(x) = 6 \sum_{n=0}^{\infty} x^{2n+1} \quad (4.1.23)$$

$$q(x) = -4 \sum_{n=0}^{\infty} x^{2n} \quad (4.1.24)$$

for stability we see, $x \ll |1|$

$$y(x) = C_1 \sum_{n=0}^{\infty} a_n x^n + C_2 \sum_{n=0}^{\infty} b_n x^n \quad (4.1.25)$$

$$y(x) = C_1 \sum_{n=0}^{\infty} (n+1)x^{2n} + C_2 \sum_{n=0}^{\infty} \frac{2n+1}{3} x^{2n+1} \quad (4.1.26)$$

For $x < 1$

$$\sum_{n=0}^{\infty} (n+1)x^{2n} = \frac{1}{(1-x^2)^2} \quad (4.1.27)$$

$$\sum_{n=0}^{\infty} \frac{2n+1}{3} x^{2n+1} = \frac{3x - x^3}{3(1-x^2)^2} \quad (4.1.28)$$

Where we get c_1 and c_2 front the boundary conditions.

Example: Harmonic Oscillator

From the spring approximation, $x(t = 0) = 0$

$$u = \frac{kx^2}{2} \quad (4.1.29)$$

$$F = -\frac{\partial u}{\partial x} = -kx \quad (4.1.30)$$

which gives the restoring force.

From Newton's Laws, $m\mathbf{a} = \sum_i \mathbf{F}_i$

$$m \frac{d^2x}{dt^2} = -kx \quad (4.1.31)$$

$$\frac{d^2X}{dt^2} + \frac{k}{m}x = 0 \quad (4.1.32)$$

$$\frac{d^2x}{dt^2} + \lambda^2x = 0 \quad (4.1.33)$$

saying we have $\tilde{t} = \lambda t$, we again have the Helmholtz equation,

$$\frac{d^2x}{d\tilde{t}^2} + x = 0 \quad (4.1.34)$$

$$X = C_1 \cos(\tilde{t}) + C_2 \sin(\tilde{t}) \quad (4.1.35)$$

from the initial condition, $C_1 \equiv 0$

$$X = C_2 \sin(\tilde{t}) \quad (4.1.36)$$

the other constant now corresponds to the amplitude of our system.

From the *Hamiltonian* of the system,

$$E_{\text{tot}} = \frac{mv^2}{2} + \frac{kx^2}{2} \quad (4.1.37)$$

$$v = \frac{dx}{dt} = -(-C_2)\lambda \cos(\lambda t) \quad (4.1.38)$$

$$v^2 = C_2^2 \lambda^2 \cos^2(\lambda t) \quad (4.1.39)$$

$$v^2 + \frac{k}{m}x^2 = \frac{2E_{\text{tot}}}{m} \quad (4.1.40)$$

we now know that $\lambda = \frac{k}{m}$

$$C_2^2 \lambda^2 \cos^2(\lambda t) + C_2^2 \lambda^2 \sin^2(\lambda t) = \frac{2E_{\text{tot}}}{m} \quad (4.1.41)$$

$$C_2^2 \lambda^2 (\cos^2(\lambda t) + \sin^2(\lambda t)) = \frac{2E_{\text{tot}}}{m} \quad (4.1.42)$$

$$C_2^2 \lambda^2 = \frac{2E_{\text{tot}}}{m} \quad (4.1.43)$$

$$C_2^2 = \frac{2E_{\text{tot}}}{m\lambda^2} \quad (4.1.44)$$

$$C_2^2 = \frac{2E_{\text{tot}}}{k} \quad (4.1.45)$$

$$C_2 = \sqrt{\frac{2E_{\text{tot}}}{k}} \quad (4.1.46)$$

$$\boxed{x = \sqrt{\frac{2E_{\text{tot}}}{k}} \sin(\tilde{t})} \quad (4.1.47)$$

4.2 Lecture 11: September 26, 2012

Review: Harmonic Oscillator

Classical Case

1. Newton Equation $x(t)$
2. Solution for $x(t)$ in $\sin(\lambda x), \cos(\lambda x)$
3. Energy $E_{\text{tot}} \rightarrow \text{const}$, which gives the amplitude

$$A = \sqrt{\frac{2E_{\text{tot}}}{k}} \quad (4.2.1)$$

$$E_{\text{tot}} = 0 \quad \rightarrow \quad A = 0 \quad (4.2.2)$$

Example: Harmonic Quantum Oscillator

For conservation of energy,

$$\hat{H}\psi = E\psi \quad (4.2.3)$$

where, ψ is the wave function, E is the energy, \hat{H} is the Hamiltonian operator.

$$\text{Energy} = E_{\text{tot}} = \frac{mv^2}{2} + \frac{kx^2}{2} \quad (4.2.4)$$

We define $\sqrt{\frac{k}{m}} = \omega_0$ with $p = mv$, and now

$$E_{\text{tot}} = \frac{p^2}{2m} + \frac{m\omega_0^2}{2}x^2 \quad (4.2.5)$$

For 1D,

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m\omega_0^2}{2}x^2 \quad (4.2.6)$$

thus,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + \frac{m\omega_0^2}{2}x^2 \psi = E\psi \quad (4.2.7)$$

this is different from the classical case of

$$m \frac{d^2 x}{dt^2} + kx = 0 \quad (4.2.8)$$

With $\hbar = \frac{h}{2\pi}$,

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2mE}{\hbar^2} \psi - \frac{m^2 \omega_0^2 x^2}{2\hbar} \psi = 0 \quad (4.2.9)$$

Rescaling our length system,

$$x_0^2 = \frac{\hbar}{m\omega_0} [=] \frac{ML^2t^{-2}t}{Mt^{-1}} = L^2 \quad (4.2.10)$$

so we define,

$$\frac{x}{x_0} = \xi; \quad \varepsilon = \frac{2E}{\hbar\omega}; \quad (\varepsilon - \xi^2) \neq \text{constant} \quad (4.2.11)$$

$$\frac{\partial^2 \psi}{\partial \xi^2} + (\varepsilon - \xi^2)\psi = 0 \quad (4.2.12)$$

note this is not the same as,

$$\frac{d^2 x}{dt^2} + \lambda^2 x = 0. \quad (4.2.13)$$

For large ξ , $|\xi^2| \gg \varepsilon$

$$\frac{\partial^2 \psi_\infty}{\partial \xi^2} - (\xi^2)\psi_\infty = 0 \quad (4.2.14)$$

$$\psi_\infty(\xi) = e^{\pm \xi^2/2} \quad (4.2.15)$$

$$\frac{\partial \psi_\infty}{\partial \xi} = \pm \xi e^{\pm \xi^2/2} \quad (4.2.16)$$

$$\frac{\partial^2 \psi_\infty}{\partial \xi^2} = \xi^2 e^{\pm \xi^2/2} \pm e^{\pm \xi^2/2} \quad (4.2.17)$$

$$= (\xi^2 \pm 1) e^{\pm \xi^2/2} \quad (4.2.18)$$

Because the solution must be finite as $\xi \rightarrow \infty$, we simplify to

$$\psi(\xi) = \eta(\xi) e^{-\xi^2/2} \quad (4.2.19)$$

$$\frac{\partial \psi_\infty}{\partial \xi} = \frac{\partial \eta}{\partial \xi} e^{-\xi^2/2} + \eta e^{-\xi^2/2} (-\xi) \quad (4.2.20)$$

$$\frac{\partial^2 \psi}{\partial \xi^2} = \frac{\partial^2 \eta}{\partial \xi^2} e^{-\xi^2/2} - 2\xi \frac{\partial \eta}{\partial \xi} e^{-\xi^2/2} - \eta e^{-\xi^2/2} + \xi^2 \eta e^{-\xi^2/2} \quad (4.2.21)$$

Simplifying out the exponential terms by setting the equation equal to zero,

$$\frac{\partial^2 \eta}{\partial \xi^2} - 2\xi \frac{\partial \eta}{\partial \xi} + (\varepsilon - 1)\eta = 0 \quad (4.2.22)$$

Now we can expand by a series with the above equation as the determining identity,

$$\eta \xi = \sum_{n=0}^{\infty} C_n \xi^n \quad (4.2.23)$$

$$\frac{\partial \eta}{\partial \xi} = \sum_{n=0}^{\infty} C_n n \xi^{n-1} \quad (4.2.24)$$

$$\frac{\partial^2 \eta}{\partial \xi^2} = \sum_{n=0}^{\infty} C_n n(n-1) \xi^{n-2} \quad (4.2.25)$$

Substituting,

$$\sum_{n=0}^{\infty} C_n n(n-1)\xi^{n-2} - 2 \sum_{n=0}^{\infty} C_n n \xi^n + (\varepsilon - 1) \sum_{n=0}^{\infty} C_n \xi^n = 0 \quad (4.2.26)$$

transforming the indices of the first summation, $n(n-1) \rightarrow (n+2)(n+1)$,

$$\sum_{n=0}^{\infty} [C_{n+2}(n+2)(n+1) - 2C_n n + (\varepsilon - 1)C_n] \xi^n = 0 \quad (4.2.27)$$

This gives a recursion formula,

$$C_{n+2} = \frac{[2n - (\varepsilon - 1)] C_n}{(n+2)(n+1)} \quad (4.2.28)$$

From physical arguments we know that $C_1 = 0$, but $C_0 \neq 0$,

$$\psi(\xi) = \eta(\xi)e^{-\xi^2/2} = \sum_{n=0}^{\infty} C_{2n} \xi^{2n} e^{-\xi^2/2} \quad (4.2.29)$$

Now, observing the series of ξ^{2n} we recognize that this is in fact similar to $e^{2\xi}$. Thus our solution still blows up as we go to infinity. For n terms, $C_{n+2} = 0, C_n \neq 0$,

$$\frac{[2n - (\varepsilon - 1)] C_n}{(n+2)(n+1)} = 0 \quad (4.2.30)$$

Which gives $2n - (\varepsilon - 1) = 0$, and we have the condition,

$$\varepsilon = 2n + 1, \quad n = 0, 1, 2, 3, \dots \quad (4.2.31)$$

Now we investigate the situation for finite values of n .

$$\eta\xi = \sum_{n=0}^{n_l} C_n \xi^n \quad (4.2.32)$$

$$C_{n+2} = \frac{[2n - (\varepsilon - 1)] C_n}{(n+2)(n+1)} \quad (4.2.33)$$

We thus get the *Hermite polynomials*,

$$H_n(\xi) \rightarrow \eta_n(\xi) = A_n H_n(\xi) \quad (4.2.34)$$

where,

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n e^{-\xi^2}}{d\xi^n} \quad (4.2.35)$$

To normalize,

$$\int |\psi^2| dV = 1 \quad (4.2.36)$$

$$A_n = \sqrt{\frac{1}{2^n n! \sqrt{\pi}}} \sqrt{\frac{\hbar}{m\omega_0}} \quad (4.2.37)$$

So,

$$\varepsilon = \frac{2E}{\hbar\omega_0} = 2n + 1 \quad (4.2.38)$$

$$\begin{aligned} E &= \frac{2n + 1}{2} \hbar\omega_0 \\ &= \left(n + \frac{1}{2}\right) \hbar\omega_0 \end{aligned} \quad (4.2.39)$$

$$E_0 = \frac{1}{2} \hbar\omega_0 \quad (4.2.40a)$$

$$E_1 = \frac{3}{2} \hbar\omega_0 \quad (4.2.40b)$$

$$E_2 = \frac{5}{2} \hbar\omega_0 \quad (4.2.40c)$$

...

Comparison of Classical and Quantum Oscillators

1. Lowest energy

Classical: $E = 0$, Quantum: $E = \frac{1}{2} \hbar\omega_0$ So, even at $T = 0\text{K}$ there is still energy in the system.

$$\psi_0 = A_0 e^{-\xi^2/2}, \quad H_0(\xi) = 1 \quad (4.2.41)$$

$$\rho_0(\xi) = |\psi^2| = A_0^2 e^{-\xi^2} \quad (4.2.42)$$

$$A_0^2 \int_{-\infty}^{\infty} e^{-\psi^2} d\psi = 1 \quad (4.2.43)$$

Thus, we find things such as tunneling for the quantum particle. We also observe uncertainty,

$$\Delta p \Delta x \geq \frac{\hbar}{2} \quad (4.2.44)$$

$$\Delta p^2 \Delta x^2 \geq \frac{\hbar^2}{4} \quad (4.2.45)$$

$$\langle p \rangle = 0 \quad (4.2.46)$$

$$\langle (p - \langle p \rangle)^2 \rangle = \langle \Delta p^2 \rangle \langle \Delta x^2 \rangle \quad (4.2.47)$$

$$\langle p^2 \rangle \langle x^2 \rangle = \frac{\hbar^2}{4} \quad (4.2.48)$$

$$\langle x^2 \rangle = \frac{\hbar^2}{4 \langle p^2 \rangle} \quad (4.2.49)$$

For the energy,

$$\langle E \rangle = \frac{\langle p^2 \rangle}{2m} + \frac{m\omega_0^2}{2} \langle x^2 \rangle \quad (4.2.50)$$

$$= \frac{\langle p^2 \rangle}{2m} + \frac{m\omega_0^2 \hbar^2}{8 \langle p^2 \rangle} \quad (4.2.51)$$

With equilibrium,

$$\frac{\partial \langle E \rangle}{\partial \langle p^2 \rangle} = 0 \quad (4.2.52)$$

we get,

$$\langle p^2 \rangle = \frac{m\omega_0 \hbar}{2} \quad (4.2.53)$$

Simplifying, we can conclude,

$$E_{\min} = \frac{\hbar}{2m} \quad (4.2.54)$$

4.3 Lecture 12: October 1, 2012

Test will be take-home, the week of October 15th.

Legendre Equation

$$(1 - x^2)y''(x) - 2xy'(x) + \alpha(\alpha + 1)y(x) = 0 \quad (4.3.1)$$

where α (and $(\alpha + 1)$) is a constant.

$$y''(x) + P(x)y'(x) + q(x)y(x) = 0 \quad (4.3.2)$$

where $P(x) = \frac{-2x}{(1-x^2)}$, and $q(x) = \frac{\alpha(\alpha+1)}{(1-x^2)}$. Since we work in a coordinates which is naturally limited it is reasonable to represent this solution on a confined domain, such as $[-1, 1]$.

$$y(x) = \sum_{n=0}^{\infty} C_n x^n \quad (4.3.3)$$

By recursion, for $n \geq 0$,

$$C_{n+2} = -\frac{(\alpha - 1)(\alpha + n + 1)}{(n + 1)(n + 2)}C_n \quad (4.3.4)$$

For example,

$$C_2 = -\frac{\alpha(\alpha + 1)}{2 \times 1}C_0 \quad (4.3.5)$$

We can separate the even and the odd coefficients with even as $y_1(x)$ and odd as $y_2(x)$, or

$$y_1(x) = \sum_{n=0}^{\infty} C_{2n} x^{2n} \quad (4.3.6)$$

$$y_2(x) = \sum_{n=0}^{\infty} C_{2n+1} x^{2n+1} \quad (4.3.7)$$

What we find is that for any integer value of α , one of these series is truncated, while the other is divergent. *e.g.* for $\alpha = 0$, we get that $C_2 = 0, C_4 = 0, \dots$. For $\alpha = 1$, we find $C_3 = 0, C_5 = 0, \dots$. So we set up a formula, $f_n(x)$ where $n = \alpha$. The terms of this formula are,

$$f_0(x) = 1, \quad (4.3.8)$$

$$f_1(x) = x, \quad (4.3.9)$$

$$f_2(x) = 1 - 3x^2, \quad (4.3.10)$$

$$f_3(x) = x - 5x^3, \quad (4.3.11)$$

...

So we find the *Legendre polynomials*,

$$P_0(x) = 1, \tag{4.3.12}$$

$$P_1(x) = x, \tag{4.3.13}$$

$$P_2(x) = \frac{1}{2}(1 - 3x^2), \tag{4.3.14}$$

$$P_3(x) = \frac{1}{2}(3x - 5x^3), \tag{4.3.15}$$

...

which are generated by the formula,

$$P_n(x) = \frac{1}{2^n} \sum_{j=0}^{n/2} \frac{(-1)^j (2n - 2j)!}{j! (n - j)! (n - 2j)!} x^{n-2j} \tag{4.3.16}$$

$$x = \cos(\theta) \tag{4.3.17}$$

We find that this is useful in solving equations in spherical coordinates,

$$\nabla^2 F = 0 \tag{4.3.18}$$

$$\nabla^2 F = f(\mathbf{r}) \tag{4.3.19}$$

Series Solutions near an Ordinary Point

$$y(x) = \sum_{n=0}^{\infty} C_n x^{n+r} \tag{4.3.20}$$

For a fractional value of r , we will need to use the *Frobenius Series Method*. With

$$y''(x) + P(x)y'(x) + q(x)y(x) = 0 \tag{4.3.21}$$

we may find that $P(x)$ or $q(x)$ is divergent, or has a singularity around a value. An example is $\frac{1}{x-x_0}$, where the solution diverges at $x = x_0$. We also observe this for $\frac{1}{(x-x_0)^2}$, where the solution diverges at $x = x_0$, however, this is more strongly divergent. If both of the following conditions are fulfilled, then the Frobenius method may be used,

$$\lim_{x \rightarrow x_0} (x - x_0)P(x) \rightarrow \text{finite} \tag{4.3.22}$$

$$\lim_{x \rightarrow x_0} (x - x_0)^2 q(x) \rightarrow \text{finite} \tag{4.3.23}$$

Illustration of method

$$2xy''(x) + 3y'(x) - y(x) = 0 \quad (4.3.24)$$

Rewriting into standard form,

$$y''(x) + \frac{3}{2x}y'(x) - \frac{1}{2x}y(x) = 0 \quad (4.3.25)$$

Now investigating the limiting behavior around the singularities,

$$\lim_{x \rightarrow 0} x \frac{3}{2x} = \frac{3}{2} \rightarrow \text{finite}, \quad (4.3.26)$$

and

$$\lim_{x \rightarrow 0} x^2 \frac{-1}{2x} = 0 \rightarrow \text{finite}. \quad (4.3.27)$$

Thus, we have a good candidate for applying the Frobenius method.

Substituting the series form,

$$a_0 r(2r+1)x^{r-1} + \sum_{n=1}^{\infty} [(n+r)(2n+2r+1)a_n - a_{n-1}]x^{n+r-1} = 0 \quad (4.3.28)$$

We know find the indicial equation (when $n = 0$), where we have non-trivial solutions

$$a_0 r(2r+1) = 0. \quad (4.3.29)$$

Since a_0 cannot be zero,

$$r(2r+1) = 0, \quad (4.3.30)$$

and we get solutions of $r_1 = 0$ and $r_2 = -\frac{1}{2}$. These correspond to two different power series solutions.

$$y_1(x) = \sum_{n=0}^{\infty} b_n x^n \quad (4.3.31)$$

$$y_2(x) = x^{1/2} \sum_{n=0}^{\infty} c_n x^n \quad (4.3.32)$$

From the first equation we get a recursion formula of,

$$n(2n+1)b_n - b_{n-1} = 0 \quad (4.3.33)$$

$$b_n = \frac{b_{n-1}}{n(2n+1)} \quad (4.3.34)$$

$$b_n = \frac{2^n}{(2n+1)!} b_0 \quad (4.3.35)$$

Similarly, for the second series ($r = -1/2$),

$$c_n = \frac{2^n c_0}{(2n)!} \quad (4.3.36)$$

Finally, we have the solution,

$$y(x) = b_0 \sum_{n=0}^{\infty} \frac{2^n}{(2n+1)!} x^n + c_0 x^{-1/2} \sum_{n=0}^{\infty} \frac{2^n}{(2n)!} x^n \quad (4.3.37)$$

For repeated roots $r_1 = r_2$ see pages 595–599.

Bessel Equation and Bessel Functions

The *Bessel equation*,

$$x^2 y''(x) + xy'(x) + (x^2 - \nu^2) y(x) = 0 \quad (4.3.38)$$

the constant, $\nu \geq 0$, (pronounced ‘nu’), gives the order of the Bessel equation. In standard form,

$$y''(x) + P(x)y'(x) + q(x)y(x) = 0 \quad (4.3.39)$$

where $P = \frac{1}{x}$, and $q(x) = 1 - \frac{\nu^2}{x^2}$. We see that $xP(x) = 1$, and $x^2q(x) = x^2 - \nu^2$ and we can use the method of Frobenius. So we have a series $y(x) = \sum_{n=0}^{\infty} a_n x^{n+r}$. Substituting,

$$(r^2 - \nu^2) a_0 x^r + \sum_{n=1}^{\infty} \{[(r+n)^2 - \nu^2] a_n + a_{n-2}\} x^{n+r} = 0 \quad (4.3.40)$$

We get $r^2 - \nu^2 = 0$, or $r = \pm\nu$. For $n \geq 2$

$$[(r+n)^2 - \nu^2] a_n - a_{n-2} = 0 \quad (4.3.41)$$

We find in our case, for $\nu = 0$ that $r_1 = r_2 = 0$. In this special case,

$$y_1(x) = \sum_{n=0}^{\infty} a_n x^n \quad (4.3.42)$$

$$y_2(x) = y_1(x) \ln(x) + x \sum_{n=0}^{\infty} b_n x^n \quad (4.3.43)$$

With the solution of,

$$y(x) = c_1 y_1(x) + c_2 y_2(x) \quad (4.3.44)$$

$$y_1(x) = J_0(x) \quad (4.3.45)$$

which is the zeroth order Bessel function of the first kind. In total there are four different kinds of *Bessel function*.

$$J_0(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(n!)^2} \left(\frac{x}{2}\right)^{2n} \quad (4.3.46)$$

In complex form, it is also,

$$J_0(x) = \frac{1}{2\pi} \int_0^{2\pi} e^{ix \cos(\theta)} d\theta \quad (4.3.47)$$

$$= \frac{1}{2\pi} \int_0^{2\pi} \cos(x \sin(\theta)) d\theta \quad (4.3.48)$$

$$y_2(x) = Y_0(x) \ln(x) + \sum_{n=1}^{\infty} \frac{(-1)^n H_n x^{2n}}{(2n)^2 (2n-2)^2 \cdot (2)^2} \quad (4.3.49)$$

where $H_n = \sum_{i=1}^n \frac{1}{i}$. Thus we have our solution for

$$y(x) = c_1 J_0(x) + c_2 Y_0(x) \quad (4.3.50)$$

$$Y_0(x) = \frac{2}{\pi} \left(\gamma + \ln\left(\frac{x}{2}\right) \right) J_0(x) \quad (4.3.51)$$

where the *Euler constant* is $\gamma = 0.5772\dots$, which is $\gamma = \lim_{n \rightarrow \infty} (H_n - \ln(n))$

For general values of n

$$J_n(x) = \sum_{j=0}^{\infty} \frac{(-1)^j}{\Gamma(j+1)\Gamma(j+1+n)} \left(\frac{x}{2}\right)^{2j+1} \quad (4.3.52)$$

UNIT 5

Chapter 14—Orthogonal Functions and Sturm–Liouville Theory

5.1 Lecture 13: October 3, 2012

Orthogonal Functions

$$(f, g) = \int fg \, dx \quad (5.1.1)$$

where (f, g) is known as the inner product. There are similarities between the inner integral product and a vector inner product.

For vectors, with an inner product $\mathbf{a} \cdot \mathbf{b}$, where the vectors may be a function of the three dimensional coordinates

$$\begin{aligned} \mathbf{a}(x, y, z) \\ \mathbf{b}(x, y, z) \end{aligned}$$

orthogonal is defined using the inner product by

$$\mathbf{a} \cdot \mathbf{b} = 0. \quad (5.1.2)$$

For functions $f(x), g(x)$ with the inner product,

$$(f, g) = \int_{\text{FD}} fg \, dx \quad (5.1.3)$$

orthogonal is defined by

$$(f, g) = 0. \quad (5.1.4)$$

The Cochy–Schwarz inequality;

$$(f, g)^2 \leq (f, f)(g, g). \quad (5.1.5)$$

Since, $(f, f) = \int f f \, dx$, we know have norms,

$$Nf = (f, f) = \int f^2 \, dx \quad (5.1.6)$$

A normalized function is,

$$Nf = 1 \quad (5.1.7)$$

Normalized Orthogonal Functions,

$$\varphi_1(x), \varphi_2(x), \varphi_3(x), \dots$$

$$(\varphi_i, \varphi_j) = \delta_{ij} \quad (5.1.8)$$

$$\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases} \quad (5.1.9)$$

This system of normalized, orthogonal vectors is known as a *Hilbert space* after David Hilbert.

Some examples of orthogonal functions

$$\frac{1}{\sqrt{2\pi}}, \frac{\cos(x)}{\sqrt{\pi}}, \frac{\sin(x)}{\sqrt{\pi}}, \frac{\cos(2x)}{\sqrt{\pi}}, \frac{\sin(2x)}{\sqrt{\pi}}, \dots$$

Fundamental Integration Domain, $[0, 2\pi]$.

$$\frac{1}{\sqrt{2\pi}}, \frac{e^{ix}}{\sqrt{\pi}}, \frac{e^{i2x}}{\sqrt{\pi}}, \dots$$

$$(f, \bar{g}) = (\bar{f}, g) \quad (5.1.10)$$

$$Nf = \int |f|^2 \, dx = \int f \bar{f} \, dx \quad (5.1.11)$$

$$\frac{1}{\sqrt{2\pi}} \int e^{i(\mu-\nu)x} \, dx = \delta_{\mu\nu} \quad (5.1.12)$$

$$f_1, f_2, f_3, \dots, f_r$$

Linearly independent at least in x

$$\sum_{i=1}^r c_i f_i \neq 0 \quad (5.1.13)$$

$$\sum_{i=1}^r c_i f_i = 0 \quad \text{for each } x \quad (5.1.14)$$

When f is any function,

$$f = \sum_{\nu=1}^{\infty} c_{\nu} \varphi_{\nu} \quad (5.1.15)$$

$$c_{\nu} = (f, \varphi) = \int_{FD} f \varphi_{\nu} dx \quad (5.1.16)$$

for each ν .

Bessel Inequality (as $n \rightarrow \infty$)

$$\sum_{\nu=1}^n c_{\nu}^2 \leq Nf \quad (5.1.17)$$

for a complete set,

$$\sum_{\nu=1}^n c_{\nu}^2 = Nf \quad (5.1.18)$$

Legendre Polynomials

$$\int_{-1}^1 P_n(x) P_m(x) dx = 0, \quad \text{for } n \neq m \quad (5.1.19)$$

A generating function for the Legendre polynomials, G ,

$$G(x, t) = \sum_{n=0}^{\infty} P_n(x) t^n \quad (5.1.20)$$

$$(n+1) P_{n+1}(x) - (2n+1)x P_n(x) + n P_{n-1}(x) = 0 \quad (5.1.21)$$

Multiply by t^n and sum over n ,

$$\sum_{n=0}^{\infty} (n+1) P_{n+1}(x) t^n - \sum_{n=0}^{\infty} (2n+1)x P_n(x) t^n + \sum_{n=0}^{\infty} n P_{n-1}(x) t^n = 0 \quad (5.1.22)$$

Now we can see what our terms are,

$$\sum_{n=0}^{\infty} (n+1) P_{n+1}(x) t^n \quad (5.1.23)$$

$$\frac{\partial}{\partial t} \left(\sum_{n=0}^{\infty} P_n(x) t^n \right) = \sum_{n=0}^{\infty} n P_n(x) t^{n-1} = \frac{\partial G}{\partial t} \quad (5.1.24)$$

$$- \sum_{n=0}^{\infty} (2n+1)x P_n(x) t^n = -2 \sum_{n=0}^{\infty} n x P_n(x) t^n - \sum_{n=0}^{\infty} x P_n(x) t^n \quad (5.1.25)$$

$$- \sum_{n=0}^{\infty} x P_n(x) t^n = -x \sum_{n=0}^{\infty} P_n(x) t^n = -xG \quad (5.1.26)$$

$$-2 \sum_{n=0}^{\infty} x P_n(x) t^n = -2t \sum_{n=0}^{\infty} x P_n(x) t^n = -2t \sum_{n=0}^{\infty} x P_n(x) \frac{\partial t^n}{\partial n} = -2tx \frac{\partial G}{\partial t} \quad (5.1.27)$$

$$\sum_{n=0}^{\infty} n P_{n-1}(x) t^n = (tG)' = \left(\sum_{n=0}^{\infty} P_n(x) t^n \right) = \sum_{n=0}^{\infty} n P_n(x) t^{n-1} \quad (5.1.28)$$

$$\frac{\partial G}{\partial t} - 2xt \frac{\partial G}{\partial t} - xG + t \frac{\partial tG}{\partial t} = 0 \quad (5.1.29)$$

$$\frac{\partial G}{\partial t} = \frac{(x-t)G}{(1-2xt+t^2)} \quad (5.1.30)$$

Separating the variables,

$$\frac{dG}{G} = \frac{(x-t)}{(1-2xt+t^2)} dt \quad (5.1.31)$$

$$\ln(G) = -\frac{1}{2} \ln [1+t^2-2tx] + C_1 \quad (5.1.32)$$

$$\ln(G) = \ln \left(\frac{1}{(1+t^2-2tx)^{1/2}} \right) + C_1 \quad (5.1.33)$$

$$G = \frac{C_2}{(1+t^2-2tx)^{1/2}} \quad (5.1.34)$$

IC $t = 0$, $G(t=0) = C_2$ For $P_0(x) = 1$

$$G = \sum_{n=0}^0 P_0 t^0 = P_0 t_0 = C_2 = 1 \quad (5.1.35)$$

So we find that the generating function has the following form,

$$G(x, t) = \frac{1}{(1+t^2-2tx)^{1/2}} \quad (5.1.36)$$

Expanding $G(x)$ in a Taylor Series around $t = 0$,

$$G(x, 1) = G(x, 0) + \frac{1}{1!} \frac{\partial}{\partial t} (G(x, t)) \Big|_{t=0} t + \frac{1}{2!} \frac{\partial^2}{\partial t^2} (G(x, t)) \Big|_{t=0} t^2 + \frac{1}{3!} \frac{\partial^3}{\partial t^3} (G(x, t)) \Big|_{t=0} t^3 + \dots \quad (5.1.37)$$

$$P_n(x) = \frac{1}{n!} \left(\frac{\partial^n G}{\partial t^n} \right)_{t=0} \quad (5.1.38)$$

Example: Electrostatics

$$V = \frac{q}{4\pi\epsilon_0|\mathbf{r} \cdot \mathbf{l}|} \quad (5.1.39)$$

$$|\mathbf{r} \cdot \mathbf{l}| = (r^2 + l^2 - 2rl \cos(\theta))^{1/2} \quad (5.1.40)$$

$$V = \frac{q}{4\pi\epsilon_0 (r^2 + l^2 - 2rl \cos \theta)^{1/2}} \quad (5.1.41)$$

Observing similar forms,

$$G = \frac{1}{(1 - 2xt + t^2)^{1/2}} \quad (5.1.42)$$

where, $x = \cos(\theta)$ and $t = \frac{l}{r}$. So,

$$\begin{aligned} V &= \frac{q}{4\pi\epsilon_0 r} \sum_{n=0}^{\infty} P_n(\cos(\theta)) \left(\frac{l}{r}\right)^n \\ &= \frac{q}{4\pi\epsilon_0} \sum_{n=0}^{\infty} P_n(\cos(\theta)) \frac{l^n}{r^{n+1}} \end{aligned} \quad (5.1.43)$$

For multiple charges,

$$V = \frac{q}{4\pi\epsilon_0} \sum_{n=0}^{\infty} \frac{1}{r^{n+1}} \left[\sum_j q_j l_j^n P_n(\cos(\theta)) \right] \quad (5.1.44)$$

this is known as a multipole expansion series. Defining the “Multipole Moments”

$$M_n = \sum_j q_j l_j^n P_n(\cos(\theta)) \quad (5.1.45)$$

Thus,

$$V = \frac{q}{4\pi\epsilon_0} \sum_{n=0}^{\infty} \frac{M_n}{r^{n+1}} \quad (5.1.46)$$

For the zeroth moment, we find

$$M_0 = q - q = 0 \quad (5.1.47)$$

$$M_1 = \frac{ql}{2} \cos(0) - \frac{ql}{2} \cos(\theta) \quad (5.1.48)$$

$$= \mu \cos(\theta) \quad (5.1.49)$$

where μ is the dipole moment, $\frac{ql}{2}$.

The Dipole,

$$V_d = \frac{\mu \cos(\theta)}{4\pi\epsilon_0 r^2} \quad (5.1.50)$$

for Coulombic,

$$V_c = \frac{q}{4\pi\epsilon_0 r} \quad (5.1.51)$$

thus dipole interactions drop off much more quickly than the Coulombic forces.

$$\mathbf{E} = \nabla V \quad (5.1.52)$$

$$= \frac{\partial V}{\partial r} \mathbf{e}_r + \frac{1}{r} \frac{\partial V}{\partial \theta} \mathbf{e}_\theta \quad (5.1.53)$$

$$= -\frac{\mu \cos(\theta)}{4\pi\epsilon_0 r^3} \mathbf{e}_r - \frac{\mu \sin(\theta)}{4\pi\epsilon_0 r^3} \mathbf{e}_\theta \quad (5.1.54)$$

$$f(x) = \sum_{n=0}^{\infty} a_n P_n(x) \quad \times \quad P_m(x) \quad (5.1.55)$$

where m is a fixed number,

$$\int_{-1}^1 f(x) P_m(x) dx = \sum_{n=0}^{\infty} a_n \int_{-1}^1 P_n P_m dx \quad (5.1.56)$$

$$\int_{-1}^1 P_n P_m dx = \frac{2}{2n+1} \delta_{nm} \quad (5.1.57)$$

$$a_m = \frac{2m+1}{2} \int_{-1}^1 f(x) P_m(x) dx \quad (5.1.58)$$

This gives the rule for obtaining the coefficients in the expansion.

5.2 Lecture 14: October 8, 2012

Orthogonal Polynomials, A General Case

Given a set of orthogonal polynomials,

$$\phi_0(x), \phi_1(x), \phi_2(x), \dots$$

if $\int_a^b r(x)\phi_i(x)\phi_j(x) dx = 0$ for $i \neq j$ and $r(x)$ as the weight function.

$$\phi_0(x) = 1 \tag{5.2.1}$$

$$\phi_1(x) = C_1x + C_2 \tag{5.2.2}$$

$$\int_a^b r(x)\phi_0(x)\phi_1(x) dx = C_1 \int r(x)x dx + C_2 \int r(x) dx = 0 \tag{5.2.3}$$

$$C_1 = \frac{-C_2 \int r(x) dx}{\int r(x)x dx} \tag{5.2.4}$$

Gramm–Schmidt Orthogonalization

In *Gramm–Schmidt orthogonalization* we can take an infinite number of linearly independent functions,

$$v_1, v_2, v_3, \dots$$

we want an orthonormal basis set of functions,

$$\varphi_1, \varphi_2, \varphi_3, \dots$$

$$\varphi_1 = \frac{v_1}{\sqrt{Nv_1}} \tag{5.2.5}$$

where the normal is,

$$Nv_1 = \int v_1^2 dx \tag{5.2.6}$$

Now,

$$\varphi_2 = V_2 - C'_1\varphi_1 \tag{5.2.7}$$

where we must find C'_1 .

$$\int \varphi_1(v_2 - C'_1\varphi_1) dx = 0 \tag{5.2.8}$$

Rearranging,

$$\int \varphi_1\varphi_2 dx = C'_1 \int \varphi_1^2 dx \tag{5.2.9}$$

$$\int \varphi_1^2 dx = 1 \quad (5.2.10)$$

$$C_1' = \int \varphi_1 v_2 dx = (\varphi_1, v_2) \quad (5.2.11)$$

$$\varphi_3 = v_3 - C_1'' - C_2'' \varphi_2 \quad (5.2.12)$$

Again we want the third term to be orthogonal to both, φ_1, φ_2 . Going through the same derivation, we quickly may find that,

$$C_1'' = (\varphi_1, v_3) \quad (5.2.13)$$

$$C_2'' = (\varphi_2, v_3) \quad (5.2.14)$$

Sturm–Liouville Theory

In *Sturm–Liouville theory*, we consider a second order ordinary differential equation of the form,

$$[p(x)y'(x)]' + [q(x) + \lambda r(x)]y(x) = 0, \quad (5.2.15)$$

where by the product rule of differentiation, the first term may alternatively be expressed

$$[p(x)y'(x)]' = p(x)y''(x) + p'(x)y'(x). \quad (5.2.16)$$

We have a parameter λ to be used in the solution. We are on a domain $[a, b]$ with boundary conditions

$$\alpha_1 y(a) + \alpha_2 y'(a) = 0, \quad (5.2.17)$$

$$\alpha_1 y(b) + \alpha_2 y'(b) = 0. \quad (5.2.18)$$

These terms are zero valued on the right hand side, or homogeneous, so they are not the most general (although these are Robin boundary conditions—a super-set of Dirichlet and Neumann boundary conditions). What is important is that these boundary conditions are real and non-zero. Now we understand that we must find values for λ which are non-trivial. These values which give real functional solutions to the differential equation are the *eigenvalues*. The solutions, y , which correspond to the eigenvalues are the *eigenfunctions*.

$$\mathcal{L}y(x) = \lambda r(x)y(x) \quad (5.2.19)$$

$$\mathcal{L}y(x) = -[p(x)y'(x)]' - [q(x)]y(x) \quad (5.2.20)$$

for $r(x) = 1$

$$\mathcal{L}y(x) = \lambda y(x) \quad (5.2.21)$$

$$\hat{H}\psi = E\psi \quad (5.2.22)$$

where we have E_n with $n = 1, 2, 3, \dots$

$$\hat{H} = \frac{-\hbar}{2m} \nabla^2 + U(x, y, z) \quad (5.2.23)$$

$$= \frac{-\hbar}{2m} \frac{d^2}{dx^2} + U(x) \quad (5.2.24)$$

We now have to solve the Helmholtz equation. This equation has numerous common applications in heat transfer, diffusion, fluid transport, and other topics. For a one dimensional system, this is reduced to

$$\frac{d^2 y}{dx^2} + \lambda y = 0 \quad (5.2.25)$$

$$-\frac{d^2 y}{dx^2} = \lambda y \quad (5.2.26)$$

Where our linear operator is $\mathcal{L} = -\frac{d^2}{dx^2}$. This problem is very common and the solution is known to be of the form,

$$y(x) = C_1 \cos(\sqrt{\lambda} x) + C_2 \sin(\sqrt{\lambda} x). \quad (5.2.27)$$

For n

$$\mathcal{L}y_n(x) = \lambda_n r(x) y_n(x) \quad (5.2.28)$$

For m

$$\mathcal{L}y_m^*(x) = \lambda_m^* r(x) y_m^*(x) \quad (5.2.29)$$

Multiplying by the opposite functions and integrating,

$$\int y_m^*(x) \mathcal{L}y_n(x) dx = \lambda_n \int r(x) y_n(x) y_m^*(x) dx \quad (5.2.30)$$

Similarly for the equation for m ,

$$\int y_n(x) \mathcal{L}y_m^*(x) dx = \lambda_m^* \int r(x) y_n(x) y_m^*(x) dx \quad (5.2.31)$$

Subtracting the two previous equations, we get,

$$\int y_m^*(x) \mathcal{L}y_n(x) dx - \int y_n(x) \mathcal{L}y_m^*(x) dx = (\lambda_n - \lambda_m^*) \int r(x) y_n(x) y_m^*(x) dx \quad (5.2.32)$$

Returning to

$$\mathcal{L}y(x) = -[p(x)y'(x)]' - [q(x)]y(x)$$

we see,

$$\int y_m^*(x) \mathcal{L}y_n(x) dx - \int y_n(x) \mathcal{L}y_m^*(x) dx = [p(x) \{y_m^*{}' y_n - y_m^* y_n'\}]_a^b \quad (5.2.33)$$

Now we work with the boundary conditions,

$$\alpha_1 y(a) + \alpha_2 y'(a) = 0 \quad (5.2.34)$$

$$\alpha_1 y(b) + \alpha_2 y'(b) = 0 \quad (5.2.35)$$

We begin with the boundary at a ,

$$\alpha_1 y(a) + \alpha_2 y'(a) = 0 \quad (5.2.36)$$

$$\alpha_1 y(a) = -\alpha_2 y'(a) \quad (5.2.37)$$

$$y(a) = -\frac{\alpha_2}{\alpha_1} y'(a) \quad (5.2.38)$$

Substituting,

$$P(a) \frac{\alpha_1}{\alpha_2} y_m^*(a) y_n(a) - P(a) y_m^*(a) \frac{\alpha_1}{\alpha_2} y_n(a) \quad (5.2.39)$$

Types of Sturm–Liouville Problems

We now have different possible cases for the Sturm–Liouville problem,

1. Regular Sturm–Liouville problem on $[a, b]$ where $P(x) > 0$. We require $P(a) \neq 0$ and $P(b) \neq 0$.
2. Singular Sturm–Liouville problem on $[a, b]$ where $P(x) \geq 0$. Here $P(a) = 0$.
3. Periodic Sturm–Liouville problem on $[a, b]$. $P(a) = P(b)$

For our linear operator,

$$\int_a^b y_m^* \mathcal{L} y_n \, dx = \int_a^b y_n \mathcal{L} y_m^* \, dx \quad (5.2.40)$$

Self-adjoint operators (also known as *Hermitian operators*);

$$(\lambda_n - \lambda_m^*) \int r(x) y_n(x) y_m^*(x) \, dx = \int y_m^*(x) \mathcal{L} y_n(x) \, dx - \int y_n(x) \mathcal{L} y_m^*(x) \, dx \quad (5.2.41)$$

for $n = m$ with $I \neq 0$,

$$\lambda_n = \operatorname{Re}(\lambda_n) + i \operatorname{Im}(\lambda_n) \quad (5.2.42)$$

$$\lambda_n^* = \operatorname{Re}(\lambda_n) - i \operatorname{Im}(\lambda_n) \quad (5.2.43)$$

So,

$$\lambda_n = \lambda_m^* \quad (5.2.44)$$

Thus we cannot have an imaginary system, and thus our λ_n are real. If, however, $\lambda_n \neq \lambda_m$, $(\lambda_n - \lambda_m) \neq 0$.

$$\int_a^b r(x) y_m^*(x) y_n(x) \, dx = 0 \quad (5.2.45)$$

Thus, we have eigenfunctions which are orthogonal.

For the system

$$a(x)y''(x) + b(x)y'(x) + c(x)y(x) + \lambda d(x)y(x) = 0 \quad (5.2.46)$$

Then,

$$[p(x)y'(x)]' + [p(x) + \lambda r(x)]y(x) = 0 \quad (5.2.47)$$

$$p(x) = e^{\int \frac{b(x)}{a(x)} dx} \quad (5.2.48)$$

$$q(x) = \frac{p(x)c(x)}{a(x)} \quad (5.2.49)$$

$$r(x) = \frac{p(x)d(x)}{a(x)} \quad (5.2.50)$$

We know that $a(x) \neq 0$ else we have encountered a difficult singularity.

Eigenfunctions

Eigenfunctions are linearly independent and orthonormal.

$$f(x) = \sum_{n=0}^{\infty} a_n y_n(x) \quad (5.2.51)$$

multiplying by y_m and integrating

$$\int_a^b f(x)y_m(x) dx = \int_a^b \sum_{n=0}^{\infty} a_n y_n(x)y_m(x) dx \quad (5.2.52)$$

since we know that we have orthogonality, $m \neq n$. Removing the sums we can solve for the coefficients,

$$\int_a^b f(x)y_m(x) dx = a_m \int_a^b y_m^2(x) dx \quad (5.2.53)$$

and we find

$$a_m = \frac{\int_a^b f(x)y_m(x) dx}{\int_a^b y_m^2(x) dx} \quad (5.2.54)$$

5.3 Lecture 15: October 10, 2012

Greens Functions for Non-homogeneous Equations

$$\mathcal{L}y(x) - \mu r(x)y(x) = g(x) \quad (5.3.1)$$

The Greens function of an equation gives you the solution of the whole left hand side equations. This speeds up the solution because it allows for changing the right hand sides, however this procedure is boundary-condition specific. Say,

$$\alpha_1 y(a) + \alpha_2 y'(a) = 0 \quad (5.3.2)$$

$$\beta_1 y(b) + \beta_2 y'(b) = 0 \quad (5.3.3)$$

$\phi_n(x)$ are Eigenfunctions which satisfy the eigenvalue problems. So,

$$\mathcal{L}\phi_n(x) = \lambda_n r(x)\phi_n(x) \quad (5.3.4)$$

This is the eigenvalue problem. It is in essence a homogeneous problem, which uses the given boundary conditions. We represent our function as,

$$g(x) = r(x)f(x) \quad (5.3.5)$$

or,

$$f(x) = \frac{g(x)}{r(x)} \quad (5.3.6)$$

We want to use the first equation because this is more useful for the general case where $r(x) \neq 1$.

$$\mathcal{L}y(x) - \mu r(x)y(x) = \lambda_n r(x)f(x) \quad (5.3.7)$$

$$y(x) = \sum_{n=1}^{\infty} a_n \phi_n(x) \quad (5.3.8)$$

$$f(x) = \sum_{n=1}^{\infty} f_n \phi_n(x) \quad (5.3.9)$$

The coefficients will be

$$f_n = \int_a^b r(x)f(x)\phi_n(x) dx \quad (5.3.10)$$

multiplying the expression for $f(x)$ by $r(x)\phi_m$,

$$\int_a^b r(x)f(x)\phi_n(x) dx = \int_a^b r(x) \sum_{n=1}^{\infty} f_n(x)\phi_n(x)\phi_m(x) dx \quad (5.3.11)$$

With orthogonality we know that for $\int_a^b r(x)\phi_n(x)\phi_m(x) dx = 0$ for $n \neq m$. Substituting in for our eigenvalues,

$$\sum_{n=1}^{\infty} \lambda_n r(x)\phi_n(x) - \sum_{n=1}^{\infty} \mu r(x)a_n \phi_n(x) = \sum_{n=1}^{\infty} r(x)f_n(x)\phi_n(x) \quad (5.3.12)$$

for this equation, we only need to know a_n , so we can do the multiplication by ϕ_l and integrate. This once again shows by orthogonality that $n = l$ because all other solutions are zero. *i.e.*

$$\int_a^b r(x)\phi_n(x)\phi_l(x) dx = 0 \quad \text{for } n \neq l \quad (5.3.13)$$

thus with $\phi_l \neq 0$,

$$\lambda_l a_l - \mu a_l = f_l \quad (5.3.14)$$

$$a_l = \frac{f_l}{\lambda_l - \mu} \quad (5.3.15)$$

We can substitute now to get our solution,

$$y(x) = \sum_{n=1}^{\infty} \frac{f_n}{\lambda_n - \mu} \phi_n(x) \quad (5.3.16)$$

Procedure

1. Solve the eigenvalue problem (with B.C.s)

$$\mathcal{L}\phi_n(x) = \lambda_n r(x)\phi_n(x)$$

because the set of the eigenfunctions are linearly independent and orthogonal.

2. Expand the Non-homogeneous term in series of the eigenfunctions.
3. Substitute the solution in the form

$$y = \sum_{n=1}^{\infty} a_n \phi_n(x)$$

4. Multiply by one (arbitrarily selected) ϕ_l ,

$$\int_a^b r(x)\phi_n(x)\phi_l(x) dx \neq 0, \quad \text{only for } n = l$$

5. The remaining equation is for a_l

6. the whole solution is now the infinite series

$$a_l = \frac{f_l}{\lambda_l - \mu} \quad (5.3.17)$$

if $\mu \neq \lambda_n$ for all n there is only one unique solution. If $\mu = \lambda_k$, which occurs only if $f_k = 0$, then there is not a unique solution. If we have a unique solution that is well behaved, we get,

$$y(x) = \sum_{n=1}^{\infty} \frac{\phi_n(x)}{\lambda_n - \mu} \int_a^b r(x)f(x)\phi_n(x) dx \quad (5.3.18)$$

$$= \int_a^b G(x, x')g(x') dx', \quad (5.3.19)$$

where $g(x) = r(x)f(x)$.

$$G(x, x') = \sum_{n=1}^{\infty} \frac{\phi_n(x)\phi_n(x')}{\lambda_n - \mu} \quad (5.3.20)$$

We have thus defined the Greens function for this problem.

Example of a Greens function problem

Let $y_n(x)$ is a set of EF for the Sturm–Liouville equation. Our function,

$$\frac{d}{dx} \left(f \frac{dy}{dx} \right) + \lambda w y = 0 \quad (5.3.21)$$

Show that $y'_n = u_n$ for certain boundary conditions. What are the boundary conditions?

We know there is a solution for the simpler Helmholtz equation,

$$\frac{d^2 y}{dx^2} + \lambda y = 0 \quad (5.3.22)$$

gives $\cos(\lambda x), \sin(\lambda x)$.

Now,

$$\frac{d}{dx} \left(f \frac{dy_m}{dx} \right) + \lambda w y_m = 0 \quad \times \left(\frac{y_n}{\lambda} \right) \quad (5.3.23)$$

$$\frac{d}{dx} \left(f \frac{dy_n}{dx} \right) + \lambda w y_n = 0 \quad \times \left(\frac{y_m}{\lambda} \right) \quad (5.3.24)$$

Subtracting the two equations,

$$\frac{y_n}{\lambda} \frac{d}{dx} \left(f \frac{dy_m}{dx} \right) + \frac{y_n}{\lambda} \lambda w y_m - \frac{y_m}{\lambda} \frac{d}{dx} \left(f \frac{dy_n}{dx} \right) - \frac{y_m}{\lambda} \lambda w y_n = 0 \quad (5.3.25)$$

the second terms cancel and,

$$\frac{y_n}{\lambda} \frac{d}{dx} \left(f \frac{dy_m}{dx} \right) - \frac{y_m}{\lambda} \frac{d}{dx} \left(f \frac{dy_n}{dx} \right) = 0 \quad (5.3.26)$$

$$\frac{y_n}{\lambda} \frac{d}{dx} \left(f \frac{dy'_m}{dx} \right) - \frac{y_m}{\lambda} \frac{d}{dx} \left(f \frac{dy'_n}{dx} \right) = 0 \quad (5.3.27)$$

integrating,

$$\int_a^b \left[\frac{y_n}{\lambda} \frac{d}{dx} (f y'_m) - \frac{y_m}{\lambda} \frac{d}{dx} (f y'_n) \right] dx = 0 \quad (5.3.28)$$

Integrating by parts,

$$\int_a^b \left[\frac{y_n}{\lambda} \frac{d}{dx} (f y'_m) - \frac{y_m}{\lambda} \frac{d}{dx} (f y'_n) \right] dx = f \left(\frac{y_n}{\lambda_m} y'_m - \frac{y_m}{\lambda_n} y'_n \right) \Big|_a^b - \left(\frac{1}{\lambda_m} - \frac{1}{\lambda_n} \right) \int_a^b f y'_n y'_m dx = 0 \quad (5.3.29)$$

$u_n = y'_n$ which are orthogonal if the last integral is 0. Returning to the first term,

$$f \left(\frac{y_n}{\lambda_m} y'_m - \frac{y_m}{\lambda_n} y'_n \right) \Big|_a^b \quad (5.3.30)$$

Now we have several cases,

1. $f(a) = f(b) = 0$, we get Legendre polynomials for the solution
2. $y(a) = y(b) = 0$, we have a trivial case
3. $y(a) = 0, y'(b) = 0$, we have a trivial case
4. $y'(a) = 0, y(b) = 0$, we have a trivial case
5. $y'(a) = 0, y'(b) = 0$, we have a trivial case

Example: Non-homogeneous Helmholtz equation

What is the Greens function for:

$$\frac{d^2 y}{dx^2} + y(x) = f(x) \quad (5.3.31)$$

1. Start with

$$\frac{d^2 y}{dx^2} + y(x) = 0 \quad (5.3.32)$$

$$y = \sum_{n=1}^{\infty} a_n \phi_n(x) \quad (5.3.33)$$

$$\frac{d^2 \phi_n}{dx^2} + \phi_n(x) = 0 \quad (5.3.34)$$

We get the solutions, then with $\cos(\sqrt{\lambda_n} x), \sin(\sqrt{\lambda_n} x)$.

Now say our boundary conditions are $\phi_n(0) = 0$ and $\phi'_n(1) = 0$. The first BC gives that the $\cos(\sqrt{\lambda_n} x)$ is not necessary. With the second boundary condition, we can now find values for λ_n

$$\left[\sin(\sqrt{\lambda_n} x) \right]' = \sqrt{\lambda_n} \cos(\sqrt{\lambda_n} x) \quad (5.3.35)$$

which shows from the boundary condition that,

$$\cos(\sqrt{\lambda_n} (1)) = 0 \quad (5.3.36)$$

Therefore,

$$\sqrt{\lambda_n} = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \dots \quad (5.3.37)$$

$$\sqrt{\lambda_n} = \frac{(2n-1)}{2} \pi, \quad n = 1, 2, 3, \dots \quad (5.3.38)$$

Our solution terms are thus expressed,

$$\sin\left(\frac{(2n-1)}{2}\pi x\right), \quad n = 1, 2, 3, \dots \quad (5.3.39)$$

for $\sqrt{N\phi}$

$$N\phi = \int_a^b \phi_n^2 dx = \int_0^1 \phi_n^2 dx \quad (5.3.40)$$

$$\begin{aligned} \int_0^1 \sin^2\left(\frac{(2n-1)}{2}\pi x\right) dx &= \frac{1}{2} + \frac{\cos(n\pi) \sin(n\pi)}{\pi(1-2n)} \\ &= \frac{1}{2}, \quad \text{for integer values of } n \end{aligned} \quad (5.3.41)$$

Thus the normalized eigenfunction is $\sqrt{2} \sin\left(\frac{(2n-1)}{2}\pi x\right)$.

We now can find our Greens function,

$$G(x, x') = \sum_{n=1}^{\infty} \frac{\phi_n(x)\phi_n(x')}{\lambda_n - \mu} \quad (5.3.42)$$

In this example $\mu = 1$, so we can fully express the function by,

$$G(x, x') = 2 \sum_{n=1}^{\infty} \frac{\sin\left(\frac{(2n-1)}{2}\pi x\right) \sin\left(\frac{(2n-1)}{2}\pi x'\right)}{\left(\frac{(2n-1)}{2}\pi\right)^2 - 1} \quad (5.3.43)$$

Therefore our solution is generally,

$$y(x) = 2 \int_0^1 \sum_{n=1}^{\infty} \frac{\sin\left(\frac{(2n-1)}{2}\pi x\right) \sin\left(\frac{(2n-1)}{2}\pi x'\right)}{\left(\frac{(2n-1)}{2}\pi\right)^2 - 1} f(x') dx' \quad (5.3.44)$$

UNIT 6

Chapter 15—Fourier Series

6.1 Lecture 16: October 15, 2012

An expanded series solution with,

$$\begin{aligned} &\sin\left(\sqrt{\lambda_n}x\right) \\ &\cos\left(\sqrt{\lambda_n}x\right) \end{aligned}$$

where we are solving,

$$\frac{d^2\phi_n}{dx^2} + \lambda_n\phi_n = 0 \quad (6.1.1)$$

This stems from using imaginary exponential basis functions, *e.g.* $e^{\pm\sqrt{\lambda_n}x}$ where we credit $\phi_n = e^{\alpha x}$ to Euler.

$$\alpha^2 e^{\alpha x} + \lambda_n e^{\alpha x} = 0 \quad (6.1.2)$$

$$\alpha^2 = -\lambda_n \quad (6.1.3)$$

$$\alpha = \pm i\sqrt{\lambda_n} \quad (6.1.4)$$

So we can represent the solution as,

$$C_1 e^{+i\sqrt{\lambda_n}x} + C_2 e^{-i\sqrt{\lambda_n}x} \quad (6.1.5)$$

$$2C_1 = 2C_2 = C \rightarrow \cos\left(\sqrt{\lambda_n}x\right) \quad (6.1.6)$$

$$C_1 = -2C_2 \rightarrow \sin\left(\sqrt{\lambda_n}x\right) \quad (6.1.7)$$

Case 1. Homogeneous boundary conditions

$$\phi_n(0) = \phi_n(L) = 0$$

Our system is simplified to $\sin(\sqrt{\lambda_n}x)$ because of the symmetry of the problem. *i.e.* from the first boundary condition

$$\sin(\sqrt{\lambda_n}0) = 0 \quad (6.1.8)$$

while the cosine cannot be zero. The first boundary condition gives which boundary conditions we will be using; the second value gives what we will actually do with it. So from $\phi_n(L) = 0$, we get

$$\lambda_n = \frac{n\pi}{L}, \quad n = 1, 2, 3, \dots \quad (6.1.9)$$

Our solution will now be of the form,

$$\phi(x) = \sum_{n=1}^{\infty} \phi_n(x) \quad (6.1.10)$$

$$= \sum_{n=1}^{\infty} C_n \sin\left(\frac{n\pi}{L}x\right) \quad (6.1.11)$$

So

$$\int_0^L \phi(x) \sin\left(\frac{n\pi}{L}x\right) dx = \sum_{n=1}^{\infty} C_n \int_0^L \sin\left(\frac{n\pi}{L}x\right) \sin\left(\frac{m\pi}{L}x\right) dx \quad (6.1.12)$$

by orthogonality the terms of the right hand side only matter for $m = n$. The integral on the right hand side can be simplified further by,

$$\int_0^L \sin^2\left(\frac{m\pi}{L}x\right) dx = \frac{L}{2} \left(1 - \frac{\sin(2m\pi)}{2m\phi}\right)$$

But with m being integer values this simplifies to,

$$\int_0^L \sin^2\left(\frac{m\pi}{L}x\right) dx = \frac{L}{2} \quad (6.1.13)$$

Case 2. Newman boundary conditions

$$\phi'(0) = \phi'(L) = 0$$

In this case, we apply the first boundary condition and we find that the $\cos(x)$ function satisfies the boundary conditions correctly. Thus, we will have the *cosine* function as our basis function.

$$\begin{aligned} \int_0^L \cos^2\left(\frac{m\pi}{L}x\right) dx &= \frac{L}{2} \left(1 + \frac{\sin(2m\pi)}{2m\phi}\right) \\ &= \frac{L}{2} \end{aligned} \quad (6.1.14)$$

$$\phi_n = \sqrt{\frac{L}{2}} \cos\left(\frac{n\pi}{L}x\right) \quad (6.1.15)$$

$$\phi_n(-L) = \phi_n(L) \quad (6.1.16)$$

$$\phi'_n(-L) = \phi'_n(L) \quad (6.1.17)$$

Note: you may solve a problem by exponential series directly, however you will find that the exponentials will have imaginary terms again and may look similar to,

$$\frac{e^{i\frac{n\pi}{L}x} - e^{-i\frac{n\pi}{L}x}}{2i} = \sin\left(\frac{n\pi}{L}x\right)$$

or

$$\frac{e^{i\frac{n\pi}{L}x} + e^{-i\frac{n\pi}{L}x}}{2i} = \cos\left(\frac{n\pi}{L}x\right)$$

$$\sqrt{\lambda_n} = \frac{n\pi}{L}$$

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[a_n \cos\left(\frac{n\pi}{L}x\right) + b_n \sin\left(\frac{n\pi}{L}x\right) \right] \quad (6.1.18)$$

the first term comes from the zeroth-order term in the cosine expansion.

$$a_0 = \frac{1}{L} \int_{-L}^L f(x) dx \quad (6.1.19)$$

observe that if $f(x) = 1$, then $a_0 = 2$.

Example using Dirac Delta function

Note that $e^{i\pi} = \cos(\pi) + i \sin(\pi)$ and $i \ln(i) = \frac{\pi}{2}$

$$f(x) = \sum_{n=-\infty}^{\infty} C_n e^{i\frac{n\pi}{L}x} \quad (6.1.20)$$

multiplying by $e^{i\frac{k\pi}{L}x}$,

$$\begin{aligned} & \int_{-L}^L f(x) e^{-i\frac{k\pi}{L}x} dx \\ & \int_{-L}^L f(x) e^{-i\frac{k\pi}{L}x} dx \\ & \int_{-L}^L f(x) e^{-i\frac{(n-k)\pi}{L}x} dx = 2L \frac{\sin((n-k)\pi)}{(n-k)\pi} \end{aligned} \quad (6.1.21)$$

This turns out to be the Kronecker delta, because $\lim_{x \rightarrow 0} \frac{\sin(x)}{x} = \lim_{x \rightarrow 0} \frac{\cos(x)}{1} = 1$

$$C_k = \frac{1}{2L} \int_{-L}^L f(x) e^{-i\frac{k\pi}{L}x} dx \quad (6.1.22)$$

Now if we do the delta function,

$$C_k = \frac{1}{2L} \int_{-L}^L \delta(x) e^{-i\frac{k\pi}{L}x} dx = \frac{1}{2L} \quad (6.1.23)$$

as it is constant for any C_k we have, in fact, shown the production of white noise. This is similar for any “delta-correlated” function, *e.g.*

$$C_k = \frac{1}{2L} \int_{-L}^L \delta(x) f(x) e^{-i\frac{k\pi}{L}x} dx = f(0) \quad (6.1.24)$$

There are three common classes; even, odd, and neither (or mixed). These are defined by,

- Even, $f(-x) = f(x)$
- Odd, $f(-x) = -f(x)$

As cosines are even and sines are odd, we find that this can be used to simplify the solution system. The Dirac delta function is an even function. If you have an even function, then

$$\int_{-L}^L f_e(x) dx = 2 \int_0^L f_e(x) dx \quad (6.1.25)$$

for odd functions,

$$\int_{-L}^L f_o(x) dx = 0 \quad (6.1.26)$$

for function expansions,

$$\int_{-L}^L f_e(x) \cos\left(\frac{n\pi}{L}x\right) dx = 2 \int_0^L f_e(x) \cos\left(\frac{n\pi}{L}x\right) dx \quad (6.1.27)$$

However, we have an interesting phenomena where

$$\int_{-L}^L f_o(x) \sin\left(\frac{n\pi}{L}x\right) dx = 2 \int_0^L f_o(x) \sin\left(\frac{n\pi}{L}x\right) dx \quad (6.1.28)$$

because the negatives cancel out. Mixing the systems

$$\int_{-L}^L f_o(x) \cos\left(\frac{n\pi}{L}x\right) dx = 0 \quad (6.1.29)$$

and

$$\int_{-L}^L f_e(x) \sin\left(\frac{n\pi}{L}x\right) dx = 0. \quad (6.1.30)$$

Returning to the sine and cosine expansion,

$$a_n = \frac{1}{L} \int_{-L}^L f(x) \cos\left(\frac{n\pi}{L}x\right) dx \quad (6.1.31)$$

$$b_n = \frac{1}{L} \int_{-L}^L f(x) \sin\left(\frac{n\pi}{L}x\right) dx \quad (6.1.32)$$

If $f(x)$ is odd, $a_n = 0$ and if $f(x)$ is even, $b_n = 0$.

We want the series to be convergent. So we know the Bessel inequality,

$$\frac{1}{L} \int_{-L}^L f^2(x) dx \geq \frac{a_0^2}{2} + \sum_{n=1}^{\infty} (a_n^2 + b_n^2) \quad (6.1.33)$$

one example of a divergent integral is given by setting $f(x) = \frac{1}{x}$

6.2 Lecture 17: October 17, 2012

“A big part of math problems is that you get trained to recognize patterns.” —Dr. Petsev

Newton’s Equation of Gravitational Motion

The solution of the second problem of the second homework is as follows; in the x -direction

$$m \frac{d^2x}{dt^2} = -\frac{kx}{(x^2 + y^2)^{3/2}} \quad (6.2.1a)$$

in the y -direction,

$$m \frac{d^2y}{dt^2} = -\frac{ky}{(x^2 + y^2)^{3/2}} \quad (6.2.1b)$$

To transform to polar coordinates,

$$x = r \cos(\theta), \quad (6.2.2a)$$

$$y = r \sin(\theta). \quad (6.2.2b)$$

We also know $r^2 = x^2 + y^2$ and $\theta = \arctan\left(\frac{y}{x}\right)$. Now substituting directly into the system, for the right hand side

$$-\frac{kx}{(x^2 + y^2)^{3/2}} = -\frac{kr \cos(\theta)}{(r^2)^{3/2}} = -\frac{k \cos(\theta)}{r^2}, \quad (6.2.3a)$$

$$-\frac{ky}{(x^2 + y^2)^{3/2}} = -\frac{kr \sin(\theta)}{(r^2)^{3/2}} = -\frac{k \sin(\theta)}{r^2}. \quad (6.2.3b)$$

Now, the left hand sides may also be substituted,

$$m \frac{d^2r \cos(\theta)}{dt^2} = -\frac{k \cos(\theta)}{r^2}, \quad (6.2.4a)$$

$$m \frac{d^2r \sin(\theta)}{dt^2} = -\frac{k \sin(\theta)}{r^2}. \quad (6.2.4b)$$

Expanding the LHS of the x ,

$$\cos(\theta) \frac{d^2r}{dt^2} - 2 \sin(\theta) \frac{d\theta}{dt} \frac{dr}{dt} - r \cos(\theta) \left(\frac{d\theta}{dt}\right)^2 - r \sin(\theta) \frac{d^2\theta}{dt^2} = -\frac{k \cos(\theta)}{m r^2}, \quad (6.2.5a)$$

$$\sin(\theta) \frac{d^2r}{dt^2} + 2 \cos(\theta) \frac{d\theta}{dt} \frac{dr}{dt} - r \sin(\theta) \left(\frac{d\theta}{dt}\right)^2 + r \cos(\theta) \frac{d^2\theta}{dt^2} = -\frac{k \sin(\theta)}{m r^2}. \quad (6.2.5b)$$

Multiplying the first by $\cos(\theta)$ and the second by $\sin(\theta)$, we find by adding the two

$$(\cos^2(\theta) + \sin^2(\theta)) \frac{d^2r}{dt^2} - (\cos^2(\theta) + \sin^2(\theta)) r \left(\frac{d\theta}{dt}\right)^2 = -\frac{k \cos^2(\theta) + \sin^2(\theta)}{m r^2}. \quad (6.2.6)$$

So we have our solution for the radial coordinate,

$$\boxed{\frac{d^2r}{dt^2} - r \left(\frac{d\theta}{dt} \right)^2 = -\frac{k}{m} \frac{1}{r^2}}. \quad (6.2.7)$$

Now doing essentially the opposite, we multiply the first by $\sin(\theta)$ and the second by $\cos(\theta)$ and then subtracting the two,

$$-2(\cos^2(\theta) + \sin^2(\theta)) \frac{d\theta}{dt} \frac{dr}{dt} - r(\cos^2(\theta) + \sin^2(\theta)) \frac{d^2\theta}{dt^2} = 0, \quad (6.2.8a)$$

$$-2 \frac{d\theta}{dt} \frac{dr}{dt} - r \frac{d^2\theta}{dt^2} = 0; \quad (6.2.8b)$$

which may also be expressed by,

$$\boxed{\frac{1}{r} \frac{d}{dt} \left(mr^2 \frac{d\theta}{dt} \right) = 0}. \quad (6.2.8c)$$

Elliptic Coordinates

Reviewing the first problem in the second homework,

$$x = a \cosh(\eta) \cos(\psi), \quad (6.2.9a)$$

$$y = a \sinh(\eta) \sin(\psi). \quad (6.2.9b)$$

part (d) was a little more trouble, $\nabla \cdot \mathbf{A}$. So we need to find the metric coefficients,

$$h_\eta = \left[\left(\frac{\partial x}{\partial \eta} \right)^2 + \left(\frac{\partial y}{\partial \eta} \right)^2 \right]^{1/2} = a \sqrt{\cosh^2(\eta) \sin^2(\psi) + \cos^2(\psi) \sinh^2(\eta)}, \quad (6.2.10a)$$

$$h_\psi = \left[\left(\frac{\partial x}{\partial \psi} \right)^2 + \left(\frac{\partial y}{\partial \psi} \right)^2 \right]^{1/2} = a \sqrt{\cosh^2(\eta) \sin^2(\psi) + \cos^2(\psi) \sinh^2(\eta)}, \quad (6.2.10b)$$

and we find,

$$h_\eta = h_\psi. \quad (6.2.10c)$$

This further may be simplified to,

$$h_\eta = h_\psi = a (\cosh^2(\eta) - \cos^2(\psi))^{1/2}. \quad (6.2.11)$$

Now returning to the divergence,

$$\nabla \cdot \mathbf{A} = \frac{1}{h_\eta h_\psi} \left[\frac{\partial(h_\psi A_\eta)}{\partial \eta} + \frac{\partial(h_\eta A_\psi)}{\partial \psi} \right]. \quad (6.2.12)$$

The laplacian is,

$$\nabla^2 f = \frac{1}{h_\eta h_\psi} \left[\frac{\partial}{\partial \eta} \left(\frac{h_\psi}{h_\eta} \frac{\partial A_\eta}{\partial \eta} \right) + \frac{\partial}{\partial \psi} \left(\frac{h_\eta}{h_\psi} \frac{\partial A_\psi}{\partial \psi} \right) \right]. \quad (6.2.13)$$

Fourier Series Solution of Non-homogeneous Ordinary Differential Equations

A simple second order linear differential equation,

$$y''(x) + y(x) = f(x), \quad (6.2.14)$$

where we have the linear operator $\mathcal{L} = \frac{d^2}{dx^2} + 1$, which has eigenfunctions in terms of $\sin(x)$ and $\cos(x)$. So we expand the right hand side,

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(\frac{n\pi}{L}x\right) + \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi}{L}x\right) \quad (6.2.15)$$

with our solution,

$$y(x) = \frac{A_0}{2} + \sum_{n=1}^{\infty} A_n \cos\left(\frac{n\pi}{L}x\right) + \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi}{L}x\right). \quad (6.2.16)$$

Thus the left hand side can be expanded as well and set equal to the right hand side. This gives,

$$\begin{aligned} \frac{A_0}{2} + \sum_{n=1}^{\infty} \left[A_n \left(1 - \frac{n^2\pi^2}{L^2}\right) \cos\left(\frac{n\pi}{L}x\right) + B_n \left(1 - \frac{n^2\pi^2}{L^2}\right) \sin\left(\frac{n\pi}{L}x\right) \right] &= \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(\frac{n\pi}{L}x\right) \\ &+ \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi}{L}x\right). \end{aligned}$$

We find that our coefficients are simply,

$$A_n = \frac{a_n L^2}{L^2 - n^2\pi^2}, \quad (6.2.17a)$$

$$B_n = \frac{b_n L^2}{L^2 - n^2\pi^2}. \quad (6.2.17b)$$

With our boundary conditions of $y(x=0) = y(x=L) = 0$, we know that we do not need the cosine terms because those functions have the correct symmetry,

$$y(x) = \sum_{n=1}^{\infty} \frac{b_n L^2}{L^2 - n^2\pi^2} \sin\left(\frac{n\pi}{L}x\right). \quad (6.2.18)$$

Integrating and multiplying with sine on both sides,

$$\int_0^L f(x) \sin\left(\frac{n\pi}{L}x\right) dx = b_m \frac{L^2}{L^2 - n^2\pi^2} \int_0^L \sin^2\left(\frac{n\pi}{L}x\right) dx. \quad (6.2.19)$$

The integral on the right hand side is simplified

$$\int_0^L \sin^2\left(\frac{n\pi}{L}x\right) dx = L \left[\frac{1 - \cos(m\pi)}{m\pi} \right] \quad (6.2.20)$$

where m is an integer. So we can simplify the system, $m = 1$ gives $\frac{2}{\pi}$, $m = 2$ gives 0, $m = 3$ gives $\frac{1}{3}\frac{2}{\pi}$. Then

$$\frac{1 - \cos(m\pi)}{m\pi} = \frac{[1 + (-1)^{m+1}]}{m\pi}. \quad (6.2.21)$$

Example: Wave equation

A general oscillator with the friction term, $\gamma \frac{dx}{dt}$, and source term, $F(x)$,

$$m \frac{d^2x}{dt^2} + \gamma \frac{dx}{dt} + kx = F(x). \quad (6.2.22)$$

We know from the system symmetry that the eigenfunctions are $\sin\left(\frac{2(n-1)\pi t}{t_0}\right)$, $n = 1, 2, 3, \dots$

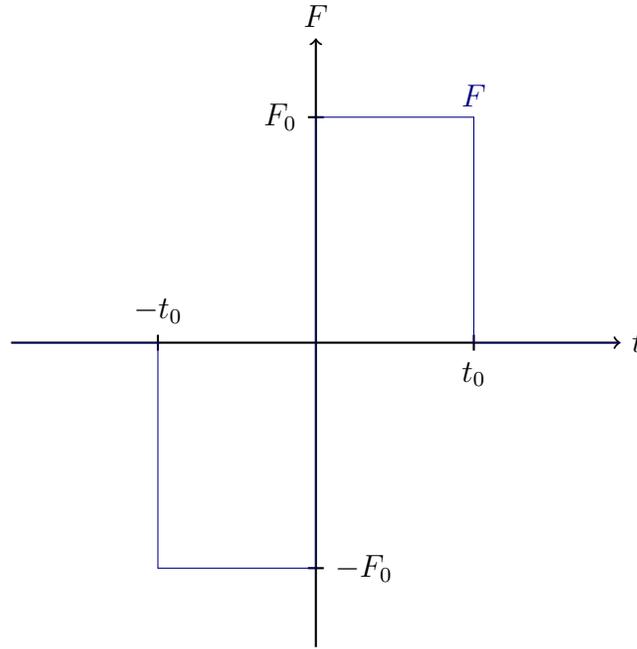


Figure 6.1. Forcing function

So we may manipulate the equation forms,

$$\begin{aligned} \int_{-t_0}^{t_0} F(t) \sin\left(\frac{2(n-1)\pi}{t_0}t\right) dt &= \int_{-t_0}^0 F(t) \sin\left(\frac{2(n-1)\pi}{t_0}t\right) dt + \int_0^{t_0} F(t) \sin\left(\frac{2(n-1)\pi}{t_0}t\right) dt \\ &= -F_0 \int_{-t_0}^0 \sin\left(\frac{2(n-1)\pi}{t_0}t\right) dt + F_0 \int_0^{t_0} \sin\left(\frac{2(n-1)\pi}{t_0}t\right) dt \\ &= 2F_0 \int_0^{t_0} \sin\left(\frac{2(n-1)\pi}{t_0}t\right) dt. \end{aligned} \quad (6.2.23)$$

For the integrals on the right hand side of the equation,

$$\frac{2 \cos^2(n\pi)}{\pi (2n-1)} + \frac{2 \cos^2(n\pi)}{\pi (2n-1)} = \frac{4}{\pi} \frac{1}{(2n-1)}. \quad (6.2.24)$$

Integrating the left hand side of the equation,

$$F_n(t) = \frac{4}{\pi} \frac{1}{(2n-1)} \sin\left(\frac{2(n-1)\pi}{t_0}t\right). \quad (6.2.25)$$

Now we may substitute back into the original differential equation,

$$m \frac{d^2 x_n}{dt^2} + \gamma \frac{dx_n}{dt} + kx_n = \frac{4}{\pi} \frac{1}{(2n-1)} \sin\left(\frac{2(n-1)\pi}{t_0} t\right). \quad (6.2.26)$$

Clearly this matches well with solutions of the form,

$$x_n = e^{-\frac{\gamma t}{2m}} (C_1 \sin(\Omega t) + C_2 \cos(\Omega t)) + C_n [\sin(\omega_n t + \phi_n)], \quad (6.2.27)$$

where $\Omega = \frac{(4km-\gamma)^{1/2}}{2m}$ and $\psi_n = \text{const.}$ For the solution,

$$\frac{-b_m m [\gamma \omega_n \cos(\omega_n t) + (\omega^2 m - k) \sin(\omega_n t)]}{k^2 - 2k\omega_n^2 m + \gamma^2 m - \omega_n^4 m^2} = C_n. \quad (6.2.28)$$

Now,

$$\sin(\omega_n t + \phi_n) = \sin(\omega_n t) \cos(\phi_n) + \cos(\omega_n t) \sin(\phi_n), \quad (6.2.29)$$

$$= \gamma \omega_n \cos(\omega_n t) + (\omega^2 m - k) \sin(\omega_n t), \quad (6.2.30)$$

because

$$\sin(\phi_n) = \gamma \omega_n, \quad (6.2.31a)$$

$$\cos(\phi_n) = (\omega_n^2 m - k); \quad (6.2.31b)$$

$$\tan(\phi_n) = \frac{\gamma \omega_n}{(\omega_n^2 m - k)}. \quad (6.2.31c)$$

Thus,

$$\phi_n = \arctan\left(\frac{\gamma \omega_n}{\omega_n^2 m - k}\right), \quad (6.2.32)$$

and

$$\omega_n = \frac{(2n-1)\pi}{t_0}; \quad (6.2.33)$$

where our terms,

$$C_n = (\omega_n t + \phi_n). \quad (6.2.34)$$

UNIT 7

Chapter 16—Partial Differential Equations

7.1 Lecture 18: October 22, 2012

Now we may have functions of several variables, *e.g.* $F(x, t)$, or $F(x, y, z, t)$. There are multiple classes of PDEs,

1. Homogeneous or Non-homogeneous
2. Linear and Nonlinear
3. Constant or variable coefficients

1. Elliptic PDEs

Two major examples include the Laplace and Poisson equations;

$$\nabla^2 F = 0, \tag{7.1.1}$$

and

$$\nabla^2 F = f(x, y, z). \tag{7.1.2}$$

In three dimensions the Laplacian operator is,

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}. \tag{7.1.3}$$

Helmholtz equation is another common example,

$$\nabla^2 F + \kappa^2 F = 0. \tag{7.1.4}$$

This system often describes the steady-state nature of some systems.

2. Hyperbolic PDEs

One very notable hyperbolic equation is the wave equation

$$\nabla^2 F = \frac{1}{\alpha^2} \frac{\partial^2 F}{\partial t^2} \tag{7.1.5}$$

This type of system is least common in chemical and nuclear engineering.

3. Parabolic PDEs

These are often mixed form equations such as,

$$a\nabla^2 F = \frac{\partial F}{\partial t}. \quad (7.1.6)$$

This category is very commonly used in our disciplines.

- Heat Transfer (Energy)
- Diffusion (Mass Transfer)
- Fluid flow (Viscosity)
- Schrodinger's Equation (Electron Structure)

Initial and Boundary Conditions

Need to have the boundary and initial conditions to complete the problem. The nature of a PDE is that it is only the description of the physical variable balance around a particle. This however needs to be further specified by the values at the edges of our solution space.

Example: Oscillating String

Assuming small amplitude for the string oscillation, considering only oscillates in one direction. Observing two nearby points, P and Q, on the string, we have angles α and β to give the projection onto x . $\tau_1 \cos \alpha = \tau_2 \cos \beta$, $\tau_2 \sin \beta - \tau_1 \sin \alpha = \text{net tension}$.

$$\tau_2 \sin \beta - \tau_1 \sin \alpha = m\mathbf{a} \quad (7.1.7)$$

$$\rho\Delta x = m \quad (7.1.8)$$

$$\tau_2 \sin \beta - \tau_1 \sin \alpha = m\mathbf{a} \quad (7.1.9)$$

$$m\mathbf{a} = \rho\Delta x \frac{\partial^2 u}{\partial t^2} \quad (7.1.10)$$

$$\tau_2 \sin \beta - \tau_1 \sin \alpha = \rho\Delta x \frac{\partial^2 u}{\partial t^2} \quad (7.1.11)$$

$$\tan \alpha = \frac{\Delta u}{\Delta x} = \left. \frac{\partial u}{\partial x} \right|_x \quad (7.1.12)$$

$$\tan \beta = \frac{\Delta u}{\Delta x} = \left. \frac{\partial u}{\partial x} \right|_{x+\Delta x} \quad (7.1.13)$$

$$\left. \frac{\partial u}{\partial x} \right|_{x+\Delta x} - \left. \frac{\partial u}{\partial x} \right|_x = \frac{\rho\Delta x}{\tau} \frac{\partial^2 u}{\partial t^2} \quad (7.1.14)$$

$$\frac{\frac{\partial u}{\partial x}|_{x+\Delta x} - \frac{\partial u}{\partial x}|_x}{\Delta} = \frac{\partial^2 u}{\partial x^2} = \frac{\rho}{\tau} \frac{\partial^2 u}{\partial t^2} \quad (7.1.15)$$

for $\tau/\rho = v^2$,

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 u}{\partial t^2} \quad (7.1.16)$$

Now we have boundary conditions, $u(0, t) = u(L, t) = 0$, and initial conditions, $u(x, 0) = f(x)$ and $u_t(x, 0) = g(x)$.

Solution with separation of variables

$$u(x, t) = X(x)T(t) \quad (7.1.17)$$

Substituting into the main equation we get the equation,

$$T \frac{d^2 X}{dx^2} = \frac{1}{v^2} X \frac{d^2 T}{dt^2} \quad (7.1.18)$$

Dividing by XT , we simplify to,

$$\frac{v^2}{X} \frac{d^2 X}{dx^2} = \frac{1}{T} \frac{d^2 T}{dt^2} = -\omega^2 \quad (7.1.19)$$

Now splitting into two equations,

$$\frac{v^2}{X} \frac{d^2 X}{dx^2} = -\omega^2 \quad (7.1.20)$$

and

$$\frac{1}{T} \frac{d^2 T}{dt^2} = -\omega^2 \quad (7.1.21)$$

These equations are of the Helmholtz type, with solutions of sin, cos. So, $\frac{d^2 T}{dt^2} + \omega^2 T = 0$. Then the solutions are, $T(t) = A \sin(\omega t) + B \cos(\omega t)$. For the x directions we have similarly that, $\frac{d^2 X}{dx^2} + \kappa^2 X = 0$ where $k^2 = \text{enable } \kappa^2 = \frac{\omega^2}{v^2}$. This also gives solution,

$$X(x) = C \sin(kx) = C \sin(vx) + D \cos(\kappa x) \quad (7.1.22)$$

$$X_n(x) = C_n \sin\left(\frac{n\pi}{L} x\right) \quad (7.1.23)$$

$$\int_0^L X_n X_n dx = \sqrt{\frac{2}{L}} \quad (7.1.24)$$

$$X_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right) \quad (7.1.25)$$

$$k = \frac{\omega}{v} = \frac{2\pi}{\lambda_n} \quad (7.1.26)$$

$$u_n = [A_n \sin(\omega_n t) + B_n \cos(\omega_n t)] \sin\left(\frac{n\pi}{L}x\right) \sqrt{\frac{2}{L}} \quad (7.1.27)$$

$$\lambda_n = \frac{2L}{n}, \quad n = 1, 2, 3, \dots \quad (7.1.28)$$

$$u(x, 0) = \sum_{n=1}^{\infty} B_n X_n(x) \quad (7.1.29)$$

Now multiplying by X_m ,

$$\int_0^L f(x) X_m(x) dx = \sum_{n=1}^{\infty} B_n \int_0^L X_m(x) X_n(x) dx, \quad (7.1.30)$$

$$= \sum_{n=1}^{\infty} B_n \delta_{nm}, \quad (7.1.31)$$

$$= B_m. \quad (7.1.32)$$

Thus,

$$B_m = \int_0^L f(x) X_m(x) dx \quad (7.1.33)$$

For the second conditions with the derivative of u

$$u_t(x, 0) = g(x) = \sum_{n=1}^{\infty} \omega_n A_n X_n(x) \quad (7.1.34)$$

$$A_m = \frac{1}{\omega_n} \int_0^L g(x) X_m dx \quad (7.1.35)$$

Our final solution,

$$u(x, t) = \sum_{n=1}^{\infty} \left\{ \left[\frac{1}{\omega_n} \int_0^L g(x) X_m dx \right] \sin(\omega_n t) + \left[\int_0^L f(x) X_m(x) dx \right] \cos(\omega_n t) \right\} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) \quad (7.1.36)$$

Now for example we can say $f(x) = 2 \sin\left(\frac{\pi}{2}x\right)$ and $g(x) = x^2$, we get

$$B_n = \int \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) 2 \sin\left(\frac{\pi}{2}x\right) dx \quad (7.1.37)$$

$$= \frac{8\sqrt{2L} \sin(L\pi/2)}{\pi(L^2 - 4n^2)} \quad (7.1.38)$$

$$A_n = \frac{1}{\omega_n} \int_0^L x^2 \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) dx \quad (7.1.39)$$

$$= \frac{1}{\omega_n} \frac{\sqrt{2L^5} [(2 - n^2\pi^2) \cos(n\pi) - 2]}{n^3\pi^3} \quad (7.1.40)$$

7.2 Lecture 19: October 24, 2012

Example: Membrane vibration in cylindrical coordinates

Say we have an $a \times b$ in x and y rectangular membrane, we see the system is described by

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} = 0. \quad (7.2.1)$$

Boundary conditions (homogeneous) $u(\text{boundaries}, t) = 0$, where the boundaries are, $x = 0, x = a, y = 0, y = b$. Our initial conditions are

$$u(x, y, t=0) = S(x, y), \quad (7.2.2a)$$

$$u'(x, y, t=0) = V(x, y); \quad (7.2.2b)$$

where $S(x, y)$ and $V(x, y)$ are known. We have a limited system so we want to look for a solution using separation of variables, or

$$U(x, y, t) = X(x)Y(y)T(t). \quad (7.2.3)$$

Substituting this form,

$$Y(y)T(t) \frac{d^2 X(x)}{dx^2} + X(x)T(t) \frac{d^2 Y(y)}{dy^2} - \frac{1}{c^2} X(x)Y(y) \frac{d^2 T(t)}{dt^2} = 0. \quad (7.2.4)$$

Dividing the equation by $X(x)Y(y)T(t)$ and rearranging,

$$\frac{1}{X(x)} \frac{d^2 X(x)}{dx^2} + \frac{1}{Y(y)} \frac{d^2 Y(y)}{dy^2} = \frac{1}{c^2} \frac{1}{T(t)} \frac{d^2 T(t)}{dt^2} = -\alpha^2 \quad (7.2.5)$$

where we have set it equal to a constant.

Focussing on the time component,

$$\frac{d^2 T(t)}{dt^2} + \alpha^2 c^2 T(t) = 0, \quad (7.2.6)$$

or in a more standard form

$$\frac{d^2 T(t)}{dt^2} + \omega^2 T(t) = 0, \quad \text{where } \omega^2 = \alpha^2 c^2. \quad (7.2.7)$$

We again know the form of the solution to this equation is,

$$T(t) = A \sin(\omega t) + B \cos(\omega t). \quad (7.2.8)$$

Now returning to our spacial system,

$$\frac{1}{X(x)} \frac{d^2 X(x)}{dx^2} + \frac{1}{Y(y)} \frac{d^2 Y(y)}{dy^2} = -\alpha^2 \quad (7.2.9)$$

say, each of the terms are also constants,

$$\frac{1}{X(x)} \frac{d^2 X(x)}{dx^2} = -p^2, \quad (7.2.10a)$$

$$\frac{1}{Y(y)} \frac{d^2 Y(y)}{dy^2} = -q^2, \quad (7.2.10b)$$

with $p^2 + q^2 = \alpha^2$. So we now have reduced our solutions to the following ordinary differential equations,

$$\frac{d^2 X(x)}{dx^2} + p^2 X(x) = 0, \quad (7.2.11a)$$

$$\frac{d^2 Y(y)}{dy^2} + q^2 Y(y) = 0. \quad (7.2.11b)$$

From the boundary conditions, we know that we can reduce the solutions in x and in y to the eigenvalue problem

$$X_n(x) = \sin(px), \quad (7.2.12a)$$

$$Y_n(y) = \sin(qy), \quad (7.2.12b)$$

with $p = \frac{n\pi}{a}$ and $q = \frac{m\pi}{b}$. This gives $\alpha_{nm} = \sqrt{\frac{n^2}{a^2} + \frac{m^2}{b^2}}$ or $\omega = c\pi \sqrt{\frac{n^2}{a^2} + \frac{m^2}{b^2}}$. Now we have the form of the solution,

$$u(x, y, t) = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} u_n(x, y, t) \quad (7.2.13)$$

$$= \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} [A_{nm} \sin(\omega_{nm}t) + B_{nm} \cos(\omega_{nm}t)] \sin\left(\frac{n\pi}{a}x\right) \sin\left(\frac{m\pi}{b}y\right) \quad (7.2.14)$$

Expanding our initial condition,

$$S(x, y) = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} B_{nm} \sin\left(\frac{n\pi}{a}x\right) \sin\left(\frac{m\pi}{b}y\right) \quad (7.2.15)$$

using orthogonality we can solve the coefficients, B_{nm} . So multiplying by $\sin\left(\frac{p'\pi}{a}x\right) \sin\left(\frac{q'\pi}{b}y\right)$, with p' and q' being index integers (not related to p and q above). We have a double integration,

$$\text{LHS} = \int_0^a \int_0^b S(x, y) \sin\left(\frac{p'\pi}{a}x\right) \sin\left(\frac{q'\pi}{b}y\right) dy dx \quad (7.2.16)$$

$$\text{RHS} = B_{p'q'} \int_0^a \int_0^b \sin^2\left(\frac{p'\pi}{a}x\right) \sin^2\left(\frac{q'\pi}{b}y\right) dy dx \quad (7.2.17)$$

we know,

$$\int_0^a \sin^2\left(\frac{p'\pi}{a}x\right) dx = \frac{a}{2} - \frac{\sin(2p'\pi)}{4p'\pi} = \frac{a}{2}, \quad \text{for integers, } p'$$

and similarly

$$\int_0^b \sin^2\left(\frac{q'\pi}{b}y\right) dy = \frac{b}{2} - \frac{\sin(2q'\pi)}{4q'\pi} = \frac{b}{2}$$

This greatly simplifies the right hand side. We thus have an expression,

$$B_{p'q'} = \frac{2}{a} \frac{2}{b} \int_0^a \int_0^b S(x, y) \sin\left(\frac{p'\pi}{a}x\right) \sin\left(\frac{q'\pi}{b}y\right) dy dx \quad (7.2.18)$$

We finally only have to find the A_{nm} coefficients. This follows the same methodology as before, with,

$$V(x, y) = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} (A_{nm}\omega_{nm} \cos(\omega_{nm}t) + B_{nm}\omega_{nm} \sin(\omega_{nm}t)) \sin\left(\frac{n\pi}{a}x\right) \sin\left(\frac{m\pi}{b}y\right) \quad (7.2.19)$$

but the B_{nm} term goes away because of the sin term, so

$$V(x, y) = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} A_{nm}\omega_{nm} \cos(\omega_{nm}t) \sin\left(\frac{n\pi}{a}x\right) \sin\left(\frac{m\pi}{b}y\right) \quad (7.2.20)$$

This gives the very similar result of,

$$A_{p'q'} = \frac{4}{ab\omega_{p'q'}} \int_0^a \int_0^b V(x, y) \sin\left(\frac{p'\pi}{a}x\right) \sin\left(\frac{q'\pi}{b}y\right) dy dx \quad (7.2.21)$$

Thus, we have solved the problem when we simply substitute our coefficients into the full expression of the solution.

If we had a slightly simpler problem, where $a = b$ and cylindrical coordinates, we would have a greater symmetry to the problem and our differential equation would be able to be written

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right) - \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} = 0 \quad (7.2.22)$$

This classic problem is discussed in the textbook and is solved by Bessel functions.

Maxwell Equations and Propagation of Electromagnetic Waves

The Maxwell equations state, the electrical field is conservative,

$$\nabla \cdot \mathbf{E} = 0 \quad (7.2.23)$$

the magnetic field is conservative as well,

$$\nabla \cdot \mathbf{B} = 0 \quad (7.2.24)$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad (7.2.25)$$

and the rotation of the magnetic field is related to the electric field,

$$\nabla \times \mathbf{B} = \varepsilon_0 \mu_0 \frac{\partial \mathbf{E}}{\partial t} \quad (7.2.26)$$

We have defined, \mathbf{E} as the electric field, \mathbf{B} is the magnetic field. The dielectric permittivity is ε_0 and the magnetic permeability is μ_0 . The speed of light is $\varepsilon_0 \mu_0 = \frac{1}{c^2}$.

$$-\nabla \phi = \mathbf{E} \quad (7.2.27)$$

and ρ_r is the charge density.

So from taking the curl the third Maxwell equation,

$$\nabla \times \nabla \times \mathbf{E} = -\nabla \times \frac{\partial \mathbf{B}}{\partial t} = -\frac{\partial}{\partial t}(\nabla \times \mathbf{B}) = -\varepsilon_0 \mu_0 \frac{\partial^2 \mathbf{E}}{\partial t^2}, \quad (7.2.28)$$

since

$$-\frac{\partial}{\partial t}(\nabla \times \mathbf{B}) = -\varepsilon_0 \mu_0 \frac{\partial^2 \mathbf{E}}{\partial t^2}. \quad (7.2.29)$$

Thus,

$$\nabla \times \nabla \times \mathbf{E} = -\varepsilon_0 \mu_0 \frac{\partial^2 \mathbf{E}}{\partial t^2}, \quad (7.2.30)$$

$$\nabla \times \nabla \times \mathbf{E} = \nabla(\nabla \cdot \mathbf{E}) - \nabla \cdot (\nabla \mathbf{E}), \quad (7.2.31)$$

because, in general

$$\mathbf{A} \times \mathbf{B} \times \mathbf{C} = \mathbf{B}(\mathbf{A} \cdot \mathbf{C}) - (\mathbf{A} \cdot \mathbf{C})\mathbf{B}. \quad (7.2.32)$$

We know,

$$\nabla \cdot \mathbf{E} = 0. \quad (7.2.33)$$

So, we now have an equation similar to the wave equation, where

$$\boxed{\nabla^2 \mathbf{E} = \varepsilon_0 \mu_0 \frac{\partial^2 \mathbf{E}}{\partial t^2}}. \quad (7.2.34)$$

Now,

$$\nabla \cdot \mathbf{E} = \frac{\rho_e}{\varepsilon_0} \quad (7.2.35)$$

$$\nabla \times \mathbf{B} - \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} = \mu_0 \mathbf{J} \quad (7.2.36)$$

where

$$\mathbf{B} = \nabla \times \mathbf{A} \quad (7.2.37)$$

is the definition of \mathbf{A} .

$$-\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \frac{\partial \mathbf{A}}{\partial t} \quad (7.2.38)$$

$$\nabla \times \left(\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} \right) = \nabla \times (\mu_0 \mathbf{J}) \quad (7.2.39)$$

since $\nabla \times \mathbf{J} = 0$, we simplify to

$$\nabla \times \left(\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} \right) = 0 \quad (7.2.40)$$

Calling,

$$-\nabla \phi = \mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} \quad (7.2.41)$$

rearranging,

$$\nabla \cdot \mathbf{E} = -\nabla^2 \phi - \frac{\partial}{\partial t}(\nabla \cdot \mathbf{A}) \quad (7.2.42)$$

From Lorentz, we want to decouple the systems so

$$\nabla \cdot \mathbf{A} + \frac{1}{c^2} \frac{\partial \phi}{\partial t} = 0 \quad (7.2.43)$$

$$\nabla \cdot \mathbf{E} = -\nabla^2 \phi - \frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} = \frac{\rho_e}{\epsilon_0} = 0 \quad (7.2.44)$$

$$\frac{1}{c^2} \frac{\partial^2 \mathbf{A}}{\partial t^2} - \nabla^2 \mathbf{A} = \mu_0 \mathbf{J} = 0 \quad (7.2.45)$$

7.3 Lecture 20: October 29, 2012

Returned HW and Midterm.

Parabolic and Elliptic Differential Equations

1D, time-dependent heat equation

$$\frac{\partial F}{\partial t} = \alpha \frac{\partial^2 F}{\partial x^2} \quad (7.3.1)$$

we have boundary conditions on the spacial domain of $[0, L]$. It is important to have homogeneous boundary conditions, *i.e.* we want to have our values at the boundaries to be $F = 0$. We can redefine our dependent variable if adjust for the values at the boundaries if we have a non-homogeneous system, or $\tilde{F} = \text{const} = F$. This then allows for a super-position solution. In the real world, we may have that $F = T$ for temperature distributions or $F = C_i$ for a concentration in a solution. Now our initial condition is

$$F(t=0) = f(t)$$

We may use separation of variables,

$$F = X(x)\Theta(t) \quad (7.3.2)$$

substituting,

$$X \frac{d\Theta}{dt} = \alpha \Theta \frac{d^2 X}{dx^2} \quad (7.3.3)$$

deciding by $X\Theta$,

$$\frac{1}{\alpha \Theta(t)} \frac{d\Theta}{dt} = \frac{1}{X(x)} \frac{d^2 X}{dx^2} = -\lambda^2 \quad (7.3.4)$$

Separating for our equation of time,

$$\frac{d\Theta}{dt} + \alpha \lambda^2 \Theta = 0 \quad (7.3.5)$$

we may solve this system easily by rearranging and integrating,

$$\int \frac{1}{\Theta} d\Theta = - \int \alpha \lambda^2 dt \quad (7.3.6)$$

and

$$\Theta = \Theta_0 e^{-\alpha \lambda^2 t} \quad (7.3.7)$$

This solution will show that we can reach a steady state in time, which is a very natural result.

The spacial part of the problem is solved very similarly to the previous hyperbolic example. So with the Helmholtz equation,

$$\frac{d^2 X}{dx^2} + \lambda^2 X = 0 \quad (7.3.8)$$

where our solution will be expressed by

$$X(x) = C_1 \cos(\lambda x) + C_2 \sin(\lambda x) \quad (7.3.9)$$

From the first boundary condition, we realize that $C_1 = 0$. From the second boundary equation we get the solution of the eigenvalues gives,

$$\lambda = \frac{n\pi}{L}, \quad n = 1, 2, 3, \dots \quad (7.3.10)$$

Now,

$$F_n = C_{2n} \sin\left(\frac{n\pi}{L}x\right) \Theta_0 e^{-\alpha\lambda^2 t} \quad (7.3.11)$$

We can combine the constants $C_{2n} \Theta_0 = B_n$ to simplify. We will naturally assume this type of simplification in all future derivations. Thus, our solution looks like,

$$F(x, t) = \sum_{n=1}^{\infty} F_n = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi}{L}x\right) e^{-\alpha\lambda^2 t} \quad (7.3.12)$$

Now we must find the values of the B_n from the initial condition. So,

$$f(x) \sin\left(\frac{m\pi}{L}x\right) = B_n \sin\left(\frac{n\pi}{L}x\right) \sin\left(\frac{m\pi}{L}x\right) \quad (7.3.13)$$

Integrating both sides and using orthogonality

$$\int_0^L f(x) \sin\left(\frac{m\pi}{L}x\right) dx = B_n \int_0^L \sin^2\left(\frac{m\pi}{L}x\right) dx \quad (7.3.14)$$

For the sake of example, let's say that $f(x) = \text{constant}$. In this case,

$$\int_0^L f(x) \sin\left(\frac{m\pi}{L}x\right) dx = \frac{L}{m\pi} (1 - \cos(m\pi)) \quad (7.3.15)$$

for different m

$$\text{LHS } (m=1) = \frac{2L}{\pi}$$

$$\text{LHS } (m=2) = 0$$

$$\text{LHS } (m=3) = \frac{2L}{3\pi}$$

For the right hand side,

$$\begin{aligned} \text{RHS} &= \int_0^L \sin^2\left(\frac{m\pi}{L}x\right) dx \\ &= \frac{L}{2} \left(1 - \frac{\sin(2m\pi)}{2m\pi}\right) \\ &= \frac{L}{2} \end{aligned} \quad (7.3.16)$$

Thus, for a constant initial condition of F_0 we have

$$B_m = \frac{4F_0}{m\pi}, \quad m = 1, 3, 5, \dots \quad (7.3.17)$$

This can now be placed into our form of the equation while substituting a new m by $2n - 1$ where $m = 1, 3, 5, \dots$ and $n = 1, 2, 3, \dots$. We find that

$$F(x, t) = \frac{4F_0}{\pi} \sum_{n=1}^{\infty} \frac{1}{2n-1} \sin\left(\frac{n\pi}{L}x\right) e^{-\alpha\left(\frac{(2n-1)\pi}{L}\right)^2 t} \quad (7.3.18)$$

Example: Elliptic partial differential equation

Another good example in the book is two-dimensional steady-state heat transfer. This is useful, and we will modify the example for our own use. We will have a two-dimensional domain, but we shall modify it to have a semi-infinite y dimension, and a limited x . Thus, our domains are $[0, L]$ and $[0, \infty]$ in x and y , respectively. The general heat transport equation is,

$$\frac{\partial F}{\partial t} = \alpha \nabla^2 F \quad (7.3.19)$$

which is simplified in steady state to

$$\nabla^2 F = 0 \quad (7.3.20)$$

The first equation is a parabolic equation, while the second is an elliptic equation. In two dimensional Cartesian coordinates, we must now solve

$$\frac{\partial^2 F}{\partial x^2} + \frac{\partial^2 F}{\partial y^2} = 0. \quad (7.3.21)$$

For our boundary conditions,

$$F(x=0, y) = 0, \quad (7.3.22a)$$

$$F(x=L, y) = 0, \quad (7.3.22b)$$

$$F(x, y=0) = f(x), \quad (7.3.22c)$$

$$F(x, y \rightarrow \infty) \rightarrow \infty. \quad (7.3.22d)$$

Separating the variables,

$$F(x, y) = X(x)Y(y) \quad (7.3.23)$$

by substituting,

$$Y \frac{d^2 X}{dx^2} + X \frac{d^2 Y}{dy^2} = 0$$

and rearranging

$$\frac{1}{X} \frac{d^2 X}{dx^2} = -\frac{1}{Y} \frac{d^2 Y}{dy^2} = -k^2. \quad (7.3.24)$$

This will give us the Helmholtz equation again in the x spacial direction, so

$$\frac{d^2X}{dx^2} + k^2X = 0, \quad (7.3.25)$$

with a solution of

$$X = C_1 \cos(kx) + C_2 \sin(kx). \quad (7.3.26)$$

In the y direction we the the *modified* Helmholtz equation where we have the sign is now negative,

$$\frac{d^2Y}{dy^2} - k^2Y = 0. \quad (7.3.27)$$

The solution may be expressed as either hyperbolic sines and cosines or as exponentials. In principle either should give us the same solutions, however looking at the physical system, we expect the solution to die out. Thus, it seems most convenient to express the solution as a function of exponentials.

$$Y = C_3 e^{ky} + C_4 e^{-ky}. \quad (7.3.28)$$

From the boundary conditions, as usual

$$C_1 = 0, \quad (7.3.29a)$$

$$k = \frac{n\pi}{L}, \quad n = 1, 2, 3, \dots; \quad (7.3.29b)$$

$$C_3 = 0. \quad (7.3.29c)$$

So we have

$$X_n = C_{2n} \sin\left(\frac{n\pi}{L}x\right), \quad (7.3.30a)$$

$$Y_n = C_{4n} e^{-\frac{n\pi}{L}y}. \quad (7.3.30b)$$

A solution may be expressed in the form,

$$F_n = B_n \sin\left(\frac{n\pi}{L}x\right) e^{-\frac{n\pi}{L}y}. \quad (7.3.31)$$

We observe that the exponential has a constant which is now not squared as is the case in time-dependent solutions. The full solution

$$F = \sum_{n=1}^{\infty} F_n \quad (7.3.32)$$

$$= \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi}{L}x\right) e^{-\frac{n\pi}{L}y} \quad (7.3.33)$$

for $y = 0$ the exponential term is simply 1. Thus, we have our bottom boundary condition,

$$f(x) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi}{L}x\right) \quad (7.3.34)$$

Multiplying by sine and integrating, we find that

$$B_m = \frac{\int f(x) \sin\left(\frac{m\pi}{L}x\right) dx}{\int \sin^2\left(\frac{m\pi}{L}x\right) dx} \quad (7.3.35)$$

Again if we set $f(x) = F_0$, a constant, we get the same terms for B_n as in the previous problem. Finally our solution is

$$F(x, y) = \frac{4F_0}{\pi} \sum_{n=1}^{\infty} \frac{1}{2n-1} \sin\left(\frac{(2n-1)\pi}{L}x\right) e^{-\frac{n\pi}{L}y} \quad (7.3.36)$$

This solution is very similar to the previous problem, only with the different form for the exponential. The terms of the series are very quickly converging in most cases. Say we choose the point $(L/2, L/2)$. The first term is 0.2079, the second term is -0.0144 , the third term 0.0018, the fourth term -0.000267 . We see now that we generally are dropping an order of magnitude with each term and alternating sign. This shows very strong convergence.

Example: Transient parabolic equation with source term

An example of a parabolic problem may also include a source term,

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} + f(x, t). \quad (7.3.37)$$

The initial and boundary conditions are homogeneous,

$$T(x=0, t) = 0, \quad (7.3.38a)$$

$$T(x=L, t) = 0, \quad (7.3.38b)$$

$$T(x, t=0) = 0. \quad (7.3.38c)$$

We are implicitly assuming that we have uniform temperature initially and that this temperature has been subtracted to make our variable T . So now we ask “How do we separate the variables here?” We choose to create a homogeneous problem in x . But, we know that there are eigenfunctions where

$$X_n \sim \sin\left(\frac{n\pi}{L}x\right), \quad n = 1, 2, 3, \dots \quad (7.3.39)$$

So we can assume a solution of the form,

$$T(x, t) = \sum_{n=1}^{\infty} R_n(t) \sin\left(\frac{n\pi}{L}x\right). \quad (7.3.40)$$

We may also expand the source as a sine–Fourier expansion to

$$f(x, t) = \sum_{n=1}^{\infty} \beta_n(t) \sin\left(\frac{n\pi}{L}x\right). \quad (7.3.41)$$

The values of the coefficients is quickly found by,

$$\beta_n(t) = \frac{2}{L} \int_0^L f(x, t) \sin\left(\frac{n\pi}{L}x\right) dx. \quad (7.3.42)$$

The next step is to take the solution and the expansion and place them into the original differential equation.

$$\frac{\partial T}{\partial t} = \sum_{n=1}^{\infty} \frac{\partial R_n}{\partial t} \sin\left(\frac{n\pi}{L}x\right); \quad (7.3.43)$$

$$\frac{\partial T}{\partial x} = \sum_{n=1}^{\infty} R_n(t) \frac{n\pi}{L} \cos\left(\frac{n\pi}{L}x\right);$$

$$\frac{\partial^2 T}{\partial x^2} = - \sum_{n=1}^{\infty} R_n(t) \left(\frac{n\pi}{L}\right)^2 \sin\left(\frac{n\pi}{L}x\right). \quad (7.3.44)$$

We observe an important feature that we have our solution only in terms of sines. Substituting,

$$\sum_{n=1}^{\infty} \frac{\partial R_n}{\partial t} \sin\left(\frac{n\pi}{L}x\right) = -\alpha \sum_{n=1}^{\infty} R_n(t) \left(\frac{n\pi}{L}\right)^2 \sin\left(\frac{n\pi}{L}x\right) + \sum_{n=1}^{\infty} \beta_n(t) \sin\left(\frac{n\pi}{L}x\right). \quad (7.3.45)$$

Since each individual equation of n^{th} order should be correct.

$$\frac{dR_n}{dt} \sin\left(\frac{n\pi}{L}x\right) = -\omega_n^2 R_n(t) \sin\left(\frac{n\pi}{L}x\right) + \beta_n(t) \sin\left(\frac{n\pi}{L}x\right). \quad (7.3.46)$$

where $\omega_n^2 = \alpha \frac{n^2\pi^2}{L^2}$ and the sines cancel out to give us a simple first order ordinary differential equation for $R_n(t)$.

$$\frac{dR_n}{dt} = -\omega_n^2 R_n(t) + \beta_n(t). \quad (7.3.47)$$

The solution is

$$R_n(t) = \int_0^t \beta_n(\tau) e^{-\omega_n^2(t-\tau)} d\tau. \quad (7.3.48)$$

We see that we have in fact a Greens function with the exponential term. We interestingly were able to find it with other arguments. So with our knowledge of $\beta_n(t)$ from above, the complete solution is,

$$T(x, t) = \sum_{n=1}^{\infty} \left\{ \int_0^t \left[\frac{2}{L} \int_0^L f(x, \tau) \sin\left(\frac{n\pi}{L}x\right) dx \right] e^{-\omega_n^2(t-\tau)} d\tau \right\} \sin\left(\frac{n\pi}{L}x\right). \quad (7.3.49)$$

In two dimensions this can still be solved similarly.

7.4 Lecture 21: November 5, 2012

In review, last week we solved, by separation of variables over $[0, L]$, with BC: $F(x=0) = 0$ and $F(x=L) = 0$

$$\frac{\partial F}{\partial t} = \alpha \frac{\partial^2 F}{\partial x^2}, \quad (7.4.1)$$

and

$$\frac{\partial F}{\partial t} = \alpha \frac{\partial^2 F}{\partial x^2} + f(x, t). \quad (7.4.2)$$

by using the eigenfunctions of $\sin(\lambda x)$. We can also solve this over an interval of $[-\frac{L}{2}, \frac{L}{2}]$ to reduce the symmetry in another way. Our BC; $\frac{\partial F}{\partial x}|_{x=0} = 0$ and $F(x=\frac{L}{2}) = 0$. This solution will be of the form, $\cos(\frac{2n\pi}{L}x)$.

Example: Heat transport in spherical coordinates

Now we are interested in solving a parabolic differential equation in spherical coordinates. For we have a metal ball in a tank with temperature at the surface of T_s

$$\frac{\partial(T - T_s)}{\partial t} = \alpha \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial(T - T_s)}{\partial r} \right) \quad (7.4.3)$$

Simplifying for our differential temperature: $\tilde{T} = T - T_s$,

$$\frac{\partial \tilde{T}}{\partial t} = \alpha \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \tilde{T}}{\partial r} \right) \quad (7.4.4)$$

we substitute for $\omega = rT$ or $T = \frac{\omega}{r}$ and simplify our problem to

$$\frac{\partial \omega}{\partial t} = \alpha \frac{\partial^2 \omega}{\partial r^2} \quad (7.4.5)$$

Our boundary conditions are $(\frac{\partial T}{\partial r})_{r=0} = 0$ and $\tilde{T}(r=R) = 0$, with an initial condition of $T(t=0) = T_0$.

We begin solving the equation with separation of variables,

$$\omega = \rho(r)\theta(t) \quad (7.4.6)$$

$$\rho \frac{d\theta}{dt} = \alpha \theta \frac{d^2 \rho}{dr^2} \quad (7.4.7)$$

$$\frac{1}{\alpha \theta} \frac{d\theta}{dt} = \frac{1}{\rho} \frac{d^2 \rho}{dr^2} = -\lambda^2 \quad (7.4.8)$$

Clearly the form of the solution for the time will be

$$\theta = \theta_0 e^{-\alpha \lambda^2 t}. \quad (7.4.9)$$

Now for our spacial system,

$$\frac{d^2\rho}{dr^2} + \lambda^2\rho = 0. \quad (7.4.10)$$

Our spacial function will thus be expressed with,

$$\rho = C_1 \cos(\lambda r) + C_2 \sin(\lambda r), \quad (7.4.11)$$

or

$$\frac{\rho}{r} = C_1 \frac{\cos(\lambda r)}{r} + C_2 \frac{\sin(\lambda r)}{r}. \quad (7.4.12)$$

Here a new boundary condition is expressed by $\left. \frac{\partial(\rho/r)}{\partial r} \right|_{r=0} = 0$. The solutions are,

$$\frac{\partial(\cos(\lambda r)/r)}{\partial r} = -\frac{\cos(\lambda r)}{r^2} - \lambda \frac{\sin(\lambda r)}{r} \quad (7.4.13)$$

$$\frac{\partial(\sin(\lambda r)/r)}{\partial r} = -\frac{\sin(\lambda r)}{r^2} + \lambda \frac{\cos(\lambda r)}{r} \quad (7.4.14)$$

taking a limiting case for the first equation we see,

$$\lim_{r \rightarrow 0} \left[-\frac{\cos(\lambda r)}{r^2} - \lambda \frac{\sin(\lambda r)}{r} \right] = -\infty - \lambda = \infty \quad (7.4.15)$$

for the second equation, using L'Hospital's rule

$$\lim_{r \rightarrow 0} \left[\lambda \frac{\cos(\lambda r)}{r} - \frac{\sin(\lambda r)}{r^2} \right] = \lim_{r \rightarrow 0} \left[\frac{1}{r^2} (\lambda r \cos(\lambda r) - \sin(\lambda r)) \right] \quad (7.4.16)$$

$$= \lim_{r \rightarrow 0} \left[\frac{1}{2r} (\lambda r \cos(\lambda r) - \lambda^2 r \sin(\lambda r) - \lambda \cos(\lambda r)) \right] \quad (7.4.17)$$

$$= \lim_{r \rightarrow 0} \left[\frac{1}{2r} (-\lambda^2 r \sin(\lambda r)) \right] \quad (7.4.18)$$

$$= \lim_{r \rightarrow 0} \left[\frac{1}{2} (-\lambda^2 \sin(\lambda r)) \right] \quad (7.4.19)$$

$$= 0 \quad (7.4.20)$$

Special functions

$$\frac{\sin x}{x} = j_0(x) \quad (7.4.21)$$

which is the spherical Bessel function

$$\frac{\cos x}{x} = y_0(x) \quad (7.4.22)$$

which is the spherical Neumann function. These are generalized by,

$$j_n(x) = \sqrt{\frac{\pi}{2x}} J_{n+1/2}(x) \quad (7.4.23)$$

$$y_n(x) = \sqrt{\frac{\pi}{2x}} Y_{n+1/2}(x) \quad (7.4.24)$$

With our boundary conditions, we get simply

$$\rho = C_2 \frac{\sin(\lambda r)}{r} \quad (7.4.25)$$

Thus our solution gives eigenvalues of $\lambda_n = \frac{n\pi}{R}$ and is

$$\omega_n = C_n \sin\left(\frac{n\pi}{R}r\right) e^{-\alpha\lambda^2 t} \quad (7.4.26)$$

Now,

$$F_0 = \sum_{n=1}^{\infty} \frac{C_n}{r} \sin\left(\frac{n\pi}{R}r\right) \quad (7.4.27)$$

integrating and rearranging for the coefficients

$$C_n = \frac{\int_0^R F_0 r \sin\left(\frac{n\pi}{R}r\right) dr}{\int_0^R \sin^2\left(\frac{n\pi}{R}r\right) dr} \quad (7.4.28)$$

$$= \frac{2}{R} \int_0^R F_0 r \sin\left(\frac{n\pi}{R}r\right) dr \quad (7.4.29)$$

The integral simplifies,

$$\int_0^R F_0 r \sin\left(\frac{n\pi}{R}r\right) dr = \frac{R^2}{m^2\pi^2} (\sin(m\pi) - m\pi \cos(m\pi)) \quad (7.4.30)$$

$$= \frac{R^2}{m^2\pi^2} (-m\pi \cos(m\pi)) \quad (7.4.31)$$

Thus,

$$C = \frac{r^2}{\pi}, \quad \text{for } m = 1, \quad (7.4.32)$$

$$C = \frac{-r^2}{2\pi}, \quad \text{for } m = 2, \quad (7.4.33)$$

$$C = \frac{r^2}{3\pi}, \quad \text{for } m = 3. \quad (7.4.34)$$

Thus, the left hand side is $(-1)^{m+1} \frac{R^2}{m\pi}$ and our solution is

$$\tilde{T} = \frac{2F_0 R}{\pi r} \sum_{n=1}^{\infty} \frac{(-1)^{m+1}}{m} \sin\left(\frac{m\pi}{R}r\right) e^{-\alpha\left(\frac{m\pi}{R}\right)^2 t} \quad (7.4.35)$$

Example: Flow in a cylindrical pipe

We now turn to the more difficult situation of solving for cylindrical coordinates. This will require the use of Bessel functions to solve the system in general. Our system is

$$\frac{\partial v_z}{\partial t} = \nu \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial v_z}{\partial r} \right) - \frac{1}{\rho} \frac{\partial P}{\partial z} \quad (7.4.36)$$

where $\nu = \mu/\rho$. We know that $-\frac{1}{\rho} \frac{\partial P}{\partial z} = \text{const.}$

1. Homogeneous Equation

Using our separation of variables,

$$v_z = X(r)T(t) \quad (7.4.37)$$

$$X \frac{dT}{dt} = \nu \left[T \frac{1}{r} \frac{d}{dr} \left(r \frac{dX}{dr} \right) \right] \quad (7.4.38)$$

also,

$$\frac{1}{T} \frac{dT}{dt} = \frac{\nu}{X} \frac{1}{r} \frac{d}{dr} \left(r \frac{dX}{dr} \right) = -\alpha^2 \quad (7.4.39)$$

Solving for the time, we again get

$$T = T_0 e^{-\alpha^2 t} \quad (7.4.40)$$

In our spacial coordinates,

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{dX}{dr} \right) + \frac{\alpha^2}{\nu} X = 0 \quad (7.4.41)$$

The Bessel equation for $n = 0$ is in fact a solution of this system,

$$X = C_1 J_0 \left(\frac{a}{\sqrt{\nu}} r \right) + C_2 Y_0 \left(\frac{a}{\sqrt{\nu}} r \right) \quad (7.4.42)$$

for our boundary conditions, we recognize that $J_0 \left(\frac{a}{\sqrt{\nu}} r \right) \rightarrow \text{finite}$, while $Y_0 \left(\frac{a}{\sqrt{\nu}} r \right) \rightarrow \text{infinite}$. Thus our solution simplifies to,

$$X = C_1 J_0 \left(\frac{a}{\sqrt{\nu}} r \right) \rightarrow \text{finite} \quad (7.4.43)$$

Our alpha is found from the roots of the Bessel function, or $a_n = \alpha_n \sqrt{\nu}$. These are tabulated and can also be accessed in Mathematica[®] or MATLAB[®]. So we have our solution is of the form

$$\rho(r) = \sum_{n=1}^{\infty} C_n J_0 \left(\frac{\alpha_n}{R} r \right) e^{-\frac{\alpha_n^2 \nu}{k} t} \quad (7.4.44)$$

2. Inhomogeneous Solution

Now we need to solve our steady state solution,

$$v_z = v'_{z,\infty} + v'_z, \quad (7.4.45)$$

which gives our large time result

$$v'_{z,\infty}(r) = \sum_{n=1}^{\infty} C_n J_0\left(\frac{\alpha_n}{R} r\right). \quad (7.4.46)$$

Then, for our pressure relation and our parabolic flow,

$$v'_{z,\infty}(r) = -\frac{R^2}{4\mu} \frac{dP}{dz} \left(1 - \frac{r^2}{R^2}\right) \quad (7.4.47)$$

$$= \sum_{n=1}^{\infty} C_n J_0\left(\frac{\alpha_n}{R} r\right) \quad (7.4.48)$$

Since $J_0\left(\frac{\alpha_n}{R} r\right)$ are orthogonal, we can integrate to get

$$\begin{aligned} C_m \int_0^R \left[J_0\left(\frac{\alpha_n}{R} r\right) \right]^2 r dr &= C_m \frac{R^2}{2} [J_0(\alpha_m) + J_1(\alpha_m)], \\ &= C_m \frac{R^2}{2} J_1(\alpha_m). \end{aligned}$$

Rearranging,

$$\begin{aligned} C_m &= \frac{R^2}{4\mu} \frac{dP}{dz} \frac{2R^2}{\alpha_m^2} \frac{J_2(\alpha_m)}{R^2} \frac{2}{J_1(\alpha_m)}, \\ &= \frac{R^2}{\mu} \frac{dP}{dz} \frac{J_2(\alpha_m)}{\alpha_m^2 J_1(\alpha_m)}. \end{aligned} \quad (7.4.49)$$

Thus, we can find a final for our equation with,

$$v_z = \sum_{n=1}^{\infty} \frac{R^2}{\mu} \frac{dP}{dz} \frac{J_2(\alpha_m)}{\alpha_m^2 J_1(\alpha_m)} J_0\left(\frac{\alpha_n}{R} r\right) \left[1 - e^{-\frac{\alpha_n^2 \nu}{R^2} t}\right].$$

or

$$\boxed{v_z = \frac{R^2}{\mu} \frac{dP}{dz} \sum_{n=1}^{\infty} \frac{J_2(\alpha_m)}{\alpha_m^2 J_1(\alpha_m)} J_0\left(\frac{\alpha_n}{R} r\right) \left[1 - e^{-\frac{\alpha_n^2 \nu}{R^2} t}\right]} \quad (7.4.50)$$

UNIT 8

Chapter 17—Integral Transforms

8.1 Lecture 22: November 7, 2012

The general form of *integral transforms*,

$$\int_a^b K(p, x) f(x) dx = \hat{F}(p) \quad (8.1.1)$$

A common transform is the *Laplace transform*.

$$\hat{F}(s) = \int_0^\infty e^{-st} f(t) dt \quad (8.1.2)$$

The *Fourier transform* is

$$\hat{F}(k) = \frac{1}{(2\pi)^{1/2}} \int_0^\infty e^{-ikx} f(x) dx \quad (8.1.3)$$

In the case of a Fourier transform of time, we get that we are working in the frequency domain. For a spacial domain we work in the wavevector domain. A great benefit of a Laplace transform is that we convert derivatives into algebraic equations. This allows us to simplify some more difficult problems because the problems are easier to manipulate in these different spaces.

Laplace transform

Say we have $f(t) = e^{\alpha t}$,

$$\int_0^\infty e^{-st} f(t) dt = \int_0^\infty e^{-st} e^{\alpha t} dt \quad (8.1.4)$$

$$= \int_0^\infty e^{-(s-\alpha)t} dt$$

$$= \frac{1}{(s-\alpha)} \left[e^{-(s-\alpha)t} \right]_0^\infty$$

$$= \frac{1}{(s-\alpha)}, \quad \text{for } s > \alpha \quad (8.1.5)$$

Now say that we transform the differential operator *i.e.* $f(t) = \frac{df}{dt}$,

$$\int_0^{\infty} e^{-st} f(s) dt = \int_0^{\infty} e^{-st} \frac{df}{dt} dt \quad (8.1.6)$$

$$\begin{aligned} &= [e^{-st} f]_0^{\infty} - \int_0^{\infty} f d(e^{-st}) \\ &= -f(0) - \int_0^{\infty} f e^{-st} d(-st) \\ &= -f(0) + s \int_0^{\infty} f e^{-st} dt \\ &= s\hat{F}(s) - f(0) \end{aligned} \quad (8.1.7)$$

This shows the power of the Laplace transform for solving initial value problems. The $f(0)$ corresponds to the initial condition and we have got rid of the derivative. Let's say we have $f^{(n)}(t)$, then in general

$$\mathcal{L}\{f^{(n)}(t)\} = s^n \hat{F}(s) - s^{n-1} f(0) - \dots - s^{n-n} f^{(n-1)}(0) \quad (8.1.8)$$

which is thus dependent on the initial conditions. A constant is transformed, $\int_0^{\infty} e^{-st} f(t) dt$, to $\hat{F}(s) = \frac{c}{s}$.

For a second order derivative,

$$\mathcal{L}\left\{\frac{d^2 f}{dt^2}\right\} = s^2 \hat{F}(s) - sf(0) - f'(0) \quad (8.1.9)$$

where $f'(0) = \left(\frac{df}{dt}\right)_{t=0}$.

Example: Oscillator equation

The oscillator equation may be transformed using the Laplace transform.

$$m \frac{d^2 x}{dt^2} + \zeta \frac{dx}{dt} + kx = f(t) \quad (8.1.10)$$

where the terms are the acceleration, friction, elastic and external forces, respectively. In the case of a random external force we can have a Brownian Oscillation. So we are now interested in a solution.

$$\frac{d^2 x}{dt^2} + \beta \frac{dx}{dt} + \omega_0^2 x = \lambda(t) \quad (8.1.11)$$

where $\beta = \zeta/m$; $\zeta = 6\pi\eta a$, $\omega_0^2 = k/m$, and $\lambda(t) = f(t)/m$. For solving for the Green function we have

$$\frac{d^2 G}{dt^2} + \beta \frac{dG}{dt} + \omega_0^2 G = \delta(t) \quad (8.1.12)$$

transforming the Dirac delta function,

$$\begin{aligned} \mathcal{L}\{\delta(t)\} &= \int_0^{\infty} e^{-st} \delta(t) dt \\ &= \frac{1}{s} \end{aligned} \quad (8.1.13)$$

Taking the transform of the other terms in our equation,

$$\mathcal{L}\left\{\frac{d^2G}{dt^2}\right\} = s^2\hat{G}(s) - sG(0) - G'(0) \quad (8.1.14)$$

$$\mathcal{L}\left\{\frac{dG}{dt}\right\} = s\hat{G}(s) - G(0) \quad (8.1.15)$$

$$\mathcal{L}\{G(t)\} = \hat{G}(s) \quad (8.1.16)$$

Let's say that we have simple initial condition so the $\hat{G}(0)$ terms go away. Then substituting into our differential equation for the Green function,

$$\begin{aligned} s^2\hat{G}(s) + \beta s\hat{G}(s) + \omega_0^2\hat{G}(s) &= \frac{1}{2} \\ \hat{G}(s^2 + \beta s + \omega_0^2) &= \frac{1}{2} \\ \hat{G} &= \frac{1}{2(s^2 + \beta s + \omega_0^2)} \end{aligned} \quad (8.1.17)$$

We now care about inverting the system into the real variables, which is a tricky process. To invert,

$$f(t) = \frac{1}{2\pi i} \oint_{\gamma-i\infty}^{\gamma+i\infty} \hat{F}(s)e^{+st} ds \quad (8.1.18)$$

This requires the method of residues. There are also many tables of the (inverse) Laplace transforms in books such as Korn and Korn. Also in Mathematica[®] you can use the command `LaplaceTransform[f(t), t, s]` and `InverseLaplaceTransform[F(s), s, t]`. Returning to our problem we find by inversion that,

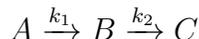
$$\begin{aligned} \mathcal{L}^{-1}\{\hat{G}(s)\} &= \frac{e^{-\frac{\beta t}{2}} \left[e^{\frac{1}{2}t\sqrt{\beta^2 - 4\omega_0^2}} - e^{-\frac{1}{2}t\sqrt{\beta^2 - 4\omega_0^2}} \right]}{2\sqrt{\beta^2 - 4\omega_0^2}} \\ &= \frac{e^{-\frac{\beta t}{2}} \sin(\omega_1 t)}{2\omega_1} \end{aligned} \quad (8.1.19)$$

where $\omega_1 = \sqrt{\omega_0^2 - \frac{\beta^2}{4}}$ and we recall $\beta = \zeta/m$. Thus we have found the Green function and can solve our system by,

$$x(t) = \int_0^\infty G(t-t')f(t') dt' \quad (8.1.20)$$

Example: System of chemical reactions

Laplace transforms may be used on systems of linear differential equations. It is not generally usable for nonlinear equations. Say we have the reactions,



So we have at $t = 0$ that $N_A = N$, and $N_B = N_C = 0$. Our reaction scheme becomes,

$$\begin{aligned}\frac{dN_A}{dt} &= -k_1 N_A \\ \frac{dN_B}{dt} &= k_1 N_A - k_2 N_B \\ \frac{dN_C}{dt} &= k_2 N_B\end{aligned}$$

Now this makes it clear why we can only be using a first-order set of reactions, or else we would be dealing with a system of non-linear equations and could not use the Laplace transform. Each of the equations above can be used to get equations in time for each of the components. Transforming these equations, we get,

$$\begin{aligned}s\hat{F}_A(s) - N &= -k_1\hat{F}_A(s) \\ s\hat{F}_B(s) &= k_1\hat{F}_A(s) - k_2\hat{F}_B(s) \\ s\hat{F}_C(s) &= k_2\hat{F}_B(s)\end{aligned}$$

Separating the terms and substituting we get the following system of independent equations,

$$\begin{aligned}\hat{F}_A(s) &= \frac{N}{s + k_1} \\ \hat{F}_B(s) &= \frac{k_1 N}{(s + k_1)(s + k_2)} \\ \hat{F}_C(s) &= \frac{k_1 k_2 N}{s(s + k_1)(s + k_2)}\end{aligned}$$

Now we find from inverting that

$$N_A(t) = N e^{-k_1 t} \tag{8.1.21}$$

$$N_B(t) = \frac{k_1 N}{k_1 - k_2} (e^{-k_2 t} - e^{-k_1 t}) \tag{8.1.22}$$

$$N_C(t) = \frac{N [k_1 (1 - e^{-k_2 t}) - k_2 (1 - e^{-k_1 t})]}{k_1 - k_2} \tag{8.1.23}$$

where the third equation follows because $N_A + N_B + N_C = N$. These solutions may be plotted easily to show the behavior of the system, where we observe A decaying, B increasing and then decreasing, and C increasing to a steady quantity.

Example: Heat transfer

Partial differential equations application to heat transfer.

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\alpha} \frac{\partial T}{\partial t} \tag{8.1.24}$$

with initial and boundary conditions of,

$$\begin{aligned}T(x, 0) &= 0 \\T(0, t) &= T_0 \\T(\infty, t) &\rightarrow 0\end{aligned}$$

On a practical note: this equation is not perfectly physical because of the heat far away seems to propagate infinitely fast which is non-physical. Now let's transform the time with the Laplace transform.

$$\begin{aligned}\mathcal{L}\left\{\frac{\partial T}{\partial t}\right\} &= s\hat{T} - T(0) \\ \mathcal{L}\left\{\frac{\partial^2 T}{\partial x^2}\right\} &= \frac{\partial^2}{\partial x^2}(\mathcal{L}\{T\}) = \frac{\partial^2 \hat{T}}{\partial x^2}\end{aligned}$$

so we have an ordinary differential equation,

$$\frac{d^2 \hat{T}}{dx^2} = \frac{s}{\alpha} \hat{T} \quad (8.1.25)$$

Also,

$$\mathcal{L}\{T_0\} = \frac{T_0}{s}$$

This gives

$$\frac{d^2 \hat{T}}{dx^2} - \frac{s}{\alpha} \hat{T} = 0 \quad (8.1.26)$$

where $\hat{T}(x=0) = \frac{T_0}{s}$. We will continue the solution next lecture.

8.2 Lecture 23: November 12, 2012

Example: Diffusion Equation

As an example of Laplace transforms we will explore the solution of Fourier's and Fick's Laws,

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad (8.2.1)$$

$$\frac{\partial C}{\partial t} = \mathcal{D} \frac{\partial^2 C}{\partial x^2} \quad (8.2.2)$$

Now say we have heat next to a wall, our initial and boundary conditions are

$$\begin{aligned} T(x, 0) &= 0 \\ T(0, t) &= T_0 \\ T(x \rightarrow \infty, t) &\rightarrow \text{finite} \end{aligned}$$

Transform with respect to time,

$$\mathcal{L}\left\{\frac{\partial T}{\partial t}\right\} = s\hat{T} - T(t=0) \quad (8.2.3)$$

$$\mathcal{L}\left\{\frac{\partial^2 T}{\partial x^2}\right\} = \frac{\partial^2}{\partial x^2}(\mathcal{L}\{T\}) = \frac{\partial^2 \hat{T}}{\partial x^2} \quad (8.2.4)$$

transforming the constant,

$$\mathcal{L}\{T_0\} = \frac{T_0}{s} \quad (8.2.5)$$

We now have everything to solve the problem. This simplifies to the modified Helmholtz equation,

$$\frac{\partial^2 \hat{T}}{\partial x^2} - \frac{s}{\alpha} \hat{T} = 0 \quad (8.2.6)$$

$$\hat{T}(x, s) = C_1(s)e^{\sqrt{\frac{s}{\alpha}}x} + C_2(s)e^{-\sqrt{\frac{s}{\alpha}}x} \quad (8.2.7)$$

from the first boundary condition we know that $C_1 \equiv 0$. We simplify to

$$\hat{T}(x, s) = C_2(s)e^{-\sqrt{\frac{s}{\alpha}}x} \quad (8.2.8)$$

from the other boundary condition,

$$\hat{T}(0, s) = \frac{T_0}{s} \quad (8.2.9)$$

$$\hat{T}(x, s) = \frac{T_0}{s} e^{-\sqrt{\frac{s}{\alpha}}x} \quad (8.2.10)$$

Now we need to invert back into time. Generally we will look at tables to find the answer. We find that the inverse of the function is the *complementary error function*.

$$\mathcal{L}^{-1}\left\{\frac{e^{-\sqrt{\frac{s}{\alpha}}x}}{s}\right\} = \operatorname{erfc}\left(\frac{x}{\sqrt{4\alpha t}}\right) \quad (8.2.11)$$

$$= 1 - \frac{2}{\pi} \int_0^{x/\sqrt{4\alpha t}} e^{-z^2} dz \quad (8.2.12)$$

Our full solution,

$$T(x, t) = T_0 \left(1 - \frac{2}{\pi} \int_0^{x/\sqrt{4\alpha t}} e^{-z^2} dz\right) \quad (8.2.13)$$

In the book there are examples with heat transfer with a constant heat flux or chemical reaction with Robin boundary conditions.

Convolution Integral

Physical Examples

Some times you end up with the product of two transforms that need to be inverted. Replacing viscous fluid with Stokes Law.

$$\beta v \rightarrow 6\pi\eta av \quad (8.2.14)$$

We get for other cases that we must evaluate

$$\int_0^\tau \beta(\tau - t)v(t) dt \quad (8.2.15)$$

Mathematical description

$$\hat{F}(s) = \int_0^\infty e^{-st} f(t) dt \quad (8.2.16)$$

or in the book's notation

$$\hat{G}(s) = \int_0^\infty e^{-st} g(t) dt \quad (8.2.17)$$

On a matter of notation, in the book integration is often written as

$$\int_0^\infty dt e^{-st} f(t) = \int_0^\infty e^{-st} f(t) dt \quad (8.2.18)$$

So we are inverting a convoluted system,

$$\mathcal{L}^{-1}\left\{\hat{F}(s)\hat{G}(s)\right\} = r(t) \quad (8.2.19)$$

$$\hat{F}(s)\hat{G}(s) = \hat{F}(s) \int_0^\infty e^{-su} g(u) du \quad (8.2.20)$$

Putting $\hat{F}(s)$ inside the system,

$$\hat{F}(s)\hat{G}(s) = \int_0^\infty e^{-su}\hat{F}(s)g(u) du \quad (8.2.21)$$

Proving an auxiliary theorem about the Laplace transform. We have *translation*

$$\mathcal{L}\{e^{at}f(t)\} = \hat{F}(s-a) \quad (8.2.22)$$

This gives $\hat{F}(s)$ which is shifted by a .

$$\hat{F}(s) = \mathcal{L}\{f(t)\} \quad (8.2.23)$$

Applying the definition of a Laplace transform,

$$\mathcal{L}\{e^{at}f(t)\} = \int_0^\infty e^{at}e^{-st}f(t) dt \quad (8.2.24)$$

$$= \int_0^\infty e^{(a-s)t}f(t) dt \quad (8.2.25)$$

$$= \hat{F}(s-a) \quad (8.2.26)$$

Remember that $s > a$ is a necessary condition for convergence of the integral.

$$g(t) = \begin{cases} 0, & 0 \leq t < a \\ f(t-a), & t \geq a \end{cases}. \quad (8.2.27)$$

$$\int_0^\infty e^{-st}g(t) dt = \int_a^\infty e^{-st}f(t-a) dt \quad (8.2.28)$$

This can further be written as,

$$\int_0^\infty e^{-st}g(t) dt = e^{-sa} \int_a^\infty e^{-s(t-a)}f(t-a) d(t-a) \quad (8.2.29)$$

$$= e^{-sa}\hat{F}(s) \quad (8.2.30)$$

We may also write,

$$g(t) = H(t-a)f(t-a) \quad (8.2.31)$$

Where the *Heaviside function* is given by

$$H(t-a) = \begin{cases} 0, & 0 \leq t < a \\ 1, & t \geq a \end{cases}. \quad (8.2.32)$$

and is found through integrating the Dirac delta function,

$$H(t) = \int \delta(t) dt \quad (8.2.33)$$

or

$$H(t - a) = \int \delta(t - a) dt \quad (8.2.34)$$

from these relationships,

$$\hat{F}(s)\hat{G}(s) = \int_0^\infty e^{-su}\hat{F}(s)g(u) du \quad (8.2.35)$$

$$e^{-su}\hat{F}(s) = e^{-su} \int_0^\infty e^{-st}f(t) dt \quad (8.2.36)$$

$$= \int_0^\infty e^{-st} H(t - u)f(t - u) dt \quad (8.2.37)$$

Finally, we get that the product is,

$$\hat{F}(s)\hat{G}(s) = \int_0^\infty du \int_0^\infty dt e^{-st} H(t - u)f(t - u)g(u) \quad (8.2.38)$$

or we may simplify

$$\hat{F}(s)\hat{G}(s) = \int_0^\infty du \int_u^\infty dt e^{-st} f(t - u)g(u) \quad (8.2.39)$$

This is the form of the convolution. However, this is not sufficient for non-linear differential equations. Say that we have $f = g$, then we may suppose $fg = f^2$. But we in fact have $f(t - u)g(u) = f(t - u)f(u) \neq f^2$. Thus, it is not the same and therefore not helpful.

Note: Example memory dependent processes Markov processes do not have memory; however many systems have memory.

Fourier Transform

Our Laplace transform that is usually $\int_0^\infty e^{-st}f(t) dt$, but may be $\int_{-\infty}^\infty e^{-st}f(t) dt$ which is a double-sided Laplace Transform. Normally, we prefer in this case to use Fourier transform because it is simply obtained by $s = -i\omega$. For the sum of the series

$$f(t) = \sum_{-\infty}^{\infty} C_n e^{in\omega t} \quad (8.2.40)$$

and

$$C_n = \frac{1}{\tau} \int_{-\tau/2}^{\tau/2} f(t) e^{-in\omega_0 t} dt \quad (8.2.41)$$

where $\omega_0\tau = 2\pi$ because we need a node on both boundaries. τ is the time interval of interest and $\frac{1}{\tau} = \frac{\omega_0}{2\pi}$.

$$f(t) = \sum_{-\infty}^{\infty} \left[\frac{\omega_0}{2\pi} \int_{-\tau/2}^{\tau/2} f(t) e^{-in\omega_0 t} dt \right] e^{in\omega_0 t} \quad (8.2.42)$$

The term in brackets is in fact the coefficients of the Fourier terms. This is a finite value. If we have a large τ and a small ω_0 , we can approximate the solution as,

$$f(t) = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} F(n\Delta\omega)\Delta\omega \tag{8.2.43}$$

This is a Riemann sum evaluation and if we have $\Delta\omega \rightarrow \omega_0$, we can express the integral with a convolution,

$$F(n\Delta\omega) = \int_{-\tau/2}^{\tau/2} f(u)e^{-in\Delta\omega(t-u)} du \tag{8.2.44}$$

Continuing our sum, we see an integral

$$f(t) = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} F(n\Delta\omega)\Delta\omega \tag{8.2.45}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} F d\omega \tag{8.2.46}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} du f(u)e^{i\omega(t-u)} \tag{8.2.47}$$

This is the Fourier integral theorem.

$$C(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} du f(u)e^{-i\omega u} \tag{8.2.48}$$

$$f(t) = \int_{-\infty}^{\infty} C(\omega)e^{i\omega t} d\omega \tag{8.2.49}$$

This is similar to an electrical engineering approach. The physicist approach likes to have the $1/2\pi$ split by a square root. This is usually a little better as far as normalization goes.

To do the transform we are required that we have a function which has a continuous derivative. In many cases it is still stable as long as the function is only piecewise continuous. The Heaviside function is discontinuous, which is a more difficult. The Fourier Integral Theorem is the continuous analogue of

$$f(t) = \sum_{n=-\infty}^{\infty} C_n e^{in\omega t} \tag{8.2.50}$$

which in the limit is $\int_{-\infty}^{\infty} C(\omega)e^{i\omega t} d\omega$.

Now, for the transform $f(t) \rightarrow \hat{F}(\omega)$,

$$\hat{F}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} du f(u)e^{-i\omega u} \tag{8.2.51}$$

To do the inversion $\hat{F}(\omega) \rightarrow f(t)$.

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega \hat{F}(\omega)e^{i\omega t} \tag{8.2.52}$$

Example: Gaussian distribution

The form of the Gaussian distribution is

$$f(x) = \frac{e^{-\frac{x^2}{2\sigma^2}}}{(2\pi\sigma^2)^{1/2}}$$

This is a useful distribution because it arises from the central limit theorem. It is also interesting because its Fourier transform is also a Gaussian distribution. With k as the wavenumber

$$\hat{F}(k) = \frac{1}{2\pi\sigma} \int_{-\infty}^{\infty} dx e^{-ikx} e^{-\frac{x^2}{2\sigma^2}} \quad (8.2.53)$$

Since this is symmetric we can multiply the function by two and simply integrate over the positive axis.

$$\hat{F}(k) = \frac{1}{\pi\sigma} \int_0^{\infty} dx e^{-ikx} e^{-\frac{x^2}{2\sigma^2}} \quad (8.2.54)$$

$$= \frac{1}{2\pi} e^{-\frac{\sigma^2 k^2}{2}} \quad (8.2.55)$$

Derivative transforms

Fourier transform is also able to convert derivatives into algebraic terms.

$$\mathcal{F}\{f^{(n)}(t)\} = (i\omega)^n \hat{F}(\omega) \quad (8.2.56)$$

This inversion is simpler than the Laplace transform because we have a simpler integral. From the original transform,

$$\hat{F}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega t} f(t) dt, \quad (8.2.57)$$

our inverse transform is

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t} \hat{F}(\omega) d\omega \quad (8.2.58)$$

It is standard to have first and second order derivatives. So their transforms are

$$\mathcal{F}\{f'(t)\} = i\omega \hat{F}(\omega) \quad (8.2.59)$$

$$\mathcal{F}\{f''(t)\} = -\omega^2 \hat{F}(\omega) \quad (8.2.60)$$

Example: Infinite Insulated Rod

Looking at a variation of the earlier problem, we now have an infinite domain instead of semi-infinite. Say we supply a spike of heat at x_0 . This instantaneous heat is done at $t = 0$.

Thus we have $T(x, 0) = T_0 \delta(x - x_0)$ as our initial condition. Our boundary conditions are such that $T(x \rightarrow \pm\infty, t) \rightarrow 0$.

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad (8.2.61)$$

This may be extended to three-dimensional systems. Applying the Fourier transform with respect to the spacial variable x . So,

$$\mathcal{F} \left\{ \frac{\partial^2 T}{\partial x^2} \right\} = -k^2 \hat{T}(k, t) \quad (8.2.62)$$

and

$$\mathcal{F} \left\{ \frac{\partial T}{\partial t} \right\} = \frac{\partial \hat{T}}{\partial t} \quad (8.2.63)$$

So our equation is now

$$\frac{d\hat{T}}{dt} = -\alpha k^2 \hat{T} \quad (8.2.64)$$

and the initial condition is

$$\hat{T}(k, 0) = \frac{T_0}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \delta(x - x_0) dx \quad (8.2.65)$$

$$= \frac{T_0}{\sqrt{2\pi}} e^{-ikx_0} \quad (8.2.66)$$

The solution is in exponential form,

$$\hat{T}(k, t) = \hat{T}(k, 0) e^{-\alpha k^2 t_0} \quad (8.2.67)$$

$$= \frac{T_0}{\sqrt{2\pi}} e^{-ikx_0} e^{-\alpha k^2 t_0} \quad (8.2.68)$$

Inverting

$$T(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \hat{T}(k, t) dk \quad (8.2.69)$$

$$= \frac{T_0}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ik(x-x_0)} e^{-k^2 \alpha t} dk \quad (8.2.70)$$

$$= \frac{T_0}{\sqrt{2\pi}} e^{-\frac{(x-x_0)^2}{4\alpha t}} \quad (8.2.71)$$

8.3 Lecture 24: November 14, 2012

Convolution Theorem

The convolution theorem tells us how we can take the following integrals,

$$f * g = \int_{-\infty}^{\infty} f(u)g(x-u) du, \quad (8.3.1a)$$

$$= \int_{-\infty}^{\infty} f(x-u)g(u) du. \quad (8.3.1b)$$

So in a Fourier transform

$$\begin{aligned} \mathcal{F}\{f * g\} &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-ikx} \int_{-\infty}^{\infty} du f(u)g(x-u) \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} du g(u) \int_{-\infty}^{\infty} dx e^{-ikx} f(x-u) \end{aligned} \quad (8.3.2)$$

Defining new variables, $z = x - u$ or $x = z + u$, and gives $e^{-ikx} = e^{-ikz}e^{-iku}$. So, the convolution product is

$$\begin{aligned} \mathcal{F}\{f * g\} &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} du g(u) \int_{-\infty}^{\infty} dz e^{-ikz} e^{-iku} f(z) \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} du e^{-iku} g(u) \int_{-\infty}^{\infty} dz e^{-ikz} f(z) \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} du e^{-iku} g(u) \hat{F}(k) \\ &= \frac{1}{\sqrt{2\pi}} \hat{F}(k) \int_{-\infty}^{\infty} du e^{-iku} g(u) \\ &= \frac{1}{\sqrt{2\pi}} \hat{F}(k) \hat{G}(k) \end{aligned} \quad (8.3.3)$$

This gives a non-shifted result, which is useful if you want to remove the offset in one of the multiplying functions.

Example: Radial distribution function

$$g(r) = 1 - h(r) \quad (8.3.4)$$

The Ornstein–Zernike equation, is a special correlation function on the densities of molecules, and is an integral equation. It is difficult to solve and is of the form

$$h(\mathbf{r}) = C(\mathbf{r}) + \int_0^{\infty} h(\mathbf{r} - \mathbf{r}')C(\mathbf{r}') d\mathbf{r}' \quad (8.3.5)$$

For special cases in the Fourier space, we can simplify greatly to

$$\hat{H}(\mathbf{k}) = \hat{C}(\mathbf{k}) + \hat{H}(\mathbf{k})\hat{C}(\mathbf{k}) \quad (8.3.6)$$

The general expression of a Fourier image of a function is,

$$\hat{F}(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \int_{-\infty}^{\infty} f(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d\mathbf{r} \quad (8.3.7)$$

This can be written by components in Cartesian space

$$\hat{F}(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} f(x, y, z) e^{-i(k_x x + k_y y + k_z z)} dx dy dz \quad (8.3.8)$$

$$= \frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} f(x, y, z) e^{-ik_x x} e^{-ik_y y} e^{-ik_z z} dx dy dz \quad (8.3.9)$$

This is powerful because it allows one-dimensional solutions to be potentially composed into three dimensions.

Transform of differential operators

$$\mathcal{F}\{f''(x)\} = -k^2 \hat{F}(k) \quad (8.3.10)$$

The multi-dimensional equivalent, the Laplace operator, is,

$$\nabla^2 f(\mathbf{r}) = -4\pi \delta(\mathbf{r}) \quad (8.3.11)$$

and can be $f(\mathbf{r}) = \frac{1}{r}$. Now

$$\frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} \nabla^2 f(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d\mathbf{r} = \frac{-4\pi}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} \delta(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d\mathbf{r} \quad (8.3.12)$$

The Laplacian is

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} \quad (8.3.13)$$

This can break up the integrals,

$$\begin{aligned} & \frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} \left(\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} \right) e^{-ik_x x} e^{-ik_y y} e^{-ik_z z} dx dy dz \\ &= \frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} \left(\frac{\partial^2 f}{\partial x^2} \right) e^{-ik_x x} e^{-ik_y y} e^{-ik_z z} dx dy dz \\ & \quad + \frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} \left(\frac{\partial^2 f}{\partial y^2} \right) e^{-ik_x x} e^{-ik_y y} e^{-ik_z z} dx dy dz \\ & \quad + \frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} \left(\frac{\partial^2 f}{\partial z^2} \right) e^{-ik_x x} e^{-ik_y y} e^{-ik_z z} dx dy dz \end{aligned}$$

Or simplifying for each term

$$\frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} \left(\frac{\partial^2 f}{\partial x^2} \right) e^{-ik_x x} e^{-ik_y y} e^{-ik_z z} dx dy dz = \frac{(ik_x)^2}{(2\pi)} \iiint_{-\infty}^{\infty} f e^{-ik_x x} e^{-ik_y y} e^{-ik_z z} dx dy dz \quad (8.3.14)$$

this shows that we can simplify to a one dimensional case. Since, $(ik)^2 = -k^2$, we have,

$$\frac{-k_x^2}{(2\pi)} \iiint_{-\infty}^{\infty} \delta(\mathbf{r}) e^{-ik \cdot \mathbf{r}} d\mathbf{r} + \frac{-k_y^2}{(2\pi)} \iiint_{-\infty}^{\infty} \delta(\mathbf{r}) e^{-ik \cdot \mathbf{r}} d\mathbf{r} + \frac{-k_z^2}{(2\pi)} \iiint_{-\infty}^{\infty} \delta(\mathbf{r}) e^{-ik \cdot \mathbf{r}} d\mathbf{r} \quad (8.3.15)$$

$$= \frac{-(k_x^2 + k_y^2 + k_z^2)}{(2\pi)} \iiint_{-\infty}^{\infty} \delta(\mathbf{r}) e^{-ik_x x} e^{-ik_y y} e^{-ik_z z} dx dy dz \quad (8.3.16)$$

distributing out the square root of 2π , we get

$$= -k^2 \hat{F}(\mathbf{k}), \quad \text{where } k^2 = (k_x^2 + k_y^2 + k_z^2) \quad (8.3.17)$$

Thus,

$$\mathcal{F}\{\nabla^2 f\} = -k^2 \hat{F}(\mathbf{k}) \quad (8.3.18)$$

This is a true operation in general. Now we return to our example, where we are doing the Fourier transform of the Greens function for the Laplace operator. Note that

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \delta(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} e^{-ik0} \quad (8.3.19)$$

$$= \frac{1}{\sqrt{2\pi}} \quad (8.3.20)$$

also,

$$\delta(\mathbf{r}) = \delta(x) \delta(y) \delta(z) \quad (8.3.21)$$

So,

$$\frac{-4\pi}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} \delta(x) e^{-ik_x x} \delta(y) e^{-ik_y y} \delta(z) e^{-ik_z z} dx dy dz = \frac{4\pi}{(2\pi)^{2/3}} = -\sqrt{\frac{2}{\pi}} \quad (8.3.22)$$

$$k^2 \hat{F}(\mathbf{k}) = \sqrt{\frac{2}{\pi}} \quad (8.3.23)$$

$$\hat{F}(\mathbf{k}) = \frac{1}{k^2} \sqrt{\frac{2}{\pi}} \quad (8.3.24)$$

and finally,

$$\mathcal{F}\left\{\frac{1}{r}\right\} = \sqrt{\frac{2}{\pi}} \frac{1}{k^2} \quad (8.3.25)$$

Spherical Coordinates

If the system is symmetric we can do many simplifications from the beginning. This lets us define Fourier transforms that correspond to certain symmetries and simply use that to solve problems. Let's look at spherical coordinates. Defining

$$\hat{V}(\mathbf{k}) = \frac{1}{(2\pi)^{2/3}} \iiint_{-\infty}^{\infty} \hat{V}V(|\mathbf{r}|)e^{-i\mathbf{k}\cdot\mathbf{r}} d\mathbf{r} \quad (8.3.26)$$

Now in spherical coordinates,

$$d\mathbf{r} = r^2 dr \sin(\theta) d\theta d\phi \quad (8.3.27)$$

and

$$\mathbf{k} \cdot \mathbf{r} = kr \cos(\theta) \quad (8.3.28)$$

This works in our invariant system. Say we define our \mathbf{k} such that it is in the z -axis; then we will simply have to deal with the polar angle of our system. Now,

$$\hat{V}(\mathbf{k}) = \frac{1}{(2\pi)^{2/3}} \int_0^{\infty} \int_0^{\pi} \int_0^{2\pi} V(|\mathbf{r}|)e^{-ikr \cos(\theta)} r^2 dr \sin(\theta) d\theta d\phi \quad (8.3.29)$$

Phi can easily be integrated out of the system. So, we simplify to a two dimensional integral

$$\hat{V}(\mathbf{k}) = \frac{2\pi}{(2\pi)^{2/3}} \int_0^{\infty} \int_0^{\pi} V(|\mathbf{r}|)e^{-ikr \cos(\theta)} d\cos(\theta) r^2 dr \quad (8.3.30)$$

to integrate the $\cos(\theta)$ term observe

$$\frac{1}{\sqrt{2\pi}} e^{-ikr \cos(\theta)} d\cos(\theta) = \frac{1}{\sqrt{2\pi}} \frac{2 \sin(kr)}{kr} = \sqrt{\frac{2}{\pi}} \frac{\sin(kr)}{kr} \quad (8.3.31)$$

This is the kernel of a function in spherical coordinates. So,

$$\hat{V}(\mathbf{k}) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} V(r) \frac{\sin(kr)}{kr} r^2 dr \quad (8.3.32)$$

This simplifies us to purely radial systems. Now notice, $\frac{\sin x}{x} = j_0(x)$ is the spherical Bessel function or in our case, $\frac{\sin(kr)}{kr} = j_0(kr)$. So we can rewrite our integral,

$$\hat{V}(\mathbf{k}) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} V(r) j_0(kr) r^2 dr \quad (8.3.33)$$

We could recall in the beginning that in spherical coordinates

$$\nabla^2 = \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) \quad (8.3.34)$$

with $C(r)$,

$$\nabla^2 C(r) = \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dC(r)}{dr} \right) \quad (8.3.35)$$

so if we take the integral we notice that the r^2 terms can cancel.

$$\sqrt{\frac{2}{\pi}} \int_0^\infty \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dC(r)}{dr} \right) j_0(kr) r^2 dr = \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{d}{dr} \left(\frac{dC(r)}{dr} \right) j_0(kr) dr \quad (8.3.36)$$

$$= \sqrt{\frac{2}{\pi}} \int_0^\infty j_0(kr) d \left(r^2 \frac{dC}{dr} \right) \quad (8.3.37)$$

$$= \sqrt{\frac{2}{\pi}} \left[j_0(kr) r^2 \frac{dC}{dr} \right]_0^\infty - \sqrt{\frac{2}{\pi}} \int_0^\infty r^2 \frac{dC}{dr} d(j_0(kr)) \quad (8.3.38)$$

$$= -\sqrt{\frac{2}{\pi}} \int_0^\infty r^2 \frac{dC}{dr} d(j_0(kr)) \quad (8.3.39)$$

This can be further solved by integrating properties of the Bessel functions.

Polar Coordinates

Recall now that the radial vector is restricted to a plane,

$$\hat{V}(\mathbf{k}) = \frac{1}{2\pi} \iint_{-\infty}^{\infty} V(r) e^{-i\mathbf{k}\cdot\mathbf{r}} dx dy \quad (8.3.40)$$

$$= \frac{1}{2\pi} \int_0^\infty \int_0^{2\pi} V(r) e^{-ikr \cos(\theta)} d\theta r dr \quad (8.3.41)$$

$$= \frac{1}{2\pi} \int_0^\infty V(r) \left[\int_0^{2\pi} e^{-ikr \cos(\theta)} d\theta \right] r dr \quad (8.3.42)$$

We notice that $\int_0^{2\pi} e^{-ikr \cos(\theta)} d\theta = J_0(kr)$, and

$$\hat{V}(\mathbf{k}) = \frac{1}{2\pi} \int_0^\infty V(r) J_0(kr) r dr \quad (8.3.43)$$

Parsifal Theorem

The *Parsifal theorem* (or Parsifal Relation) is often useful in quantum mechanics. It states that the product of two product of the complex conjugate function ($f^*(t)$), we have

$$\int_{-\infty}^{\infty} f^*(t) f(t) dt = \int_{-\infty}^{\infty} |f(t)|^2 dt \quad (8.3.44)$$

Writing the transform, of the function is

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{F}(\omega) e^{i\omega t} d\omega \quad (8.3.45)$$

and of the complex conjugate is

$$f^*(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{F}^*(\omega) e^{-i\omega t} d\omega \quad (8.3.46)$$

so

$$f^*(t)f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \hat{F}^*(\omega) e^{-i\omega t} \int_{-\infty}^{\infty} d\omega' \hat{F}(\omega') e^{i\omega' t} \quad (8.3.47)$$

Integrating

$$\int_{-\infty}^{\infty} dt f^*(t)f(t) = \int_{-\infty}^{\infty} dt \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega \hat{F}^*(\omega) e^{-i\omega t} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega' \hat{F}(\omega') e^{i\omega' t} \quad (8.3.48)$$

$$= \int_{-\infty}^{\infty} d\omega \hat{F}^*(\omega) \int_{-\infty}^{\infty} d\omega' \hat{F}(\omega') \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{i(\omega' - \omega)t} \quad (8.3.49)$$

The integral at the end is simply a delta function or $\delta(\omega' - \omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{i(\omega' - \omega)t}$ and

$$= \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' \hat{F}^*(\omega) \hat{F}(\omega') \delta(\omega' - \omega) \quad (8.3.50)$$

$$= \int_{-\infty}^{\infty} d\omega \hat{F}^*(\omega) \hat{F}(\omega) \quad (8.3.51)$$

$$= \int_{-\infty}^{\infty} |\hat{F}(\omega)|^2 d\omega \quad (8.3.52)$$

Will do application example next time.

8.4 Lecture 25: November 19, 2012

Momentum Representation

$$\int \Psi^*(x)\Psi(x) dx = \int \Psi^2(x) dx \quad (8.4.1)$$

This is over $[x, x + dx]$

1. Normalization

$$\int \Psi^*(x)\Psi(x) dx = 1 \quad (8.4.2)$$

$$\int \Psi^*(x)x\Psi(x) dx = \langle x \rangle \quad (8.4.3)$$

$$\int \Psi^*(x)A\Psi(x) dx = \langle A \rangle \quad (8.4.4)$$

2. Momentum

Over $[p, p + dp]$, we have $g(p)$

$$g^*(p)g(p) dp \quad (8.4.5)$$

$$\int g^*(p)g(p) dp = 1 \quad (8.4.6)$$

3. Expected value of the momentum

(Note: $\hbar = \frac{h}{2\pi}$)

$$\langle p \rangle = \int g^*(p) p g(p) dp \quad (8.4.7)$$

$$g(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x) e^{-\frac{ipx}{\hbar}} dx \quad (8.4.8)$$

$$g^*(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi^*(x) e^{+\frac{ipx}{\hbar}} dx \quad (8.4.9)$$

In three dimensions,

$$g^*(\mathbf{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \iiint_{-\infty}^{\infty} \Psi^*(\mathbf{r}) e^{+\frac{i\mathbf{r}\cdot\mathbf{p}}{\hbar}} d\mathbf{r} \quad (8.4.10)$$

Now we ask

$$\langle p \rangle = \int_{-\infty}^{\infty} g^*(p) p g(p) dp \stackrel{?}{=} \int_{-\infty}^{\infty} \Psi^* \frac{\hbar}{i} \frac{d}{dx} (\Psi(x)) dx \quad (8.4.11)$$

So,

$$\int_{-\infty}^{\infty} g^*(p) p g(p) dp = \frac{1}{2\pi\hbar} \iiint_{-\infty}^{\infty} e^{-\frac{ip(x-x')}{\hbar}} \Psi^*(x) \Psi(x) dx dx'. \quad (8.4.12)$$

Now,

$$pe^{-\frac{ip(x-x')}{\hbar}} = \frac{d}{dx} \left(-\frac{\hbar}{i} e^{-\frac{ip(x-x')}{\hbar}} \right) \quad (8.4.13)$$

$$\langle p \rangle = \iiint_{-\infty}^{\infty} \left[-\frac{1}{2\pi\hbar} e^{-\frac{ip(x-x')}{\hbar}} dp \right] \Psi^*(x') \frac{\hbar}{i} \frac{d}{dx} (\Psi(x)) dx dx' \quad (8.4.14)$$

We recognize the term in brackets is the Dirac delta function.

$$\langle p \rangle = \iint_{-\infty}^{\infty} \delta(x-x') \Psi^*(x') \frac{\hbar}{i} \frac{d}{dx} (\Psi(x)) dx dx' \quad (8.4.15)$$

$$= \int_{-\infty}^{\infty} \Psi^*(x) \frac{\hbar}{i} \frac{d}{dx} (\Psi(x)) dx \quad (8.4.16)$$

$$= e^{ipx} \quad (8.4.17)$$

Example: Pulse Propagation

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{\nu^2} \frac{\partial^2 y}{\partial t^2} \quad (8.4.18)$$

with initial and boundary conditions,

$$y(t=0, x) = f(x)$$

and

$$f'(x) = 0$$

Using the Fourier transform,

$$\int_{-\infty}^{\infty} \frac{\partial^2 y}{\partial x^2} e^{-ikx} dx = \frac{1}{\nu^2} \int_{-\infty}^{\infty} \frac{\partial^2 y}{\partial t^2} e^{-ikx} dx \quad (8.4.19)$$

which gives the ordinary differential equation,

$$(ik)^2 \hat{y}(k, t) = \frac{1}{\nu^2} \frac{d^2 \hat{y}}{dt^2} \quad (8.4.20)$$

and is rearranged into the Helmholtz equation,

$$\frac{d^2 \hat{y}}{dt^2} + \nu^2 k^2 \hat{y}(k, t) = 0. \quad (8.4.21)$$

The solution is,

$$\hat{y}(k, t) = C(k) e^{\pm ik\nu t} \quad (8.4.22)$$

From the initial condition we get,

$$\hat{F}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \quad (8.4.23)$$

and we find $C(k) = \hat{F}(k)$ or

$$\hat{y}(k, t) = \hat{F}(k) e^{\pm ikvt} \quad (8.4.24)$$

Finally retransforming into,

$$y(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{y}(k, t) e^{ikx} dk \quad (8.4.25)$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \hat{F}(k) e^{\pm ikvt} e^{ikx} \quad (8.4.26)$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \hat{F}(k) e^{i(x \mp vt)k} \quad (8.4.27)$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \hat{F}(k) e^{izk} \quad (8.4.28)$$

$$y(x, t) = f(x \mp vt) \quad (8.4.29)$$

Example: Quantum Oscillator

Finding Greens function to the equation

$$\frac{d^2x}{dt^2} + \beta \frac{dx}{dt} + \omega_0^2 x = f(x) \quad (8.4.30)$$

To do so we will have to solve,

$$\frac{d^2G}{dt^2} + \beta \frac{dG}{dt} + \omega_0^2 G = \delta(t) \quad (8.4.31)$$

with a Fourier transform in time. The individual components become,

$$\mathcal{F} \left\{ \frac{d^2G}{dt^2} \right\} = -\omega^2 \hat{G} \quad (8.4.32)$$

$$\mathcal{F} \left\{ \frac{dG}{dt} \right\} = i\omega \hat{G} \quad (8.4.33)$$

$$\mathcal{F} \{G\} = \hat{G} \quad (8.4.34)$$

$$\mathcal{F} \{\delta(t)\} = \frac{1}{\sqrt{2\pi}} \quad (8.4.35)$$

Substituting into the original equation,

$$-\omega^2 \hat{G} - i\omega\beta \hat{G} + \omega_0^2 \hat{G} = \frac{1}{\sqrt{2\pi}} \quad (8.4.36)$$

$$\hat{G} = \frac{1}{\sqrt{2\pi} (-\omega^2 - i\omega\beta + \omega_0^2)} \quad (8.4.37)$$

To find the roots we substitute $x = i\omega$,

$$-\omega^2 - i\omega\beta + \omega_0^2 = -x^2 - \beta x + \omega_0^2 = 0 \quad (8.4.38)$$

$$x_1 = \frac{1}{2} \left(\beta - 2i\sqrt{\omega^2 - \beta^2/4} \right), \quad (8.4.39a)$$

$$x_2 = \frac{1}{2} \left(\beta + 2i\sqrt{\omega^2 - \beta^2/4} \right); \quad (8.4.39b)$$

$$x_1 = -z_1, \quad (8.4.40a)$$

$$x_2 = -z_2. \quad (8.4.40b)$$

The Greens function is now,

$$\begin{aligned} \hat{G} &= \frac{1}{\sqrt{2\pi} (z_1 + i\omega) (z_2 + i\omega)} \\ &= \frac{1}{\sqrt{2\pi}} \frac{1}{z_2 - z_1} \left(\frac{1}{z_1 + i\omega} - \frac{1}{z_2 + i\omega} \right) \end{aligned} \quad (8.4.41)$$

Transforming back to normal space

$$G = \frac{e^{z_1 t}}{z_2 - z_1} \theta(t) - \frac{e^{z_2 t}}{z_2 - z_1} \theta(t) \quad (8.4.42)$$

$$G = \frac{e^{-\beta t/2}}{\omega_1} \sin(\omega_1 t) \theta(t) \quad (8.4.43)$$

where $\omega_1 = \sqrt{\omega_0^2 - \beta^2/4}$. Thus, our solution goes to

$$\frac{d^2 x}{dt^2} + \beta \frac{dx}{dt} + \omega_0^2 x = f(x) \quad (8.4.44)$$

is

$$x(t) = \int G(t - t') f(t') dt' \quad (8.4.45)$$

where $G(t)$ is given above.

Example: Total solution of the diffusion equation

In heat, mass (diffusion), and momentum (viscous) transport we get the equation,

$$\frac{\partial F}{\partial t} = a \frac{\partial^2 F}{\partial x^2} \quad (8.4.46)$$

This equation has a fundamental solution, which is similar to the Green function. We will now derive it in a fundamental way. We will use a Laplace transform in time and a Fourier transform in space. Transforming with Laplace

$$\mathcal{L}\{F\} = \tilde{F} \quad (8.4.47)$$

$$\mathcal{L}\left\{\frac{\partial F}{\partial t}\right\} = s\tilde{F} - F_0 \quad (8.4.48)$$

$$\mathcal{L}\left\{\frac{\partial^2 F}{\partial x^2}\right\} = \frac{\partial^2 \tilde{F}}{\partial x^2} \quad (8.4.49)$$

We denote,

$$\mathcal{F}\{F\} = \hat{F} \quad (8.4.50)$$

$$\mathcal{F}\{\tilde{F}\} = \hat{\tilde{F}}$$

$$\mathcal{F}\left\{\frac{\partial^2 F}{\partial x^2}\right\} = (ik)^2 \hat{F}$$

$$\mathcal{F}\left\{\frac{\partial^2 F}{\partial x^2}\right\} = -k^2 \hat{F} \quad (8.4.51)$$

So we can transform our full equation to,

$$s\hat{\tilde{F}} - F_0 = -ak^2 \hat{\tilde{F}} \quad (8.4.52)$$

$$(s + ak^2) \hat{\tilde{F}} = F_0$$

$$\hat{\tilde{F}} = \frac{F_0}{(s + ak^2)} \quad (8.4.53)$$

We have $\hat{\tilde{F}} = \hat{\tilde{F}}(s, k)$

$$\mathcal{L}^{-1}\{\hat{\tilde{F}}\} = \hat{F} = F_0 e^{-k^2 at} \quad (8.4.54)$$

$$\mathcal{F}^{-1}\{F_0 e^{-k^2 at}\} = \frac{F_0}{\sqrt{2at}} e^{-\frac{x^2}{4at}} \quad (8.4.55)$$

or our solution is,

$$F(x, t) = \frac{F_0}{\sqrt{2at}} e^{-\frac{x^2}{4at}} \quad (8.4.56)$$

The mean-square displacement of the function is

$$\langle x^2 \rangle = \frac{\int_{-\infty}^{\infty} x^2 \frac{1}{\sqrt{2at}} e^{-\frac{x^2}{4at}} dx}{\int_{-\infty}^{\infty} \frac{1}{\sqrt{2at}} e^{-\frac{x^2}{4at}} dx} \quad (8.4.57)$$

which simplifies to,

$$\langle x^2 \rangle = 2at \tag{8.4.58}$$

UNIT 9

Chapter 20—Calculus of Variations

9.1 Lecture 26: November 26, 2012

Definitions

functionals: Consider a function as a rule; *e.g.* $y = x$ or $y = x^2$. Now a functional is where we have a number associated with a function; much like a function of functions. *e.g.* $f(x) \rightarrow$ number.

$$I = \int_0^1 f(x) dx$$

where we could have $f(x) = x$ or $y = x^2$ or $y = e^x$.

One of the most important things in calculus is finding of minima and maxima. For mechanical equilibrium (or equilibrium in general) means that the sum of all forces is zero. *i.e.*

$$\sum_i \mathbf{F}_i = 0 \quad (9.1.1)$$

in a potential field we have $\mathbf{F}_i = \nabla u_i$, and

$$\nabla \sum_i u_i = 0 \quad (9.1.2)$$

Minimizing a system also plays into thermodynamics. Entropy is the most general function useful. Gibbs (Josiah Willard Gibbs) showed that the system may be expressed by other variables and used for showing the minima of our system. Say we have our internal energy $U(S, N, V)$,

$$dU = T dS - p dV + \mu dN \quad (9.1.3)$$

or from calculus we can show the differential may be expressed as,

$$dU = \frac{\partial U}{\partial S} dS + \frac{\partial U}{\partial V} dV + \frac{\partial U}{\partial N} dN \quad (9.1.4)$$

$$0 = \left(\frac{\partial U}{\partial S} \right)_{V,N} = T \quad (9.1.5)$$

For the *Helmholtz free energy*, we want a function which is simply a function of measurable variables, *i.e.* $A(N, V, T)$. In the *Gibbs free energy*, we have a function, $G(N, p, T)$ and for the *enthalpy* we have a function, $H(S, p, N)$. From Onsager, ϕ . Now we can have a system where $A(N(z), V, T)$. This becomes a variational problem because we want to minimize the Helmholtz free energy based on the function of the position of the atoms in the system. Now one special careful consideration must be made; for using a variational expression we *must* assume the system is reversible or conservative.

The Euler Equation

Another example of variational calculus is the demonstration of the shortest distance between two points. It may be shown that the shortest distance in a Cartesian plane is in fact a straight line. So, say we define a differential distance,

$$ds^2 = dx^2 + dy^2 \quad (9.1.6)$$

or,

$$ds^2 = \left(1 + \left(\frac{dy}{dx} \right)^2 \right) dx \quad (9.1.7)$$

$$ds = \sqrt{1 + \left(\frac{dy}{dx} \right)^2} dx \quad (9.1.8)$$

Then our straight line is found by minimizing,

$$L = \int_a^b \sqrt{1 + \left(\frac{dy}{dx} \right)^2} dx \quad (9.1.9)$$

This is the Euler–Lagrange equation. In a more general form,

$$I = \int_a^b F(x, y(x), y'(x)) dx \quad (9.1.10)$$

and we care about the extrema: either I_{\min} or I_{\max} . To show the cases of minima, maxima and inflection points, we need to use second derivatives. In the calculus of variations this may be done by the “second variation”. We will not go into this in this course because it is fairly involved. So returning to the above equation, I is a functional of $y(x)$ and we usually care about a minimization problem. So say we have,

$$Y(x, \varepsilon) = y(x) + \varepsilon\eta(x) \quad (9.1.11)$$

where we also restrict $\eta(a) = \eta(b) = 0$. Now we must have that the functional is at least second-order partial differentiable. So,

$$F = F [x, Y(x, \varepsilon), Y'(x, \varepsilon)] \quad (9.1.12)$$

Let's use this for the integral,

$$I = \int_a^b F[x, Y(x, \varepsilon), Y'(x, \varepsilon)] dx \quad (9.1.13)$$

If $y(x)$ is in fact tending to an extremum then $I(\varepsilon) \rightarrow I_{ext}$ as $\varepsilon \rightarrow 0$. Or we have

$$\left. \frac{dI}{d\varepsilon} \right|_{\varepsilon=0} = 0 \quad (9.1.14)$$

$$\frac{dI}{d\varepsilon} = \int_a^b \left(\frac{\partial F}{\partial Y} \frac{\partial Y}{\partial \varepsilon} + \frac{\partial F}{\partial Y'} \frac{\partial Y'}{\partial \varepsilon} \right) dx \quad (9.1.15)$$

Now,

$$\frac{\partial Y}{\partial \varepsilon} = \eta(x) \quad (9.1.16)$$

$$\frac{\partial Y'}{\partial \varepsilon} = \frac{\partial}{\partial \varepsilon}(y'(x) + \varepsilon \eta'(x)) = \eta'(x) \quad (9.1.17)$$

$$\frac{dI}{d\varepsilon} = \int_a^b \left[\frac{\partial F}{\partial y} \eta(x) + \frac{\partial F}{\partial y'} \eta'(x) \right] dx \quad (9.1.18)$$

as our $\varepsilon \rightarrow 0$. $Y(x, \varepsilon) \rightarrow y(x)$, and $Y'(x, \varepsilon) \rightarrow y'(x)$ and $\frac{\partial F}{\partial Y} \rightarrow \frac{\partial F}{\partial y}$ and $\frac{\partial F}{\partial Y'} \rightarrow \frac{\partial F}{\partial y'}$.

$$\int_a^b \left[\frac{\partial F}{\partial y} \eta(x) + \frac{\partial F}{\partial y'} \eta'(x) \right] dx = 0 \quad (9.1.19)$$

since $\eta(a)\eta(b) = 0$ or,

$$\int_a^b \frac{\partial F}{\partial y} \frac{\partial \eta}{\partial x} dx = \int_a^b \frac{\partial F}{\partial y'} d\eta \frac{d\eta}{dx} dx \quad (9.1.20)$$

$$= \left[\frac{\partial F}{\partial y'} \right]_a^b - \int_a^b \eta(x) d \left(\frac{\partial F}{\partial y'} \right) \quad (9.1.21)$$

from the side conditions we have the left portion is simply zero.

$$= - \int_a^b \eta(x) \frac{\partial}{\partial x} \left(\frac{\partial F}{\partial y'} \right) dx \quad (9.1.22)$$

$$\int_a^b \left(\frac{\partial F}{\partial y} \eta(x) + \frac{\partial F}{\partial y'} \frac{\partial \eta}{\partial x} \right) dx = \int_a^b \left(\frac{\partial F}{\partial y} \eta(x) - \frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) \eta(x) \right) dx \quad (9.1.23)$$

$$= \int_a^b \left(\frac{\partial F}{\partial y} - \frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) \right) \eta(x) dx \quad (9.1.24)$$

which gives the Euler equation,

$$\frac{\partial F}{\partial y} - \frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) = 0 \quad (9.1.25)$$

Example 1 in the book is the shortest distance between two points in a plane. Example 2 in the book is on the great circle route, or the shortest line over a sphere; this is the geodesic line. Say our function $F(y(x), y'(x))$ but not on x explicitly. In this case,

$$\frac{d}{dx} \left(y' \frac{\partial F}{\partial y'} \right) = y' \frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) + y'' \frac{\partial F}{\partial y'} \quad (9.1.26)$$

from the Euler equation, we have $\frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) = \frac{\partial F}{\partial y}$. Using this,

$$\frac{d}{dx} \left(y' \frac{\partial F}{\partial y'} \right) = y' \frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) + y'' \frac{\partial F}{\partial y'} \quad (9.1.27)$$

$$= \frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) \frac{dy}{dx} + \frac{\partial F}{\partial y'} \frac{dy'}{dx} \quad (9.1.28)$$

$$= \frac{dF}{dx} \quad (9.1.29)$$

This gives that,

$$y' \frac{\partial F}{\partial y'} - F = \text{const} = c \quad (9.1.30)$$

The above equation is the important one for finding shapes of surfaces.

Example: Brachistrone Problem

Bernoulli (Jacob Bernoulli) asked the following question: say we have two points that are connected by a wire. What is the trajectory that gives the fastest connection? This problem is known as the *Bernoulli brachistrone*. Say we start at a ; we would have that

$$\frac{mv^2}{2} = mgy \quad (9.1.31)$$

or

$$\frac{v^2}{2} = gy \quad (9.1.32)$$

and

$$v = \sqrt{2gy} \quad (9.1.33)$$

The time,

$$\tau = \int_a^b \frac{1}{v} ds \quad (9.1.34)$$

$$ds^2 = dx^2 + dy^2$$

$$\frac{ds}{v} = \frac{(1 + (y')^2)}{\sqrt{2gy}} dx \quad (9.1.35)$$

So we are looking for a minimum of,

$$\tau = \int_a^b \frac{(1 + (y')^2)}{\sqrt{2gy}} dx \quad (9.1.36)$$

From above,

$$y' \frac{\partial F}{\partial y'} - F = \text{const} = c \quad (9.1.37)$$

$$\frac{\partial F}{\partial y'} = \frac{\partial}{\partial y'} \left(\frac{(1 + (y')^2)}{\sqrt{2gy}} \right) = \frac{y'}{[2gy(1 + (y')^2)]^{1/2}} \quad (9.1.38)$$

$$y' \frac{\partial F}{\partial y'} = \frac{(y')^2}{[2gy(1 + (y')^2)]^{1/2}} \quad (9.1.39)$$

Subtracting,

$$\frac{y' - (1 - (y')^2)}{[2gy(1 + (y')^2)]^{1/2}} = C \quad (9.1.40)$$

$$\frac{-1}{[2gy(1 + (y')^2)]^{1/2}} = C_1 \quad (9.1.41)$$

$$y(1 + (y')^2) = \frac{1}{2gC_1^2} = C_2 \quad (9.1.42)$$

$$1 + \left(\frac{dy}{dx} \right)^2 = \frac{C}{y} \quad (9.1.43)$$

$$\frac{dy}{dx} = \left(\frac{C - y}{y} \right)^{1/2} \quad (9.1.44)$$

This gives an integrable equation,

$$\left(\frac{y}{C - y} \right)^{1/2} dy = dx \quad (9.1.45)$$

with a solution of,

$$x = \sqrt{\frac{C}{y} - 1} \left(y + \frac{C\sqrt{y} \arctan\left(\sqrt{\frac{y}{C-y}}\right)}{\sqrt{C-y}} \right) \quad (9.1.46)$$

$$y = \frac{C}{2} (1 - \cos(\theta)) \quad (9.1.47)$$

$$= \frac{C}{2} (\theta - \sin(\theta)) + C_2 \quad (9.1.48)$$

9.2 Lecture 27: November 28, 2012

Example: Classical Mechanics

Lagrange was one of the original formulators of the calculus of variations. For

$$\nabla u = 0 \quad (9.2.1)$$

we have equilibrium.

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial y} = \frac{\partial u}{\partial z} = 0 \quad (9.2.2)$$

Hamilton's formulation of the *principle of least action*.

$$I = \int_{t_1}^{t_2} L(q, q', t) dt \quad (9.2.3)$$

The action I is found from the path that gives a minimal value. The Euler–Lagrange equation is,

$$\frac{\partial L}{\partial q} - \frac{d}{dt} \left(\frac{\partial L}{\partial q'} \right) = 0 \quad (9.2.4)$$

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt} \left(\frac{\partial L}{\partial q'_i} \right) = 0 \quad (9.2.5)$$

For $L = L(q_1, q_2, \dots, q_s; q'_1, q'_2, \dots, q'_s; t)$,

$$L_1(q, q', t) = L(q, q', t) + \frac{df(q, t)}{dt} \quad (9.2.6)$$

$$I_1 = \int_{t_1}^{t_2} L_1(q, q', t) dt \quad (9.2.7)$$

$$= \int_{t_1}^{t_2} L(q, q', t) dt + \int_{t_1}^{t_2} \frac{df(q, t)}{dt} dt \quad (9.2.8)$$

$$= \int_{t_1}^{t_2} L(q, q', t) dt + f(t_2) - f(t_1) \quad (9.2.9)$$

The *Lagrangian* is

$$L = K - V \quad (9.2.10)$$

and the integral over it is the action. The *Hamiltonian* is

$$E_{\text{tot}} = K + V \quad (9.2.11)$$

In a real system, q_i can be x, y, z , the kinetic energy is $K = \frac{m}{2} (x'^2 + y'^2 + z'^2)$, and $V = V(x, y, z)$.

$$\frac{\partial L}{\partial x} - \frac{d}{dt} \left(\frac{\partial L}{\partial x'} \right) = 0 \quad (9.2.12)$$

or,

$$\frac{\partial L}{\partial x} = \frac{d}{dt} \left(\frac{\partial L}{\partial x'} \right) \quad (9.2.13)$$

$$L = K - V = \frac{m}{2} (x'^2 + y'^2 + z'^2) - V(x, y, z) \quad (9.2.14)$$

Substituting into the Euler–Lagrange equation (9.2.12).

$$\frac{\partial L}{\partial x} = -\frac{\partial V}{\partial x} = F_x \quad (9.2.15)$$

$$\frac{\partial L}{\partial x'} = \frac{m}{2} 2x' = mx' \quad (9.2.16)$$

$$\frac{d}{dt} \left(\frac{\partial L}{\partial x'} \right) = \frac{d(mx')}{dt} \quad (9.2.17)$$

$$= \frac{dF_x}{dt} \quad (9.2.18)$$

$$= m \frac{dv_x}{dt} \quad (9.2.19)$$

$$m \frac{dv_x}{dt} = -\frac{\partial V}{\partial x} = F_x. \quad (9.2.20)$$

Example: Double pendulum

Find the Lagrange function for the case that we have a pendulum hanging from the ceiling with ϕ_1 angle from the ceiling and a mass, m_1 , at the end. There it is attached to another pendulum of angle ϕ_2 from the vertical and a mass, m_2 hanging from the end. So,

- m_1 : $K_1 = \frac{1}{2}m_1 l_1^2 \dot{\phi}_1^2$
- m_2 : $x_2 = l_1 \sin(\phi_1) + l_2 \sin(\phi_2)$

$$y_2 = l_1 \cos(\phi_1) + l_2 \cos(\phi_2)$$

$$K_2 = \frac{m_2}{2} (x'^2 + y'^2) = \frac{m_2}{2} [l_1^2 \dot{\phi}_1^2 + l_2^2 \dot{\phi}_2^2 + 2l_1 l_2 \cos(\phi_1 - \phi_2) \dot{\phi}_1 \dot{\phi}_2]$$

$$V_2 = -m_2 g C_1 \cos(\phi_1) - m_1 g l_2 \cos(\phi_2) \quad (9.2.21)$$

$$L = \frac{m_1 + m_2}{2} l_1^2 \dot{\phi}_1^2 + \frac{m_2}{2} l_2^2 \dot{\phi}_2^2 + m_2 l_1 l_2 \dot{\phi}_1 \dot{\phi}_2 \cos(\phi_1 - \phi_2) + (m_1 + m_2) g l_1 \cos(\phi_1) + m_2 l_2 \cos(\phi_2) \quad (9.2.22)$$

For another system of a single oscillator,

$$L = \left(\frac{m_1 + m_2}{2} \right) x'^2 + \frac{m_2}{2} (l^2 \dot{\phi}^2 + 2lx' \dot{\phi} \cos(\phi)) + m_2 g l \cos(\phi) \quad (9.2.23)$$

We apply the Euler–Lagrange equation,

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt} \left(\frac{\partial L}{\partial q_i'} \right) = 0, \quad \text{because } q_i \rightarrow x_1 \varphi \quad (9.2.24)$$

$$\frac{\partial L}{\partial x} - \frac{d}{dt} \left(\frac{\partial L}{\partial x'} \right) = 0 \quad (9.2.25)$$

$$\frac{\partial L}{\partial \varphi} - \frac{d}{dt} \left(\frac{\partial L}{\partial \varphi'} \right) = 0 \quad (9.2.26)$$

$$\frac{\partial L}{\partial x} = 0 \quad (9.2.27)$$

$$\frac{\partial L}{\partial x'} = (m_1 + m_2) x' + \frac{m_2}{2} 2l\varphi' \cos(\varphi) \quad (9.2.28)$$

$$\frac{d}{dt} \left(\frac{\partial L}{\partial x'} \right) = (m_1 + m_2) \frac{d^2 x}{dt^2} + m_2 l \frac{d^2 \varphi}{dt^2} - m_2 l \left(\frac{d\varphi}{dt} \right)^2 \sin(\varphi) = 0 \quad (9.2.29)$$

$$\frac{\partial L}{\partial \varphi} = \frac{-2m_2}{2} 2lx' \sin(\varphi) - m_2 gl \sin(\varphi) \quad (9.2.30)$$

$$\frac{\partial L}{\partial \varphi'} = m_2 l \varphi' + m_2 l x' \cos(\varphi) \quad (9.2.31)$$

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \varphi'} \right) = m_2 l \frac{d^2 \varphi}{dt^2} + m_2 l \cos(\varphi) \frac{d^2 x}{dt^2} - m_2 l \frac{dx}{dt} \sin(\varphi) \frac{d\varphi}{dt} \quad (9.2.32)$$

Integrals of Motion—Conservation of Energy

$$L = L(q, q', t) \quad (9.2.33)$$

in steady state,

$$L = L(q, q') \quad (9.2.34)$$

Then,

$$\frac{dL}{dt} = \sum_i \frac{\partial L}{\partial q_i} q_i' + \sum_i \frac{\partial L}{\partial q_i'} q_i'' \quad (9.2.35)$$

$$\frac{\partial L}{\partial q_i} = \frac{d}{dt} \left(\frac{\partial L}{\partial q_i'} \right) \quad (9.2.36)$$

$$= \sum_i q_i' \frac{d}{dt} \left(\frac{\partial L}{\partial q_i'} \right) + \sum_i \frac{\partial L}{\partial q'} q'' = \sum_i \frac{d \frac{\partial L}{\partial q'} q'}{dt} = \frac{dL}{dt} \quad (9.2.37)$$

$$\frac{d}{dt} \left(\sum \frac{\partial L}{\partial q'} q' - L \right) = 0 \quad (9.2.38)$$

$$E = \sum \frac{\partial L}{\partial q'} q' - L = \text{constant with respect to time} \quad (9.2.39)$$

$$L = K - V \quad (9.2.40)$$

$$K = \sum_{k,l} \gamma_{kl} q'_k q'_l \quad (9.2.41)$$

$$\sum_i q'_i \frac{\partial L}{\partial q'} = \frac{\partial}{\partial q'_i} \left(\sum \gamma_{kl} q'_k q'_l \right) = \frac{\partial q'_k}{\partial q'_i} = \delta_{ki} = \delta_{ik} \quad (9.2.42)$$

$$\sum \frac{\partial}{\partial q'_i} \left(\sum_k \gamma_{kl} q'_k q'_l + \sum_l \gamma_{kl} q'_k q'_l \right) q'_i = \sum_i \left(\sum_l \gamma_{kl} q'_l + \sum_k \gamma_{kl} q'_k \right) q'_i \quad (9.2.43)$$

$$= \sum_i \left(\sum_l \gamma_{il} q'_l q'_i + \sum_l \gamma_{il} q'_i q'_l \right) \quad (9.2.44)$$

$$= 2K \quad (9.2.45)$$

9.3 Lecture 28: December 3, 2012

The Variation

1.

$$\frac{df(x)}{dx} = 0 \quad (9.3.1)$$

for $x = x^*$ is similar to

$$\frac{\delta I}{\delta y} = 0 \quad (9.3.2)$$

for $y = y_{\text{ext}}$. We have

$$I = \int F(y, y', x) dx \quad (9.3.3)$$

$$\frac{\partial F}{\partial y} - \frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) = 0 \quad (9.3.4)$$

These become important for applications in density distributions, shapes of capillary surfaces, equations of motion, and the wave function in quantum mechanics.

Example: Low density gas

Assuming no viscous stress, dilute gaseous solution, we have a symmetric object flying through the air. The pressure

$$p = 2\rho v^2 \sin^2(\theta) \quad (9.3.5)$$

the total drag force on the surface is the integral of the pressure over the surface. $F = pA$ or in general $F = \iint p dA$. So from a differential ring, we get

$$\begin{aligned} \int_{F(0)}^{F(w)} dF &= 2\rho v^2 \int_0^w \sin^3(\theta) \left[2\pi y (1 + y'^2)^{1/2} \right] dx \\ F &= \int_0^w 4\pi\rho v^2 \sin^3(\theta) \left[2\pi y (1 + y'^2)^{1/2} \right] dx \end{aligned} \quad (9.3.6)$$

so $\sin(\theta) \sim \frac{y_x}{\sqrt{1+y_x^2}}$ for $y_x = \frac{dy}{dx}$ and for small y_x $\frac{y_x}{\sqrt{1+y_x^2}} \approx y_x$. This excludes the zone of the tip for the approximation.

$$F = 4\pi\rho v^2 \int_0^w y_x^3 y dx \quad (9.3.7)$$

setting $G = y_x^3 y$

$$\frac{\partial G}{\partial y} - \frac{d}{dx} \left(\frac{\partial G}{\partial y_x} \right) = 0 \quad (9.3.8)$$

Now $G(y, y_x)$, so

$$\frac{\partial G}{\partial y} = y_x^3 \quad (9.3.9)$$

$$\frac{\partial G}{\partial y_x} = y \frac{\partial y_x^3}{\partial y_x} = 3y y_x^2 \quad (9.3.10)$$

and substituting

$$y_x^3 + 3yy_x y_{xx} = 0 \quad (9.3.11)$$

$$y_x^3 y = C_1^3$$

$$\left(\frac{dy}{dx}\right)^3 y = C_1^3$$

$$\frac{dy}{dx} = \frac{C_1}{\sqrt[3]{y}} \quad (9.3.12)$$

Integrating,

$$y^{1/3} dy = C_1 dx$$

$$\frac{4}{3} \int dy^{4/3} = C_1 \int dx$$

$$y^{4/3} = C_1 x$$

$$\boxed{y = (C_1 x)^{3/4}}. \quad (9.3.13)$$

which gives the solution over the long domain. This allows for minimizing drag.

Similar to Stokes flow around a sphere $F = 6\pi\mu RU$,

$$F = \int_{\text{surface}} \boldsymbol{\sigma} \cdot \mathbf{n} dA + \int_{\text{surface}} \boldsymbol{\tau} \cdot \mathbf{n} dA \quad (9.3.14)$$

Constrained minimization and maximization

Given arbitrary function, taking a total derivative of a function $F(x, y, z)$,

$$dF = \left(\frac{\partial F}{\partial x}\right)_{y,z} dx + \left(\frac{\partial F}{\partial y}\right)_{x,z} dy + \left(\frac{\partial F}{\partial z}\right)_{x,y} dz \quad (9.3.15)$$

If we add in the function $G(x, y, z) = \text{const}$, this creates a constraint to the system and that the equation dF is not a total differential. However, $d(F - \lambda G)$ is a new function. The λ is the *Lagrange multiplier*.

From Thermodynamics, the *First Law* is

$$dU = \left(\frac{\partial U}{\partial S}\right) dS + \left(\frac{\partial U}{\partial V}\right) dV + \left(\frac{\partial U}{\partial N}\right) dN \quad (9.3.16)$$

where S, V, N are the entropy, volume, and number of molecules, respectively. This gives $\left(\frac{\partial U}{\partial S}\right) = T$, $\left(\frac{\partial U}{\partial V}\right) = -P$, and $\left(\frac{\partial U}{\partial N}\right) = \mu$. For the Helmholtz free energy we have $A(T, V, N)$. Using a simple constraint we can derive the equation for the Helmholtz free energy from the expression $U(S, V, N)$. So, say we have the condition $\lambda S = TS = \text{const}$. Say

$$d(U - TS) = dU - d(TS).$$

Then

$$d(TS) = T dS + S dT = 0 \quad (9.3.17)$$

$$\begin{aligned} d(U - TS) &= T dS - p dV + \mu dN - T dS - S dT \\ &= -S dT - p dV + \mu dN \end{aligned} \quad (9.3.18)$$

This illustrates an interesting application of constraints and minimization.

Variations with Constraints

$$I = \int_a^b F(y, y', x) dx \quad (9.3.19)$$

Now say we have some constraint,

$$J = \int_a^b G(y, y', x) dx \quad (9.3.20)$$

Interestingly, we can use the same approach to solve this problem.

Example: Hanging Cable

From the above relations, we have that J is the constraint of the length of the cable. Using the Lagrange multiplier with the definition, $K = I + \lambda J$. In this case we know for this problem that $J = 2C$ which is a simple input parameter. So substituting K , into the Euler equation,

$$\frac{\partial}{\partial y}(F + \lambda G) - \frac{d}{dx} \left(\frac{\partial}{\partial y'}(F + \lambda G) \right) = 0 \quad (9.3.21)$$

the system can be solved in the usual manner.

If $F + \lambda G$ do not depend on y then,

$$\frac{\partial}{\partial y'}(F + \lambda G) = \text{const w.r.t. } x \quad (9.3.22)$$

If $F + \lambda G$ does not depend on x explicitly,

$$y' \frac{\partial}{\partial y'}(F + \lambda G) - (F + \lambda G) = \text{const} \quad (9.3.23)$$

So with the hanging cable we have a system going from $[-a, a]$ in x and the y coordinate is the height of the cable. We have lengths l going between $[0, \pm a]$ for a total length of $2l$. The cable as a whole must minimize the potential energy or

$$I = \int \rho g y ds \quad (9.3.24)$$

We must assume constant density, perfectly flexible cable, and constant gravitational field. The constraint is

$$J = \int_{-a}^a ds = 2l$$

The expression of the differential is,

$$ds = (1 + y_x^2)^{1/2} dx \quad (9.3.25)$$

So our system and constraints are

$$I = \int_{-a}^a \rho g y (1 + y_x^2)^{1/2} dx \quad (9.3.26)$$

$$J = \int_{-a}^a (1 + y_x^2)^{1/2} dx = 2l \quad (9.3.27)$$

So we define $F(y, y', x) = \rho g y (1 + y_x^2)^{1/2}$, and $G(y, y', x) = (1 + y_x^2)^{1/2}$. By nature there is no explicit dependence of the system on x .

$$y' \frac{\partial}{\partial y'} \left(\rho g y (1 + y_x^2)^{1/2} - \lambda (1 + y_x^2)^{1/2} \right) - \left[\rho g y (1 + y_x^2)^{1/2} - \lambda (1 + y_x^2)^{1/2} \right] = C_1 \quad (9.3.28)$$

with (extensive) differentiation and simplifying, we have

$$\rho g y - \lambda = (1 + y_x^2)^{1/2} \quad (9.3.29)$$

This is then solved,

$$y_x^2 = \left(\frac{\rho g y - \lambda}{C_1} \right)^2 - 1$$

$$y_x = \sqrt{\left(\frac{\rho g y - \lambda}{C_1} \right)^2 - 1}$$

Rearranging, we get,

$$C_1 \int \frac{dy}{\sqrt{(\rho g y - \lambda)^2 - C_1^2}} = x \quad (9.3.30)$$

9.4 Lecture 29: December 5, 2012

Example: Hanging Cable, cont.

Returning to previous example; we had previously derived

$$C_1 \int \frac{dy}{\sqrt{(\rho gy - \lambda)^2 - C_1^2}} = x. \quad (9.4.1)$$

Now we substitute $(\rho gy - \lambda) = C_1 \cosh(z)$, along with

$$dy = \frac{C_1}{\rho g} \sinh(z) dz, \quad (9.4.2)$$

and rewrite the equation

$$x = \frac{C_1^2}{\rho g} \int \frac{\sinh(z)}{C_1 \sqrt{\cosh^2(z) - 1}} dz. \quad (9.4.3)$$

Substituting again $\sqrt{\cosh^2(z) - 1} = \sinh z$,

$$\begin{aligned} x &= \frac{C_1}{\rho g} \int dz \\ &= \frac{C_1}{\rho g} z + C_2. \end{aligned}$$

with

$$z = \frac{\rho g(x - C_2)}{C_1}$$

we set

$$z = \cosh^{-1} \left(\frac{(\rho gy - \lambda)}{C_1} \right), \quad (9.4.4a)$$

$$= \frac{\rho g(x - C_2)}{C_1}. \quad (9.4.4b)$$

Finally we get the solution

$$\boxed{(\rho gy - \lambda) = C_1 \cosh \left(\frac{\rho g(x - C_2)}{C_1} \right)}. \quad (9.4.5)$$

For final exam

You may use Mathematica[®], MATLAB[®], *etc.* (No help from other students). Note that solutions on this exam will be general solutions for the system (*i.e.* without numerical values).

First Problem

Cube of sides a, b, c and a non-steady state problem. IC: $T(t=0) = 0$, surfaces heated (BCs) $T(t>0) = T_s$.

Second Problem

Problem solved in class:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} + f(x, t)$$

Now solve similar,

$$\frac{\partial^2 F}{\partial x^2} + \frac{\partial^2 F}{\partial y^2} = f(x, y) \quad (9.4.6)$$

with boundary conditions,

$$\begin{aligned} F(x=0, y) &= F_0 \\ F(x=a, y) &= 0 \\ \left. \frac{\partial F}{\partial y} \right|_{y=0} &= 0 \\ \left. \frac{\partial F}{\partial y} \right|_{y=b} &= 0 \end{aligned}$$

Expand $f(x, y)$ as a series along the x axis.

Third Problem

In class we solved,



Now we have



This gives the system,

$$\frac{dC_A}{dt} = -k_1 C_A + k_2 C_B, \quad (9.4.8a)$$

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B - k_3 C_B, \quad (9.4.8b)$$

$$\frac{dC_C}{dt} = k_3 C_B, \quad (9.4.8c)$$

and may be solved similarly.

Fourth Problem

$$L = m_0 c \left(1 - \sqrt{1 - \frac{v^2}{c^2}} \right) - V(\mathbf{r}) \quad (9.4.9)$$

$$v^2 = v_x^2 + v_y^2 + v_z^2$$

$$r^2 = x^2 + y^2 + z^2$$

Perform for x component (at least) to show the generalization of Newton's Third Law. Observe that c is the speed of light.

Fifth Problem

The cylindrical Bessel (Hankel) function in

$$\int_0^\infty \left[\frac{1}{r} \frac{d}{dr} \left(r \frac{dF}{dr} \right) \right] J_0(kr) r \, dr = -k^2 \hat{F}(k) \quad (9.4.10)$$

with $\hat{F}(k) = \int_0^\infty F(r) J_0(kr) r \, dr$

You will need the identity, $J_0(kr) = \frac{2}{kr} J_1(kr) - J_2(kr)$

UNIT 10

Asymptotic Analysis and Perturbation Theory

10.1 Lecture 26: November 18, 2013

Asymptotic Perturbation Techniques for Solving Nonlinear Differential Equations

Several useful books are out there that discuss perturbation methods. Note that this material is not in the textbook, but may be found in books such as,

- Nayfeh *Introduction to Perturbation Techniques*, Wiley 1993;
- Nayfeh *Perturbation Methods*, Wiley 2000;
- Van Dyke *Perturbation Methods in Fluid Mechanics*, Parabolic Press 1975.

First we will be discussing the general idea of these methods. This will help to illustrate the power of the methods. Then we will cover some simpler problems in detail. So say we have a small parameter and take a power series around it. This will not be in terms of an independent variable or the eigenfunctions, but by the small parameter. The choice of parameter is dictated by the physics of the problem.

Asymptotic Example: Navier–Stokes Equations

One major example of the use of asymptotic methods is in the *Navier–Stokes equations* of fluid flow. The vector equation is

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\nabla P - \mu \nabla^2 \mathbf{v}. \quad (10.1.1)$$

This gives us in fact four unknowns to solve for. The equation of mass must also be included to fully describe the system;

$$\nabla \cdot \mathbf{v} = 0. \quad (10.1.2)$$

This is a difficult set of equations to solve due to the nonlinearity of the $\mathbf{v} \cdot \nabla \mathbf{v}$ term. There are many everyday situations where this term is important.

As a contrast in heat transfer (or diffusion), nearly everything can be described using a linear equation. In extreme cases, such as in very different boundary conditions, the properties of the material may vary significantly over the gradient along the domain, and then the solution would be nonlinear. However, for examples such as heat exchangers and water flows in pipes, the gradients are sufficiently mild such that the heat conduction coefficient, k , will be relatively constant.

Now consider a flow that is *time independent*. We do this only to simplify the system by removing the $\frac{\partial \mathbf{v}}{\partial t}$ term. This is reasonable because there are many systems which are steady state and will not reduce the generality of our discussion. Then we have the equation,

$$\rho \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla P - \mu \nabla^2 \mathbf{v}. \quad (10.1.3)$$

But now we must identify the characteristic scaling parameters specific to our problem. This will allow us to convert the dimensional variables into a dimensionless system. We know some characteristic velocity, u ; a standard length scale, L ; and a viscosity based pressure scale, $\frac{\mu u}{L^2}$. If we scale our variables we will replace them using

- $\mathbf{v} \rightarrow u \mathbf{v}^*$
- $\nabla \rightarrow \frac{1}{L} \nabla^*$; since $\nabla = \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}$
- $x \rightarrow Lx^*$
- $y \rightarrow Ly^*$
- $z \rightarrow Lz^*$
- $P \rightarrow \frac{\mu u}{L^2} P^*$
- $\nabla^2 \rightarrow \frac{1}{L^2} \nabla^{2*}$

To avoid complicating our lives further, however, we will simply use the dimensionless forms of the variables (without the star notation) from here on. This was simply a helpful transition to remind us of the importance of dimensionless variables. So substituting these variables we have the equation,

$$\frac{\rho u^2}{L} \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{\mu u}{L^2} \nabla P + \frac{\mu u}{L^2} \nabla^2 \mathbf{u}, \quad (10.1.4a)$$

$$\frac{\rho u L}{\mu} \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla P + \nabla^2 \mathbf{u} \quad (10.1.4b)$$

This clearly illustrates the origin of the *Reynolds number*, $\text{Re} = \frac{\rho u L}{\mu}$. This number tells us what kind of flow we have. If it is large then we have a strong nonlinear term, and if it is big enough it can dominate the flow such that the right hand side of the equation becomes almost negligible. This is because the terms $\mathbf{v} \cdot \nabla \mathbf{v}$, ∇P , and $\nabla^2 \mathbf{u}$ are all of the order of one in the dimensionless system. However, the Reynolds number can be any value. If it is

on the order of 1000 then it will be the dominant term. When it is small ($\text{Re} \ll 1$), then the flow is viscous dominated, and nearly linear; so the equation can be solved analytically.

So we are now interested in Reynolds number flow which are small, but still finite. The flow is viscous dominated, but we cannot ignore the nonlinear part. This means that $\text{Re} < 1$ and will determine how big the nonlinear effects are. This is what we want to solve; a solution that accounts for a small nonlinearity. Note at if $\text{Re} > 1$, this approach would not work.

Given $\text{Re} = 0$, we know the solution of the *Stokes flow* equation;

$$\nabla^2 \mathbf{u} = \nabla P. \quad (10.1.5)$$

So we may use this as our zero-order approximation. Then we will correct for it by adding terms such as first, second, etc, depending on our interest in how accurate we want our solution to be. Consider the expanded series of the velocity,

$$\mathbf{v} = \mathbf{v}_0 + \text{Re} \mathbf{v}_1 + \text{Re}^2 \mathbf{v}_2 + \text{Re}^3 \mathbf{v}_3 + \cdots . \quad (10.1.6)$$

In general we will truncate this series very quickly because it is prohibitively impractical to solve for very high order terms. Usually the linear term is the most interesting, and on occasion the quadratic term can help in the analysis, but in most cases the cubic term and beyond is not very helpful. We are looking for a solution for our velocity profile and our pressure in the power series form;

$$P = P_0 + \text{Re} P_1 + \text{Re}^2 P_2 + \text{Re}^3 P_3 + \cdots . \quad (10.1.7)$$

Zero Order

Now we will look into our zero order. It is so called because it is effectively the pressure/velocity multiplied by the Reynolds number to the zero power. The equations are now,

$$\nabla^2 \mathbf{v}_0 = \nabla P_0, \quad (10.1.8a)$$

$$\nabla \cdot \mathbf{v}_0 = 0. \quad (10.1.8b)$$

We also will have a specified set of boundary conditions. Then we can solve this equation (which we can do because they are linear). So, there is no principle difficulty due to the nonlinear terms of the Navier–Stokes equation, because we do not have them in this particular approximation. In fact, you have already solved examples of these equations. We will not actually solve one in this lecture because there are many cases due to geometry, boundary conditions, and so on. These could be no slip boundary conditions, stress, flux or others as long as they are well defined. Then we may find the solutions which satisfy the DE's and boundary conditions. Thus, \mathbf{v}_0 and P_0 are for all practical purposes treated as known values.

First Order

We can move on to the first order correction. The first order means that we are linear in the Reynolds number. If we were to substitute for the velocities and pressure into the full

Navier–Stokes equations, we then look only for terms which are proportional to the Re^1 and ignore all higher and lower order terms. When we do this we are trying to get rid of terms such as second order to make this solvable. So, knowing the substitutions,

$$\mathbf{v} = \mathbf{v}_0 + \text{Re } \mathbf{v}_1, \quad (10.1.9a)$$

$$P = P_0 + \text{Re } P_1; \quad (10.1.9b)$$

we can replace these in the Navier–Stokes equations,

$$\text{Re}(\mathbf{v}_0 + \text{Re } \mathbf{v}_1) \cdot \nabla(\mathbf{v}_0 + \text{Re } \mathbf{v}_1) = \nabla(P_0 + \text{Re } P_1) + \nabla^2(\mathbf{v}_0 + \text{Re } \mathbf{v}_1), \quad (10.1.10a)$$

$$= \nabla P_0 + \text{Re} \nabla P_1 + \nabla^2 \mathbf{v}_0 + \text{Re} \nabla^2 \mathbf{v}_1, \quad (10.1.10b)$$

$$= \text{Re} \nabla P_1 + \text{Re} \nabla^2 \mathbf{v}_1, \quad (10.1.10c)$$

Expanding for the full left hand side,

$$\text{Re } \mathbf{v}_0 \cdot \nabla \mathbf{v}_0 + \text{Re}^2 \mathbf{v}_0 \cdot \nabla \mathbf{v}_1 + \text{Re}^2 \mathbf{v}_1 \cdot \nabla \mathbf{v}_0 + \text{Re}^3 \mathbf{v}_1 \cdot \nabla \mathbf{v}_1 = \text{Re} \nabla P_1 + \text{Re} \nabla^2 \mathbf{v}_1. \quad (10.1.10d)$$

Since we are truncating any higher order terms, we will only keep the equation,

$$\text{Re } \mathbf{v}_0 \cdot \nabla \mathbf{v}_0 = \text{Re} \nabla P_1 + \text{Re} \nabla^2 \mathbf{v}_1. \quad (10.1.11)$$

These are smaller (though non-zero) and are negligible compared to the first order terms. So, we have a linear differential equation for \mathbf{v}_1 . Canceling out the Reynolds number, we have the equation,

$$\mathbf{v}_0 \cdot \nabla \mathbf{v}_0 = \nabla P_1 + \nabla^2 \mathbf{v}_1. \quad (10.1.12)$$

The mass conservation equation $\nabla \cdot \mathbf{v}_1 = 0$ will also be included in the system. This means that \mathbf{v}_1 will also be a conserved quantity. Now observe that we have two unknown functions \mathbf{v}_1 and P_1 . We also have the non-homogeneous term in the momentum equation, but it is known because we have determined \mathbf{v}_0 , or $\mathbf{v}_0 \cdot \nabla \mathbf{v}_0$ is a function which we can substitute as well. So to find \mathbf{v}_1 and P_1 we must solve a linear non-homogeneous equation, which we can do in principle.

We will also have to satisfy the boundary conditions. We also must consider that the sums of the zeroth, first, second order, *etc*, must add up to the boundary conditions. So usually \mathbf{v}_1 and P_1 will be zero at the boundaries, since the zeroth order will ordinarily account for any finite values of the boundary conditions.

Second Order

We move on to second order, but we will not go further because it would be impractical. The second order will keep all of the quadratic terms. The velocity and pressures will be given by,

$$\mathbf{v} = \mathbf{v}_0 + \text{Re } \mathbf{v}_1 + \text{Re}^2 \mathbf{v}_2, \quad (10.1.13a)$$

$$P = P_0 + \text{Re } P_1 + \text{Re}^2 P_2. \quad (10.1.13b)$$

This will be a longer process dealing with the Navier–Stokes equation, so we will handle the sides separately. We will only look at the terms Re^2 and lower in the simplifications

$$\text{LHS} = \text{Re} (\mathbf{v}_0 + \text{Re} \mathbf{v}_1 + \text{Re}^2 \mathbf{v}_2) \cdot \nabla (\mathbf{v}_0 + \text{Re} \mathbf{v}_1 + \text{Re}^2 \mathbf{v}_2), \quad (10.1.14a)$$

$$\begin{aligned} &= \text{Re} \mathbf{v}_0 \cdot \nabla \mathbf{v}_0 + \text{Re}^2 \mathbf{v}_1 \cdot \nabla \mathbf{v}_0 + \text{Re}^3 \mathbf{v}_2 \cdot \nabla \mathbf{v}_0 \\ &\quad + \text{Re}^2 \mathbf{v}_0 \cdot \nabla \mathbf{v}_1 + \text{Re}^3 \mathbf{v}_1 \cdot \nabla \mathbf{v}_1 + \text{Re}^4 \mathbf{v}_2 \cdot \nabla \mathbf{v}_1 \\ &\quad + \text{Re}^3 \mathbf{v}_0 \cdot \nabla \mathbf{v}_2 + \text{Re}^4 \mathbf{v}_1 \cdot \nabla \mathbf{v}_2 + \text{Re}^5 \mathbf{v}_2 \cdot \nabla \mathbf{v}_2; \end{aligned} \quad (10.1.14b)$$

where the only relevant (second order and less) terms are

$$\text{LHS} = \text{Re} \mathbf{v}_0 \cdot \nabla \mathbf{v}_0 + \text{Re}^2 \mathbf{v}_1 \cdot \nabla \mathbf{v}_0 + \text{Re}^2 \mathbf{v}_0 \cdot \nabla \mathbf{v}_1. \quad (10.1.14c)$$

Now moving on to the right hand side, we have the gradient and laplacian linear terms;

$$\text{RHS} = -\nabla P_0 - \text{Re} \nabla P_1 - \text{Re}^2 \nabla P_2 + \nabla^2 \mathbf{v}_0 + \text{Re} \nabla^2 \mathbf{v}_1 + \text{Re}^2 \nabla^2 \mathbf{v}_2. \quad (10.1.15)$$

Setting $\text{LHS} = \text{RHS}$,

$$\begin{aligned} &\text{Re} \mathbf{v}_0 \cdot \nabla \mathbf{v}_0 + \text{Re}^2 \mathbf{v}_1 \cdot \nabla \mathbf{v}_0 + \text{Re}^2 \mathbf{v}_0 \cdot \nabla \mathbf{v}_1 \\ &\quad = -\nabla P_0 - \text{Re} \nabla P_1 - \text{Re}^2 \nabla P_2 + \nabla^2 \mathbf{v}_0 + \text{Re} \nabla^2 \mathbf{v}_1 + \text{Re}^2 \nabla^2 \mathbf{v}_2. \end{aligned} \quad (10.1.16a)$$

Combining terms of each order of Reynolds number on the right hand side,

$$\begin{aligned} &\text{Re} \mathbf{v}_0 \cdot \nabla \mathbf{v}_0 + \text{Re}^2 \mathbf{v}_1 \cdot \nabla \mathbf{v}_0 + \text{Re}^2 \mathbf{v}_0 \cdot \nabla \mathbf{v}_1 \\ &\quad = \underbrace{(-\nabla P_0 + \nabla^2 \mathbf{v}_0)}_0 + \text{Re} (-\nabla P_1 + \nabla^2 \mathbf{v}_1) + \text{Re}^2 (-\nabla P_2 + \nabla^2 \mathbf{v}_2). \end{aligned} \quad (10.1.16b)$$

From the first order correction,

$$\text{Re}^2 \mathbf{v}_1 \cdot \nabla \mathbf{v}_0 + \text{Re}^2 \mathbf{v}_0 \cdot \nabla \mathbf{v}_1 = \text{Re} \mathbf{v}_0 \cdot \nabla \mathbf{v}_0 + \text{Re} \underbrace{(-\nabla P_1 + \nabla^2 \mathbf{v}_1)}_0 + \text{Re}^2 (-\nabla P_2 + \nabla^2 \mathbf{v}_2). \quad (10.1.16c)$$

Finally, what remains is

$$\text{Re}^2 \mathbf{v}_1 \cdot \nabla \mathbf{v}_0 + \text{Re}^2 \mathbf{v}_0 \cdot \nabla \mathbf{v}_1 = \text{Re}^2 (-\nabla P_2 + \nabla^2 \mathbf{v}_2). \quad (10.1.16d)$$

This gives us the principle that we may simply group terms which are of the same order to get the equation that we need to solve for that order. This gives us the new equation with the Re^2 terms canceled,

$$\mathbf{v}_1 \cdot \nabla \mathbf{v}_0 + \mathbf{v}_0 \cdot \nabla \mathbf{v}_1 = -\nabla P_2 + \nabla^2 \mathbf{v}_2, \quad (10.1.17)$$

where we will additionally have the mass conservation term $\nabla \cdot \mathbf{v}_2 = 0$. We will be solving for \mathbf{v}_2 and P_2 , but we will depend on our solution for \mathbf{v}_0 , \mathbf{v}_1 , P_0 , and P_1 . However, we have already obtained these in the previous solutions. Thus, $\mathbf{v}_1 \cdot \nabla \mathbf{v}_0 + \mathbf{v}_0 \cdot \nabla \mathbf{v}_1$ is a known function. It may or may not be tractable to solve depending on the difficulty of the expression. This is essentially how we get rid of the nonlinear term—by replacing it with something that we know. Again at the boundaries \mathbf{v}_2 and P_2 will be zero. Thus, we will have a recursion-like relation between the successive orders. \mathbf{v}_0 and P_0 will be known; then $\mathbf{v}_1 = f(\mathbf{v}_0, P_0)$ and $P_1 = f(\mathbf{v}_0, P_0)$; and $\mathbf{v}_2 = f(\mathbf{v}_0, \mathbf{v}_1, P_0, P_1)$ and $P_2 = f(\mathbf{v}_0, \mathbf{v}_1, P_0, P_1)$. If we were to move to the next correction the velocity and pressure would also be dependent on all lower order terms.

Once we have the functions $\mathbf{v}_0, \mathbf{v}_1, \mathbf{v}_2, P_0, P_1$, and P_2 , we can construct our solution;

$$\mathbf{v} = \mathbf{v}_0 + \text{Re } \mathbf{v}_1 + \text{Re}^2 \mathbf{v}_2 + \mathcal{O}(\text{Re}^3), \quad (10.1.18a)$$

$$P = P_0 + \text{Re } P_1 + \text{Re}^2 P_2 + \mathcal{O}(\text{Re}^3). \quad (10.1.18b)$$

Thus, if $\text{Re} \approx 0.1$ then the error will be approximately 0.001. If we had only done the zeroth order term, the error would be approximately 0.1, or for the linear term of the Reynolds number the approximation would be around 0.01. If the Reynolds number was, say 0.5, then stopping at the linear term the error would be about 25%. At this point you want to go further up to more terms in your approximation, or more likely, it would be better to use a computer simulation.

Remember that the nonlinear fluid flow equation is also very difficult to solve numerically as well as analytically because of many numerical stability issues. This makes the analytical approximations quite valuable. If we look at the solution, the parameters changing power is the Reynolds number, which is known. Now, the velocity and the pressures are complicated functions of the coordinates. This makes the solution different to eigenfunction expansion methods to solve the linear equations. It is similar in one way (the power series) because you will have to sum up to infinity in the Reynolds number to get the exact solution. The difference is that here it is much more complicated—we may have a series in space and a series in Reynolds number on top of that! However, recall that if $\text{Re} \geq 1$, this series will be divergent and the solution is not valid. If the Reynolds number is less than one, the series will sum up to a convergent value, but even for $\text{Re} = 1$ the series will not converge.

Asymptotic Example: Duffing Equation

Now we will solve a simple example. Note that actually solving the Navier–Stokes to the quadratic term would take us a very long time! The *Duffing equation* is much simpler and is well known;

$$\frac{d^2 u}{dt^2} + u + \varepsilon u^3 = 0. \quad (10.1.19)$$

It is an initial value problem. The equation is similar to the linear oscillator, except we have the cubic nonlinearity. Now epsilon is a parameter that tells us how strong the effect of the nonlinear term is. Epsilon is thus the term to use as the small parameter around which to take the power series.

By the way in both of our examples, the small parameter multiplies the nonlinear term, but it is not the highest order derivative. This is called a *regular perturbation* series because if we take the limit of the small parameter goes to zero we still have the same boundary value problem. But if we do multiply the highest order derivative (and there are many famous cases of this), we will change the basic physics of the problem by changing the equation to an algebraic one or into an overdetermined differential system. These are called *singular perturbation* problems.

We may start solving the Duffing equation subject to the initial conditions

$$u(t=0) = x_0, \quad (10.1.20a)$$

$$\dot{u}(t=0) = \dot{x}_0. \quad (10.1.20b)$$

So the solution will depend on time and also on ε , the small parameter.

Zeroth order

We need to begin with the zeroth order ($\varepsilon = 0$), and the equation obtained is simply

$$\frac{d^2u}{dt^2} + u = 0. \quad (10.1.21)$$

This is still a Helmholtz solution, but will look different because we are doing an initial value problem. An expression of the solution is,

$$u_0 = \alpha_0 \cos(t + \beta_0). \quad (10.1.22)$$

Substituting this into the zeroth order differential equation proves that it cancels out.

Now the total solution may be expressed,

$$u(t, \varepsilon) = u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + \varepsilon^3 u_3 + \dots. \quad (10.1.23)$$

For this example we will stop at the linear correction only. This means that the solution will be truncated to,

$$u(t, \varepsilon) = u_0 + \varepsilon u_1 + \mathcal{O}(\varepsilon^2). \quad (10.1.24)$$

First order

Using the double dot notion for a second order time derivative, we may substitute the approximation back into the full Duffing equation,

$$\ddot{u}_0 + \varepsilon \ddot{u}_1 + \mathcal{O}(\varepsilon^2) + u_0 + \varepsilon u_1 + \mathcal{O}(\varepsilon^2) + \varepsilon [u_0 + \varepsilon u_1 + \mathcal{O}(\varepsilon^2)]^3 = 0. \quad (10.1.25a)$$

To truncate the cubic term for simply the linear ε , we can approximate with,

$$[u_0 + \varepsilon u_1 + \mathcal{O}(\varepsilon^2)]^3 \approx u_0 + 3u_0^2 u_1 \varepsilon + \mathcal{O}(\varepsilon^2). \quad (10.1.25b)$$

The equation that we need to solve is,

$$\ddot{u}_0 + u_0 + \varepsilon [\ddot{u}_1 + u_1 + u_0^3] = 0. \quad (10.1.25c)$$

The left hand part which does not multiply ε has already been solved in the zeroth term so all we must solve is,

$$\ddot{u}_1 + u_1 + u_0^3 = 0. \quad (10.1.26)$$

The cubic power is now not a non-linear term because it is just a power of a known function. Thus we have a non-homogeneous equation.

$$\ddot{u}_1 + u_1 = [\alpha_0 \cos(t + \beta_0)]^3. \quad (10.1.27)$$

We will solve it using a linear combination of the homogeneous solution and the particular solution.

First, we replace the cubic cosine function by using the identity $\cos^3(\theta) = \frac{1}{4}\cos(3\theta) + \frac{3}{4}\cos(\theta)$. This identity is actually the exact Fourier expansion of the cube of the cosine function. In the original variables;

$$\ddot{u}_1 + u_1 = -\frac{3}{4}\alpha_0^3 \cos(t + \beta_0) - \frac{1}{4}\alpha_0^3 \cos(3t + 3\beta_0). \quad (10.1.28)$$

The particular solution for this differential equation is

$$u_{1p} = -\frac{3}{8}\alpha_0^3 t \sin(t + \beta_0) + \frac{1}{32}\alpha_0^3 \cos(3t + 3\beta_0). \quad (10.1.29)$$

The homogeneous solution was just the cosine function. So the general solution is,

$$u = \alpha_0 \cos(t + \beta_0) + \varepsilon \left[\alpha_1 \cos(t + \beta_1) - \frac{3}{8}\alpha_0^3 t \sin(t + \beta_0) + \frac{1}{32}\alpha_0^3 \cos(3t + 3\beta_0) \right] + \mathcal{O}(\varepsilon^2). \quad (10.1.30)$$

There may appear to be four constants, but since we had the boundary conditions,

$$x_0 = u(0) = \alpha_0 \cos(\beta_0) + \varepsilon \left[\alpha_1 \cos(\beta_1) - \frac{3}{8}\alpha_0^3 t \sin(\beta_0) + \frac{1}{32}\alpha_0^3 \cos(3\beta_0) \right], \quad (10.1.31a)$$

$$\dot{x}_0 = \dot{u}(0) = -\alpha_0 \sin(\beta_0) - \varepsilon \left[\alpha_1 \sin(\beta_1) + \frac{3}{8}\alpha_0^3 t \sin(\beta_0) + \frac{3}{32}\alpha_0^3 \sin(3\beta_0) \right]. \quad (10.1.31b)$$

Collecting the terms of the same power of epsilon; for epsilon to the zeroth power

$$x_0 = u(0) = \alpha_0 \cos(\beta_0), \quad (10.1.32a)$$

$$\dot{x}_0 = \dot{u}(0) = -\alpha_0 \sin(\beta_0). \quad (10.1.32b)$$

For the first power,

$$\alpha_1 \cos(\beta_1) = \frac{3}{8}\alpha_0^3 t \sin(\beta_0) + \frac{1}{32}\alpha_0^3 \cos(3\beta_0), \quad (10.1.33a)$$

$$\alpha_1 \sin(\beta_1) = \frac{3}{8}\alpha_0^3 t \sin(\beta_0) + \frac{3}{32}\alpha_0^3 \sin(3\beta_0). \quad (10.1.33b)$$

This gives us enough equations to find α_1 and β_1 .

The Duffing equation can be solved exactly, but we want to compare the asymptotic techniques to the exact solution.

10.2 Lecture 27: November 20, 2013

An article was sent out on the importance of analytical solutions. This is important even in these days of computers, because analytical solutions give you excellent simplified tests of the code. The fellow who wrote the article makes a good case about it.

The last homework will be sent out this afternoon.

Homework 7 problem 4

Now we will discuss the fourth problem from the previous homework. The problem number in the book is 12.4.15. We were given one particular solution of the differential equation, which is the series,

$$y_1(x) = x^{1/2} \left[1 - \frac{3}{4}x + \frac{9}{64}x^2 - \frac{3}{256}x^3 + \mathcal{O}(x^4) \right]. \quad (10.2.1)$$

The second solution may be found from the expression;

$$y_2(x) = y_1(x) \int \frac{1}{y_1^2(x)} dx. \quad (10.2.2)$$

In this case the Wronski determinant is simply 1 because $P(x) = 0$ so $W = e^0 = 1$. The integral is indeterminate and we don't worry about the constant of integration here. This equation is the first important point in solving this system.

We notice that we are dealing with a power series of $y_1(x)$. So, we must calculate the value of the square of $y_1(x)$ and this requires us to decide how many terms of the series we wish to keep. We have the terms, and

$$y_1^2(x) = x \left[1 - \frac{3}{2}x + \frac{27}{3}x^2 + \frac{15}{64}x^3 + \mathcal{O}(x^4) \right]. \quad (10.2.3)$$

We could do this by hand (if we enjoy lengthy calculations), or we could do it using a software such as Mathematica[®], Wolfram|Alpha[®], or others. This is very easy for Mathematica[®] to do!

Once this is found, we need the series expansion of the reciprocal of $y_1^2(x)$. Noting that we do not combine the x term in front so that we can expand the series around $x = 0$ with a Taylor series,

$$\frac{1}{y_1^2(x)} = \frac{1}{x \left[1 - \frac{3}{2}x + \frac{27}{3}x^2 + \frac{15}{64}x^3 + \mathcal{O}(x^4) \right]}, \quad (10.2.4a)$$

$$= \frac{1}{x} \left[1 + \frac{3}{2}x + \frac{45}{32}x^2 + \mathcal{O}(x^3) \right], \quad (10.2.4b)$$

$$= \frac{1}{x} + \frac{3}{2} + \frac{45}{32}x + \mathcal{O}(x^2) \quad (10.2.4c)$$

Next we must integrate the expression, then we will multiply by $y_1(x)$, and give our solution as the truncated series to the order of accuracy which we are interested in. We must be

careful if we want to keep to quadratic accuracy because we will get higher order terms in the process of the polynomial multiplication. Integrating the series,

$$y_2(x) = y_1(x) \ln(x) + x^{3/2} \left[\frac{3}{2} - \frac{27}{64}x + \frac{11}{256}x^2 \right]. \quad (10.2.5)$$

This is the solution of the problem.

Two things to keep in mind; we needed to use the $y_2(x) = y_1(x) \int \frac{W}{y_1^2(x)} dx$ to find the solution, then we needed to manipulate the series expressions in a sensible way to get our answer. This tedious, but the most straightforward approach to solving this problem.¹

Asymptotics Example: The Duffing Equation (cont.)

We now continue on to return to the Duffing equation. If time permits we may do another example first with asymptotic solutions, then do it exactly. Asymptotic expansions are not limited to nonlinear methods; they can be done for linear as well. However this is usually not necessary because these systems may already be solved exactly, and the solution is quite simple.

As discussed previously the Duffing equation is nonlinear. The asymptotic solution is of the form,

$$u = \alpha_0 \cos(t + \beta_0) + \varepsilon \left[\alpha_1 \cos(t + \beta_1) - \frac{3}{8}\alpha_0^3 t \sin(t + \beta_0) + \frac{1}{32}\alpha_0^3 \cos(3t + 3\beta_0) \right] + \mathcal{O}(\varepsilon^2), \quad (10.2.6)$$

where we have obtained α_0 , β_0 , α_1 , and β_1 . The α_0 and β_0 are obtained from the zero order term, (ε^0).

$$x_0 = \alpha_0 \cos(\beta_0), \quad (10.2.7a)$$

$$\dot{x}_0 = -\alpha_0 \sin(\beta_0). \quad (10.2.7b)$$

Furthermore, from the first order solution, ε^1 , we can find α_1 and β_1 with,

$$\alpha_1 \cos(\beta_1) = \frac{3}{8}\alpha_0^3 t \sin(\beta_0) + \frac{1}{32}\alpha_0^3 \cos(3\beta_0), \quad (10.2.8a)$$

$$\alpha_1 \sin(\beta_1) = \frac{3}{8}\alpha_0^3 t \sin(\beta_0) + \frac{3}{32}\alpha_0^3 \sin(3\beta_0). \quad (10.2.8b)$$

Now say we have α and β defined with the equations,

$$\alpha_0 \cos(\beta_0) + \varepsilon \alpha_1 \cos(\beta_1) = \alpha \cos(\beta), \quad (10.2.9a)$$

$$\alpha_0 \sin(\beta_0) + \varepsilon \alpha_1 \sin(\beta_1) = \alpha \sin(\beta). \quad (10.2.9b)$$

In principle, this allows us to calculate α and β simply by this relationship. It does involve the small parameter, ε , but in general this is a known value. Now, rearranging, $\alpha_0 = \alpha + \mathcal{O}(\varepsilon)$ and $\beta_0 = \beta + \mathcal{O}(\varepsilon)$ If we are interested in the zero order solution only,

$$u = \alpha \cos(t + \beta) + \mathcal{O}(\varepsilon) \quad (10.2.10)$$

¹As an alternative approach, we could assume a form of the series and then try to find the coefficients; this method is possible, but not recommended.

Exact solution of the Duffing Equation

Now the Duffing equation can be solved exactly. However, we may observe that the asymptotic solution is much simpler than the exact one. Again, the Duffing equation is

$$\frac{d^2u}{dt^2} + u + \varepsilon u^3 = 0. \quad (10.2.11)$$

We will use a similar method to previous work in solving nonlinear differential equations, and we will end up with a solution that is quite similar to what we have already seen. Introducing the new variable,

$$v = \frac{du}{dt}, \quad (10.2.12)$$

we will move through a different angle of approaching the solution. Recall that the Duffing equation is much like an oscillator equation; so u is the displacement and v is the velocity. This gives us a tangible physical meaning to these quantities and this justifies the substitution. Then clearly $\frac{d^2u}{dt^2} = \frac{dv}{dt} = \frac{dv}{du} \frac{du}{dt}$ by the chain rule for $v(u(t))$. Further, by definition of v , this simplifies to,

$$\frac{d^2u}{dt^2} = v \frac{dv}{du}. \quad (10.2.13)$$

This is analogous to the $\mathbf{v} \cdot \nabla \mathbf{v}$ term in the Navier–Stokes equations discussed previously. This is because both of them are related to acceleration and inertial motion. We have thus observed a relation between fluid motion and nonlinear oscillators; physical similarity can appear in surprising areas.

Now our equation is,

$$v \frac{dv}{du} + u + \varepsilon u^3 = 0. \quad (10.2.14)$$

This equation of two variables may be solved in a very similar way as the electrostatics equation. Integrating the rearranged form of the equation,

$$\int v \, dv = - \int (u + \varepsilon u^3) \, du, \quad (10.2.15a)$$

$$\frac{1}{2}v^2 = h - \left(\frac{1}{2}u^2 + \frac{1}{4}\varepsilon u^4 \right), \quad (10.2.15b)$$

$$= h - F(u). \quad (10.2.15c)$$

The left hand side ($\frac{1}{2}v^2$) is much like the kinetic energy, while h is the constant of integration, and $F(u) = \frac{1}{2}u^2 + \frac{1}{4}\varepsilon u^4$ for brevity. Now F is only a function of position and is related to the potential energy of the system. It only has displacement, while kinetic energy depends on the velocities alone.

Plotting the potential energy of the system with respect to displacement, we see that for positive ε the function will be everywhere increasing. It is a symmetric function. The constant, h is related to the total energy of the system. We can have different total energies, but if h changes then the plot of v with respect to u gives an oscillatory phase plot as seen by the elliptical nature of the plot. This is very typical of oscillators to have these phase plots of closed oscillations. But we have it for both linear and nonlinear oscillators. This

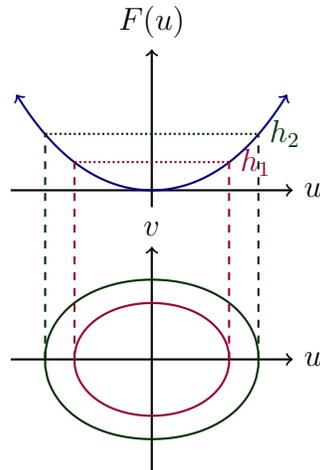


Figure 10.1. Parabolic plot of $F(u)$ versus u for positive epsilon with corresponding v and u phase diagrams

changes the shape of the parabola, but it still has the same characteristics of an increasing potential at both sides. Also note that for higher energies, the phase ellipse will be larger.

Now consider if we have a negative ϵ . If we have small displacement, the quadratic term in $f(u)$ will dominate, but as the displacement grows the quartic term multiplied by epsilon will eventually become greater. These two terms will then be competing and at large enough displacement the fourth order term will dominate. This cannot happen in a linear oscillator. Here we observe some similarities and some crucial effects the total energy has

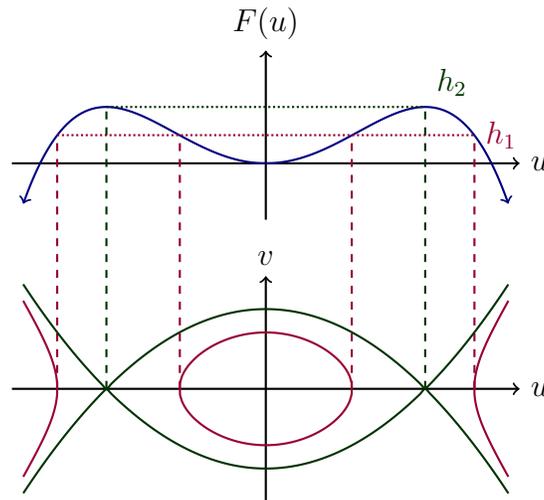


Figure 10.2. Plot of $F(u)$ versus u for negative epsilon with corresponding v and u phase diagrams

on the dynamics. If h is relatively low, the function will have a very normal oscillation, but as we approach the maxima of $F(u)$ the motion will be unlimited. The trajectories will be much more like hyperbolas as if the system is repulsive. Recall that in planetary systems,

as more kinetic energy is put in, the orbit becomes much more elongated. Consider that planets have nearly circular orbits, while comets have very elliptical orbits. If a body—such as the Voyager I and II satellites—receives sufficient energy it can be knocked away from the gravitational pull of the sun. The effect is similar here, though this is not orbital. The lines bounding these two phases are called separatrices.

Looking at the formula, we can summarize our observations (even though we are not done yet—we can do another integration). Now, rearranging

$$v = \pm\sqrt{2} (h - F(u))^{1/2}. \quad (10.2.16)$$

Thus, the velocity is real only if $h \geq F(u)$. In the plots of $F(u)$ the velocity is not real above the line of h . Concluding the phase behavior;

- For $\varepsilon > 0$ and $h = 0$ we have a closed circular, periodic trajectories.
- For $\varepsilon < 0$ we may have closed or open (separatrices).

Now the second integration may be performed; this will give us a closed form solution. However, since u is the natural variable it will be and v is the dependent variable, the implicit solution we will arrive at will look a little unusual. We will also introduce the initial conditions,

$$u(0) = x_0, \quad (10.2.17a)$$

$$\dot{u}(0) = \dot{x}_0. \quad (10.2.17b)$$

We may use these to find h . Applying the initial conditions to the first integral,

$$\frac{1}{2}\dot{x}_0^2 = h - \left(\frac{1}{2}x_0^2 + \frac{1}{4}\varepsilon x_0^4 \right), \quad (10.2.18a)$$

$$h = \frac{1}{2}\dot{x}_0^2 + \frac{1}{2}x_0^2 + \frac{1}{4}\varepsilon x_0^4. \quad (10.2.18b)$$

Clearly, the first term is the initial kinetic energy, and the second two terms are the potential energy for the nonlinear oscillator.

So, now we may solve the differential equation,

$$\frac{du}{dt} = \pm \left(2h - u^2 - \frac{1}{2}\varepsilon u^4 \right)^{1/2}, \quad (10.2.19a)$$

$$\int dt = \pm \int \frac{1}{(2h - u^2 - \frac{1}{2}\varepsilon u^4)^{1/2}} du. \quad (10.2.19b)$$

This is clearly not a trivial integral. However, such integral solutions are either tabulated or may easily be computed. Nevertheless, the behavior is not obvious by looking at the integral as is. Finally, the full solution is,

$$\boxed{\int \frac{1}{(2h - u^2 - \frac{1}{2}\varepsilon u^4)^{1/2}} du = \pm \int dt}. \quad (10.2.20)$$

We find that this is very difficult to compare to the asymptotic solution directly. In many cases the asymptotic is much easier to work with.

Comparison to the Linear Oscillator

This point is even clearer in the example of the damped linear oscillator. The equation of the linear oscillator (with stars for dimensional variables),

$$m \frac{d^2 u^*}{dt^{*2}} + \mu \frac{du^*}{dt^*} + ku^* = 0. \quad (10.2.21)$$

This is like a pendulum in a viscous fluid. The oscillations will decay with time until we reach the static case. Note that this is not a driven oscillation (the RHS is zero).

Let's change the variables. Say there is a frequency $\omega_0 = \sqrt{\frac{k}{m}}$. Then we have the dimensionless system,

- $t = \omega_0 t^*$
- $u = \frac{u^*}{v^*}$ where v^* may be the initial velocity.

This gives the dimensionless equation,

$$\ddot{u} + 2\varepsilon\dot{u} + u = 0, \quad (10.2.22)$$

where $\varepsilon = \frac{1}{2} \frac{\mu}{\sqrt{km}}$. We cannot assume that ε is small because the viscosity could be very high. But if we have low viscosity, and a strong spring constant, then it may be sufficiently small. Then we may use a perturbation technique to find an approximate solution.

So we will find the asymptotic solution, then recall the exact solution and truncate it at the same term that we have gone to in the asymptotic expansion. Then we can compare them; they should be the same. If they are not, then it is our error in the derivation.

So we look for a solution which depends on the time and small parameter;

$$u(t; \varepsilon) = u_0(t) + \varepsilon u_1(t) + \varepsilon^2 u_2(t) + \dots \quad (10.2.23)$$

Substituting this into the differential equation and combining terms of equal power of epsilon,

$$\ddot{u}_0(t) + \varepsilon \ddot{u}_1(t) + \varepsilon^2 \ddot{u}_2(t) + 2\varepsilon \dot{u}_0(t) + 2\varepsilon^2 \dot{u}_1(t) + 2\varepsilon^3 \dot{u}_2(t) + u_0(t) + \varepsilon u_1(t) + \varepsilon^2 u_2(t) = 0. \quad (10.2.24)$$

Combining the terms for increasing powers of ε ,

$$\ddot{u}_0(t) + u_0(t) = 0, \quad (10.2.25a)$$

$$\ddot{u}_1(t) + u_1(t) = -2\dot{u}_0(t), \quad (10.2.25b)$$

$$\ddot{u}_2(t) + u_2(t) = -2\dot{u}_1(t). \quad (10.2.25c)$$

Again we may observe that each equation depends on the solution of the previous order of the parameter. This hierarchical layout of the equations means that we must find the zeroth first to move on. Then we have the further orders with the non homogeneous equations.

The solution to the zeroth order is the same as the Duffing equation,

$$u_0 = \alpha \cos(t + \beta) \quad (10.2.26)$$

Then the first order becomes,

$$\ddot{u}_1(t) + u_1(t) = 2\alpha \sin(t + \beta). \quad (10.2.27a)$$

This is very similar to having a driven oscillator, even though that was not in the original form of the damped linear oscillator. The solution is

$$u_1 = -\alpha t \cos(t + \beta). \quad (10.2.27b)$$

The second order perturbation equation is then,

$$\ddot{u}_2(t) + u_2(t) = 2\alpha \cos(t + \beta) + 2\alpha t \sin(t + \beta). \quad (10.2.28a)$$

The solution of this equation is harder (it may be done by varying parameters),

$$u_2 = \frac{1}{2}\alpha t^2 \cos(t + \beta) + \frac{1}{2}\alpha t \sin(t + \beta). \quad (10.2.28b)$$

Thus the complete solution up to ε^2 is,

$$\boxed{u = \alpha \cos(t + \beta) - \varepsilon \alpha t \cos(t + \beta) + \frac{1}{2}\varepsilon^2 \alpha [t^2 \cos(t + \beta) + t \sin(t + \beta)]}. \quad (10.2.29)$$

This is the approximate solution.

Now observe that often in these terms ε is multiplied by matching powers of t . This limits how long we can go in time when using this expansion. This is because, if the product $(\varepsilon t)^n$ is not less than one, the series will diverge! Even more so if simply $\varepsilon t > 1$ this solution will diverge. This is because if we were to sum up all terms up to infinity the series sum will be infinite. So for this expansion we may only go up to times $t < \frac{1}{\varepsilon}$.

Exact Solution of Damped Linear Oscillator

Let us assume that the solution has the form $Ce^{\lambda t}$ and insert into the differential equation $\ddot{u} + 2\varepsilon\dot{u} + u = 0$;

$$C(\lambda^2 + 2\varepsilon\lambda + 1)e^{\lambda t} = 0. \quad (10.2.30)$$

The characteristic equation is simply,

$$\lambda^2 + 2\varepsilon\lambda + 1 = 0. \quad (10.2.31)$$

This quadratic equation has the two roots;

$$\lambda = -\varepsilon \pm \sqrt{\varepsilon^2 - 1}. \quad (10.2.32)$$

The trouble with this equation is that for $\varepsilon < 1$ this system will not be real. However this is ok because it will give an oscillatory behavior. We may rearrange this to more naturally express the harmonic nature of the equation,

$$\lambda = -\varepsilon \pm i\sqrt{1 - \varepsilon^2}. \quad (10.2.33)$$

Then we recognize that the first term relates to the friction decay, while the second term relates to the oscillations. Then we have a solution,

$$u = c_1 e^{-\varepsilon t + i\sqrt{1-\varepsilon^2}t} + c_2 e^{-\varepsilon t - i\sqrt{1-\varepsilon^2}t}. \quad (10.2.34)$$

Now c_2 is a complex conjugate of c_1 to have a real solution for u (except if we are dealing with quantum mechanics!). In other words if they are complex conjugates, we can write them in the following form,

$$c_1 = \frac{1}{2}\alpha e^{i\beta}, \quad (10.2.35a)$$

$$c_2 = \frac{1}{2}\alpha e^{-i\beta}. \quad (10.2.35b)$$

Remembering the exponential definition of sine and cosine functions (*e.g.* $\cos(x) = \frac{e^{ix} + e^{-ix}}{2}$), our solution becomes,

$$\boxed{u = \alpha e^{-\varepsilon t} \cos\left(\sqrt{1-\varepsilon^2}t + \beta\right)}. \quad (10.2.36)$$

This exact solution is not all that similar to the asymptotic solution. But we may expand the exact solution for small ε around $\varepsilon = 0$, then truncate the expression and compare to the asymptotic solution.

We will need to expand the exponential and the cosine function. The expansion of the exponential function is,

$$e^{-\varepsilon t} = \sum_{n=0}^{\infty} \frac{1}{n!} (-\varepsilon t)^n, \quad (10.2.37a)$$

$$= 1 - \varepsilon t + \frac{1}{2!}\varepsilon^2 t^2 - \frac{1}{3!}\varepsilon^3 t^3 + \dots. \quad (10.2.37b)$$

Then expanding the square root,

$$\sqrt{1-\varepsilon^2} = 1 - \frac{1}{2}\varepsilon^2 - \frac{1}{8}\varepsilon^4 + \dots. \quad (10.2.38)$$

So within the cosine we have, (we will expand the signs around epsilon)

$$\cos\left(\sqrt{1-\varepsilon^2}t + \beta\right) = \cos\left(t + \beta - \frac{1}{2}\varepsilon^2 t - \frac{1}{8}\varepsilon^4 t + \dots\right), \quad (10.2.39a)$$

$$= \cos(t + \beta) \cos\left(\frac{1}{2}\varepsilon^2 t + \frac{1}{8}\varepsilon^4 t + \dots\right) + \sin(t + \beta) \sin\left(\frac{1}{2}\varepsilon^2 t + \frac{1}{8}\varepsilon^4 t + \dots\right), \quad (10.2.39b)$$

$$= \cos(t + \beta) \left[1 - \frac{1}{2}\left(\frac{1}{2}\varepsilon^2 t + \dots\right)^2\right] + \sin(t + \beta) \left[\frac{1}{2}\varepsilon^2 t + \frac{1}{8}\varepsilon^4 t + \dots\right], \quad (10.2.39c)$$

$$\approx \left(\frac{1}{2}\varepsilon^2 t - \frac{1}{8}\varepsilon^4 t\right) \cos(t + \beta) + \left(\frac{1}{2}\varepsilon^2 t + \frac{1}{8}\varepsilon^4 t\right) \sin(t + \beta). \quad (10.2.39d)$$

Next we must multiply this series by the exponential expansion. Then we combine all terms of the same order. Finally,

$$u = \alpha \left(1 - \varepsilon t + \frac{1}{2} \varepsilon^2 t^2 \right) \left[\cos(t + \beta) + \frac{1}{2} \varepsilon^2 t \sin(t + \beta) \right], \quad (10.2.40a)$$

$$= \boxed{\cos(t + \beta) - \varepsilon \alpha t \cos(t + \beta) + \frac{1}{2} \varepsilon^2 \alpha [t^2 \cos(t + \beta) + t \sin(t + \beta)]}. \quad (10.2.40b)$$

We can compare this to the asymptotic solution and realize that they are the same. In this system, the asymptotic was a lot more hassle than using the regular linear solution. The only major reason for doing this is to convince us that the asymptotic techniques work correctly up to the order of magnitude that we have decided to truncate our series.

10.3 Lecture 28: November 25, 2013

Today we will discuss several examples of perturbation techniques applied to fluid mechanics. Time permitting we will cover singular perturbations.

Example from Fluid Mechanics

From undergraduate transport phenomena courses, we may recall the problems of inviscid and irrotational flows; as well as problems involving stream functions and potentials. Recalling the flow around a cylinder with a uniform flow around the cylinder, we may solve the problem exactly. The equation to solve is,

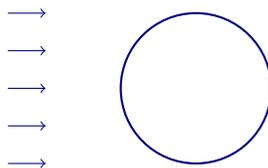


Figure 10.3. Uniform flow around a cylinder

$$\nabla^2\psi = 0, \quad (10.3.1)$$

where ψ is the stream function. Inviscid flow means that the problem does not include any viscosity. This simplifies the Navier–Stokes equations significantly, and clearly reduces the problem to a Laplace (or Poisson) problem. In general exact solutions are important because they give us a clear picture of what is going on. They also allow us to perturb each solution we have to cover a much broader range of cases (geometric, parameter space, *etc.*). Otherwise these problems may not easily be solved. This particular case is a good example.

Consider that inviscid means,

$$\nabla \cdot \mathbf{v} = 0; \quad (10.3.2)$$

in other words the rotation of the velocity is everywhere zero. Now the rotation of a vector field is not simple because when we may compare to types of flows we may not observe any overall angular change in the flow. However, the rotationally is related to whether a particle (infinitesimal point) in the flow would not collide with neighbors. There is no friction or interaction between neighboring points in the stream because each point moves along with the other in irrotational flow. In the case of parallel plate flow, a particle (such as a piece of cork) would rotate within the fluid, but in the case of a draining sink it would not change its orientation. Thus rotation is directly related to viscosity because of the friction between layers of fluids.

An inviscid fluid could also be rotational ($\nabla \cdot \mathbf{v} \neq 0$) if there is a gradient in the fluid motion imposed externally. In this case, we would solve an equation of the form,

$$\nabla^2\psi = -\omega(\psi), \quad (10.3.3)$$

where $\omega(\psi)$ is the vorticity. The vorticity is usually a nonlinear function, and particularly is a function of the stream function. This is problematic because it presents us with a

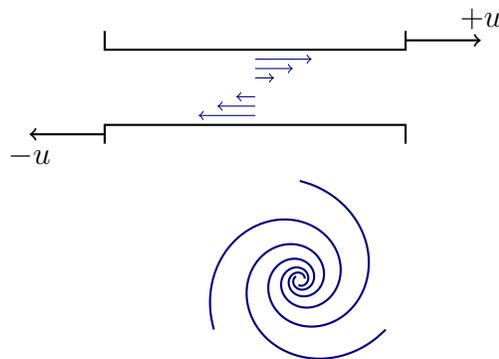


Figure 10.4. Rotational and irrotational flow systems

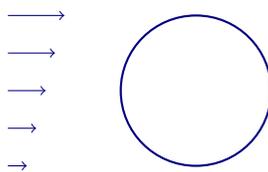


Figure 10.5. Non-uniform flow around a cylinder

nonlinear differential equation. Now recall that once we know the stream function, ψ , we can determine the components of the velocity by,

$$v_x = \frac{\partial \psi}{\partial y}, \quad (10.3.4a)$$

$$v_y = -\frac{\partial \psi}{\partial x}. \quad (10.3.4b)$$

In other words, the stream function has all the information you need to find the flow field. We, however, will limit our discussion to the stream function only for purposes of simplicity.

The first problem (uniform flow field) proposed, may be solved exactly for an idealized system. The other cannot in the general sense; however we could use the first system as a way to approximately solve the second using perturbations. In the undergraduate transport class all focus is on the simplified case, but more often we may encounter more tricky problems such as the second.

Uniform Flow Around a Cylinder

Now let's remind ourselves how we deal with the simple case. Since the velocity is coming in uniformly from infinitely far away, as it approaches the cylinder it will bend around the cylinder because the cylinder is a solid object. Calling the flow at infinity, u , we will rewrite the problem in polar coordinates because that system best relates to the symmetry of the problem. We now have radial and angular coordinates r and θ . Given the new Laplace operator, $\nabla^2 \psi = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \theta^2}$, the equation now becomes,

$$\frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r} \frac{\partial \psi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \theta^2} = 0. \quad (10.3.5)$$

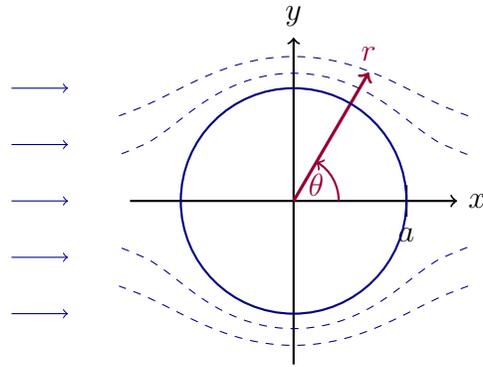


Figure 10.6. Uniform flow around a cylinder with radial coordinates

This equation would be easy to solve if it was just an ordinary differential equation because then we could multiply by twice the first order derivative and quickly solve. With this PDE, we cannot.

The boundary conditions for this problem are,

$$\psi(r \rightarrow \infty, \theta) = ur \sin \theta, \quad (10.3.6a)$$

$$\psi(r=a, \theta) = 0. \quad (10.3.6b)$$

Thus, for large distance from the cylinder the velocity will go to uniform field, and the velocity at the surface of the cylinder will be zero. The flow is symmetric around the x -axis of the system, or

$$\psi(r, \theta) = -\psi(r, -\theta). \quad (10.3.7)$$

This condition in fact simplifies the problem very significantly. We need the symmetry to eliminate the nonlinear and non-homogeneous term. Note that an problem with an arbitrary flow profile would not have any guarantee of symmetry. So the velocity would have significantly different properties of the motion.

The boundary condition suggests the nature of our solution. For example we can solve this system by considering a function of the form,

$$\psi(r, \theta) = f(r) \sin \theta. \quad (10.3.8)$$

We have reduced the problem to one of finding $f(r)$. This eliminates the dependence on θ in the differential equation and we have converted the problem into a single ordinary dimensional equation. We already know the solution of $f(r)$ elsewhere, so in the interest of time,

$$\boxed{\psi = u \left(r - \frac{a^2}{r} \right) \sin \theta.} \quad (10.3.9)$$

Here the $f(r) = u \left(r - \frac{a^2}{r} \right)$.

In general all stream functions have a corresponding potential function. So often a problem may be solved by using either function. The gradient of the velocity potential is

the velocity itself, or $\nabla\phi = \mathbf{v}$. This gives the relations,

$$v_x = \frac{\partial\phi}{\partial x}, \quad (10.3.10a)$$

$$v_y = \frac{\partial\phi}{\partial y}. \quad (10.3.10b)$$

The isopotential in this problem is,

$$\phi = u \left(r + \frac{a^2}{r} \right) \sin\theta. \quad (10.3.11)$$

The lines of isopotential are everywhere normal to the streamlines.

Non-constant Gradient of Velocity Around Cylinder

Returning to the streamlines, we now have the exact solution. Consider if the incoming flow is no longer uniform. Then we may use the exact solution and perturb it to find a new solution to account for the nonlinearities in the problem. We remain in cylindrical coordinates. Now

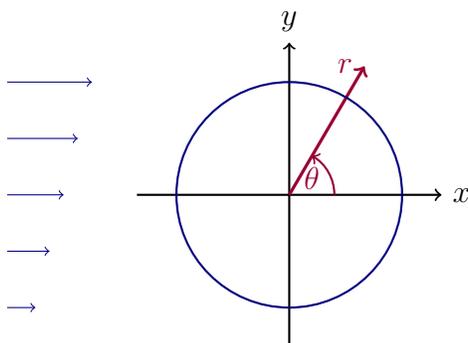


Figure 10.7. Non-uniform flow around a cylinder with radial coordinates

we must say that the vorticity function is small, otherwise the asymptotic solution will not be valid due to too large of parameters. This may make the solution diverge. Say now $v_x = \frac{\partial\psi}{\partial y}$, then say our boundary condition is and transforming into polar coordinates,

$$\left(\frac{\partial\psi}{\partial y} \right)_{\infty} = u \left(1 + \varepsilon \frac{y}{a} \right), \quad (10.3.12a)$$

$$= u \left(1 + \varepsilon \frac{r}{a} \sin\theta \right). \quad (10.3.12b)$$

So we may find the stream function boundary condition by $\psi = \int v_x dy$ from the definition of the derivatives of the stream function. We will ignore additive constants because we do not care about the value of the stream function but only the derivatives of it. So, integrating,

$$\psi = u \left(y + \frac{1}{2} \varepsilon \frac{y^2}{a} \right), \quad (10.3.13a)$$

$$= u \left(r \sin\theta + \frac{1}{4} \varepsilon \frac{r^2}{a} [1 - \cos(2\theta)] \right). \quad (10.3.13b)$$

The second part of the boundary condition is clearly a perturbation from the uniform flow profile. The vorticity at infinity will be determined from the differential equation, or

$$\omega_\infty = -\nabla^2\psi_\infty, \quad (10.3.14a)$$

$$= -\varepsilon\frac{u}{a}. \quad (10.3.14b)$$

Clearly we may now write the equation to solve,

$$\frac{\partial^2\psi}{\partial r^2} + \frac{1}{r}\frac{\partial\psi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2} = \varepsilon\frac{u}{a}. \quad (10.3.15)$$

The ε must remain less than one because this is our small parameter. The boundary conditions,

$$\psi(r \rightarrow \infty, \theta) = u \left(r \sin\theta + \frac{1}{4}\varepsilon\frac{r^2}{a} [1 - \cos(2\theta)] \right), \quad (10.3.16a)$$

$$\psi(r=a, \theta) = 0. \quad (10.3.16b)$$

Here we have an implied assumption that the circulation due to the non-homogeneous will not also include anything induced by the body itself. If we consider a viscous fluid this would further induce circulation and vorticity on the flow, because then the fluid contacting or near the wall would have a gradient because of the non-slip boundary condition. This would appear as an acceleration as we move further from the surface of the body and we observe the shear flow. Again with inviscid flow this will not be the case and the vorticity is already accounted for.

We may look for a solution in the form,

$$\psi(r, \theta; \varepsilon) = \psi_0(r, \theta) + \varepsilon\psi_1(r, \theta) + \dots. \quad (10.3.17)$$

Clearly we could add further terms, but at present we will only investigate the linear term. The substituted equation is

$$\nabla^2\psi_0 + \varepsilon\nabla^2\psi_1 = \varepsilon\frac{u}{a}. \quad (10.3.18)$$

The zero order solution ($\varepsilon = 0$) will be found with,

$$\nabla^2\psi_0 = 0. \quad (10.3.19)$$

This was found by collecting the terms of the same order in epsilon. The problem we previously solved is in fact the zero order solution for this current problem. The correction for a finite epsilon is,

$$\varepsilon\nabla^2\psi_1 = \varepsilon\frac{u}{a}. \quad (10.3.20)$$

Intriguingly this equation is simply just a constant RHS and not a function or a function of the zero order solution.

First Order Solution

We now need to solve the first order perturbation. For large radii ($r \rightarrow \infty$), the boundary conditions

$$\psi_1(r \rightarrow \infty, \theta) = \frac{1}{4} \frac{u}{a} r^2 [1 - \cos(2\theta)], \quad (10.3.21a)$$

$$\psi_1(r=a, \theta) = 0. \quad (10.3.21b)$$

This gives us a helpful form of the boundary conditions for the first order solution. We may solve this by assuming a form of the solution. We know that the boundary condition, $\frac{1}{4} \frac{u}{a} r^2 [1 - \cos(2\theta)]$, is one particular solution of the system because this is an asymptotic form which we must have at infinity. This would satisfy the homogeneous equation and be general solution for homogeneous solution.

Now we must find the particular solution, χ_1 ;

$$\psi_1 = \frac{1}{4} \frac{u}{a} r^2 [1 - \cos(2\theta)] + \chi_1(r, \theta). \quad (10.3.22)$$

The differential equation is,

$$\frac{\partial^2 \chi_1}{\partial r^2} + \frac{1}{r} \frac{\partial \chi_1}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \chi_1}{\partial \theta^2} = 0. \quad (10.3.23)$$

Now the boundary conditions are

$$\psi(r \rightarrow \infty, \theta) = \text{const}, \quad (10.3.24a)$$

$$\psi(r=a, \theta) = -\frac{1}{4} u a (1 - \cos 2\theta). \quad (10.3.24b)$$

The solution of this equation is,

$$\chi_1 = \frac{1}{4} u a \left(\frac{a^2}{r^2} \cos(2\theta) - 1 \right). \quad (10.3.25)$$

Then the total solution is,

$$\boxed{\psi = u \left(r - \frac{a^2}{r} \right) \sin \theta + \frac{1}{4} \varepsilon u \left[\frac{r^2}{a^2} (1 - \cos(2\theta)) \frac{a^3}{r^2} \cos(2\theta) - a \right]}. \quad (10.3.26)$$

So we have found a solution to our perturbation problem.

The algorithm for solving the perturbation problem:

1. Find nonlinear differential equation (NLDE) which is weakly nonlinear,
2. Approximate the solution by the series,

$$\psi = \psi_0 + \varepsilon \psi_1 + \varepsilon^2 \psi_2 + \dots. \quad (10.3.27)$$

3. Linearize the vorticity $\omega(\psi)$ by using information at infinity because the profile will have a particular form.

4. Then substitute form of ψ into original differential equation with linearized vorticity.
5. Collect terms of equal power of ε ; you will need to solve as many differential equations as the number of terms you are interested in for your solution.
6. Solve the differential equations and their respective boundary conditions.

Non-circular body

We could solve the following problem with perturbation methods as well. Now a circle is very normal, but say we do not have a perfectly circular body. If the shape is only slightly different, we can perturb the circle a small distance $a\varepsilon$ so that the minor axis of the ellipse is length $a(1 - \varepsilon)$. Then the equation of the surface of the boundary of the elliptic cylinder

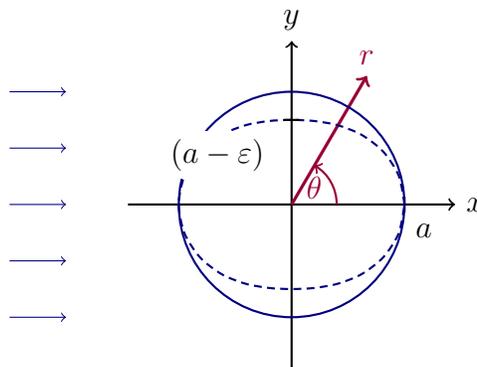


Figure 10.8. Uniform flow around an elliptical cylinder

is,

$$r = a(1 - \varepsilon \sin^2(\theta)). \tag{10.3.28}$$

So,

$$r^2 = a^2 \cos^2(\theta) + a^2(1 - \varepsilon) \sin^2(\theta), \tag{10.3.29a}$$

$$= a^2 \cos^2(\theta) + a^2 \sin^2(\theta) - \varepsilon a^2 \sin^2(\theta), \tag{10.3.29b}$$

$$= a^2 - \varepsilon a^2 \sin^2(\theta), \tag{10.3.29c}$$

$$= a^2 (1 - \varepsilon \sin^2(\theta)). \tag{10.3.29d}$$

We will be looking for a solution of the form

$$\psi(r, \theta; \varepsilon) = \psi_0(r, \theta) + \varepsilon \psi_1(r, \theta) + \dots \tag{10.3.30}$$

Thus the differential equation becomes

$$\nabla^2 \psi_0 + \varepsilon \nabla^2 \psi_1 = 0. \tag{10.3.31}$$

Notice that we have no vorticity, hence the RHS is zero. We must separate terms of the same order,

$$\nabla^2 \psi_0 = 0, \quad (10.3.32a)$$

$$\nabla^2 \psi_1 = 0. \quad (10.3.32b)$$

Then, the boundary conditions are,

$$\psi_0(r \rightarrow \infty, \theta) = ur \sin \theta, \psi_1(r \rightarrow \infty, \theta) = 0. \quad (10.3.33)$$

The first boundary condition is because the shape does not matter at significant distances from the object. This is related to the fact that a slightly deformed circle is very much like a circle from a sufficient distance. The correction for ψ_1 is zero because of the fact that there is no dependence of this condition on ε .

Now there are difficulties that still remain in the boundary condition on the surface. The surface has the condition of a zero value of the stream function at the surface. Now we may express this with the series approximation,

$$\psi_0 [a^2 (1 - \varepsilon \sin^2(\theta)), \theta] + \varepsilon \psi_1 [a^2 (1 - \varepsilon \sin^2(\theta)), \theta] = 0. \quad (10.3.34)$$

This is a difficult equation because it is an explicit function of epsilon by the ε multiplying the second term, and an implicit function of ε in both terms—most importantly the zeroth term. So we will need to expand everything, then truncate at the linear term otherwise we will get something unreal. Doing a Taylor expansion around $\varepsilon = 0$ in the zeroth order term,

$$\psi_0 [a^2 (1 - \varepsilon \sin^2(\theta)), \theta] = \psi_0 [a, \theta] + \frac{1}{1!} \left(\frac{\partial \psi_0}{\partial r} \frac{\partial r}{\partial \varepsilon} \right)_{r \neq 0} \varepsilon, \quad (10.3.35a)$$

$$= \psi_0(a, \theta) - \varepsilon \frac{\partial \psi_0}{\partial r} \sin^2(\theta). \quad (10.3.35b)$$

This is the zero order boundary term. Similarly, for the first order term, we only care about the first term in the Taylor series (since we would have ε^2 if we expanded further);

$$\psi_1 [a^2 (1 - \varepsilon \sin^2(\theta)), \theta] = \psi_1(a, \theta). \quad (10.3.36)$$

Finally the boundary condition on the surface is

$$\psi(S, t) = \psi_0(a, \theta) - \varepsilon \frac{\partial \psi_0}{\partial r} \sin^2(\theta) + \varepsilon \psi_1(a, \theta). \quad (10.3.37)$$

So we have linearized our boundary condition as well.

For $\varepsilon = 0$, $\psi_0(a, \theta) = 0$, and for the first order

$$\psi_1(a, \theta) = a \sin^2(\theta) \frac{\partial \psi_0}{\partial r}, \quad (10.3.38a)$$

$$= \frac{1}{2} a u (3 \sin(\theta) - \sin(3\theta)). \quad (10.3.38b)$$

We used our solution from the zeroth order problem to find this boundary condition ($\psi_0 = u(r - \frac{a^2}{r}) \sin \theta$) with the differentiation. We reduced the perturbation problem into the exact one with linear boundary conditions.

What we must solve now is one with difficult boundary conditions. The total solution is found to be

$$\psi = u \left(r - \frac{a^2}{r} \right) \sin \theta + \frac{1}{2} \varepsilon u \left(3 \frac{a^2}{r} \sin(\theta) - \frac{a^4}{r^3} \sin(3\theta) \right) + \mathcal{O}(\varepsilon^2). \tag{10.3.39}$$

All of these examples are of regular perturbation. This means that the equations that we generate remain consistent in terms of order. In all our examples, we start with the second order differential equations and they stay that order. This is not always the case.

Singular Perturbations

The analysis of boundary layers in fluid mechanics is an example of a singular perturbation problem. Here we have viscosity as well as flow around a large object. Sufficiently far from the obstacle, the flow behaves to varying degrees like an inviscid flow. Nearby, however, the viscosity becomes very important; the main problem with boundary layers is that we have different domains. In one domain (near the surface) $\mu \nabla^2 \mathbf{v}$ dominates, further away the curvature becomes unimportant. As we move away, then $\mathbf{v} \cdot \nabla \mathbf{v}$. In the case of greater

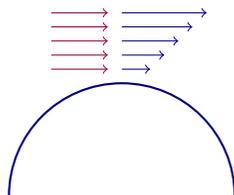


Figure 10.9. Boundary layers

distances we only care about $\mathbf{v} \cdot \nabla \mathbf{v} = -\nabla P$. If friction is ignored we don't even need to solve the equation. If we care only about the profile, then we only solve the mass conservation

$$\nabla \cdot \mathbf{v} = 0, \tag{10.3.40}$$

or

$$\nabla \times \mathbf{v} = -\omega, \tag{10.3.41}$$

more generally. So we solve a second order differential equation close to the boundary and a first order differential equation far away. This is a problem because we have one extra boundary condition that cannot be satisfied. These are complicated mathematically (even simpler asymptotics are non-trivial), but there are simple cases that illustrate the point.

Example of Singular Perturbations: Matched Asymptotic Expansion

In this example the system behaves very differently in the two subdomains we are observing. Here we may use an approach called *matched asymptotic expansion*. Here the small

parameter will multiply the highest order derivative. When we take the limit as the small parameter goes to zero, we lose a second derivative term. Now this method is generally disliked by mathematicians because there is no rigorous theory underlying it (as is the case with regular expansion). We also may not get a convergent solution! The zeroth order for example may work well, the first order might look better, but the second gets terrible, the third might get good again, and so on. It is not easy to know the convergence!

Let's look at the following equation.

$$\varepsilon \frac{d^2 f}{dx^2} + \frac{df}{dx} = a \quad (10.3.42)$$

For $\varepsilon = 0$,

$$\frac{df}{dx} = a. \quad (10.3.43)$$

This is clearly a very different equation. Say our boundary conditions are

$$f(0) = 0, \quad (10.3.44a)$$

$$f(1) = 1. \quad (10.3.44b)$$

Regular solution of the differential equation

This equation can be solved exactly so that we compare the different domains of the solution. Substituting $y = \frac{df}{dx}$ and manipulating

$$\varepsilon \frac{dy}{dx} + y = a, \quad (10.3.45a)$$

$$\frac{dy}{dx} = -\frac{1}{\varepsilon}(y - a), \quad (10.3.45b)$$

$$\int \frac{1}{y - a} dy = -\frac{1}{\varepsilon} \int dx, \quad (10.3.45c)$$

$$y - a = C_1 e^{-\frac{x}{\varepsilon}}, \quad (10.3.45d)$$

$$\frac{df}{dx} = a + C_1 e^{-\frac{x}{\varepsilon}}, \quad (10.3.45e)$$

$$\int df = a \int dx + C_1 \int e^{-\frac{x}{\varepsilon}} dx, \quad (10.3.45f)$$

$$f = ax - C_1 \varepsilon e^{-\frac{x}{\varepsilon}} + C_2. \quad (10.3.45g)$$

We have two boundary conditions remaining to determine the two constants in this equation. Substituting for these boundary conditions,

$$0 = -C_1 \varepsilon e^{-\frac{0}{\varepsilon}} + C_2, \quad (10.3.46a)$$

$$C_2 = C_1 \varepsilon; \quad (10.3.46b)$$

$$1 = a - C_1 \varepsilon e^{-\frac{1}{\varepsilon}} + C_2, \quad (10.3.46c)$$

$$1 = a - C_2 e^{-\frac{1}{\varepsilon}} + C_2, \quad (10.3.46d)$$

$$C_2 = \frac{1 - a}{1 - e^{-1/\varepsilon}}. \quad (10.3.46e)$$

The first constant is now obvious as well. The solution is,

$$f = ax - \frac{1 - a}{1 - e^{-1/\varepsilon}} e^{-\frac{x}{\varepsilon}} + \frac{1 - a}{1 - e^{-1/\varepsilon}}, \tag{10.3.47}$$

or

$$f = ax + (1 - a) \frac{1 - e^{-\frac{x}{\varepsilon}}}{1 - e^{-\frac{1}{\varepsilon}}}. \tag{10.3.48}$$

If we plot this solution We observe that near $x = 1$ the solution is close to linear and the

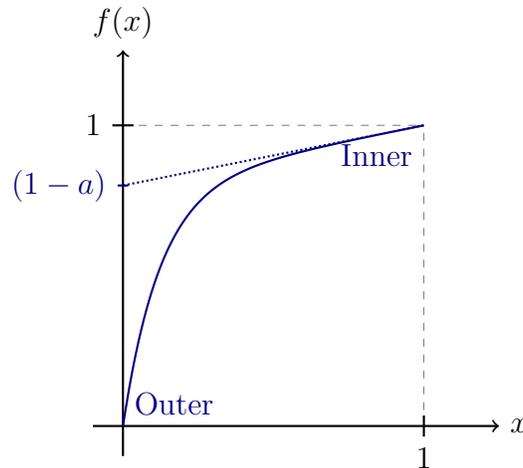


Figure 10.10. Plot second order system with small parameter

intersection with the y axis is $1 - a$. Near $x = 0$ there is a rapid change in the function up until a certain point, while beyond it is very linear. This is called the inner domain, and the linear part is the outer domain.

Asymptotic solution of the differential equation

This differential equation may also be solved using asymptotic methods. They are done in a very different way, though. Let us introduce an inner coordinates and outer coordinates systems. Effectively we will zoom into each region and solve it. Now with the new coordinates (knowing that ε is small), $X = \frac{x}{\varepsilon}$ and $f(x; \varepsilon) = F(X; \varepsilon)$. These we call the inner variables. From these coordinates the equation becomes,

$$\varepsilon \times \varepsilon \frac{d^2 f}{dx^2} + \frac{df}{dx} = a, \tag{10.3.49a}$$

$$\varepsilon^2 \frac{d^2 f}{dx^2} + \varepsilon \frac{df}{dx} = a\varepsilon, \tag{10.3.49b}$$

$$\frac{d^2 f}{d(x/\varepsilon)^2} + \frac{df}{d(x/\varepsilon)} = a\varepsilon, \tag{10.3.49c}$$

$$\frac{d^2 F}{dX^2} + \frac{dF}{dX} = a\varepsilon. \tag{10.3.49d}$$

We see that the zero order solution will be the solution of a first order differential equation while the outer solution will be of a second order differential equation. In this case we are only doing the zero order term, but we have two equations corresponding to the two different domains. We may ultimately need to solve four differential equations if we want to approximate to the linear term. Thus, we deal with nonlinear equations by doing more (easier) work!

10.4 Lecture 29: November 27, 2013

Singular Asymptotic Solution of Second Order Differential Equation (cont.)

Returning to the previous lecture on the asymptotic solution of a singular perturbation. Recall that one of our domains undergoes a rapid change, while the other is simpler and much more nearly linear. The equation we were discussing was,

$$\varepsilon \frac{d^2 f}{dx^2} + \frac{df}{dx} = a \tag{10.4.1}$$

where a is an arbitrary constant. The exact solution was

$$f = ax + (1 - a) \frac{1 - e^{-\frac{x}{\varepsilon}}}{1 - e^{-\frac{1}{\varepsilon}}} \tag{10.4.2}$$

The plot of the equation shows a linear change (with intersection at $(1 - a)$). The zero order

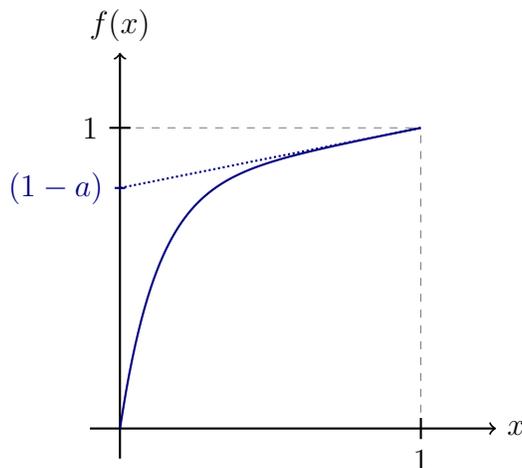


Figure 10.11. Plot second order system with small parameter

asymptotic solution is often a sufficiently accurate solution for the inner and outer solutions. Again we may zoom in to each of the solution areas, but each will give helpful descriptions of their area of interest. In the inner solution form, we set $X = \frac{x}{\varepsilon}$ and $f(x; \varepsilon) = F(X; \varepsilon)$, and get the equation,

$$\frac{d^2 F}{dX^2} + \frac{dF}{dX} = a\varepsilon. \tag{10.4.3}$$

In the zero order, we will have,

$$\frac{d^2 F_0}{dX^2} + \frac{dF_0}{dX} = 0. \tag{10.4.4}$$

In the outer domain, where we do not rescale the system and our equation would become a first order differential equation in the zeroth term. So the outer differential equation is,

$$\frac{df}{dx} = a. \tag{10.4.5}$$

From the exact solution, we can expect that the linear term will come from the inner solution. We may solve the inner term equation by setting $Y = \frac{dF}{dX}$;

$$\frac{dY}{dX} = -Y, \quad (10.4.6a)$$

$$Y = C_1 e^{-X}. \quad (10.4.6b)$$

Recall that we have a derivative,

$$\frac{dF}{dX} = C_1 e^{-X}, \quad (10.4.6c)$$

$$F = C_2 - C_1 e^{-X}. \quad (10.4.6d)$$

We can apply the boundary conditions and,

$$0 = F(X=0), \quad (10.4.7a)$$

$$C_1 = C_2 = C. \quad (10.4.7b)$$

Then the solution simplifies to,

$$F = C(1 - e^{-X}). \quad (10.4.8)$$

For the second boundary condition,

$$1 = F(X=\frac{1}{\varepsilon}), \quad (10.4.9a)$$

$$C = \frac{1}{1 - e^{-\frac{1}{\varepsilon}}} \quad \text{for } \varepsilon \rightarrow 0; C = 1. \quad (10.4.9b)$$

If we took $\varepsilon \rightarrow 0$ then $C = 1$, we would get.

$$F_{\text{in}} = 1 - e^{-X}. \quad (10.4.10)$$

This fails to match the appropriate boundary conditions. Here we must now recognize that we do not want to push our solutions (inner/outer) to be true at the opposite boundaries. This generally won't work. The inner solution will fulfill the condition at $x = 0$, while the outer will match the condition at $x = 1$. In the transition regions we will match the two equations.

Now the outer solution will easily give us,

$$f_{\text{out}} = ax + C_3. \quad (10.4.11)$$

For $x = 1$,

$$1 = a + C_3, \quad (10.4.12a)$$

$$C_3 = 1 - a. \quad (10.4.12b)$$

Thus the outer solution,

$$f_{\text{out}} = ax + (1 - a). \quad (10.4.13)$$

At this point we have both of the solutions forms. For $x \rightarrow 0$ the inner solution will fulfill the left boundary condition for any value of C . We also may observe that the outer solution clearly explains the asymptotic extrapolation of the solution from 1 toward the intersection at $1 - a$.

Now we must have the condition that $x \rightarrow 0 F = 1$, with $X = \frac{x}{\varepsilon}$. From the meeting condition,

$$C = 1 - a. \tag{10.4.14}$$

Then the inner solution is,

$$F_{\text{in}} = (1 - a) (1 - e^{-X}); \tag{10.4.15}$$

the outer solution is,

$$f_{\text{out}} = (1 - a) + ax. \tag{10.4.16}$$

How do we find the composite solution of the inner and the outer? We must sum the two solutions and subtract them while they are written in terms of inner or outer variables. So, in inner variables

$$F_{\text{in}} + f_{\text{out}} + N = (1 - a) (1 - e^{-X}) + (1 - a) + ax - (1 - a), \tag{10.4.17a}$$

$$= (1 - a) (1 - e^{-\frac{x}{\varepsilon}}) + ax. \tag{10.4.17b}$$

If we were to plot this it would look very similar to the solution for small ε . The asymptotic solution will follow almost nearly perfectly for $\varepsilon \in [0.1, 0.5]$. This is surprising because 0.5 is not much less than one. So putting all the solutions on a single figure, we see two solutions are almost indistinguishable. We observe that the inner solution does satisfy the boundary

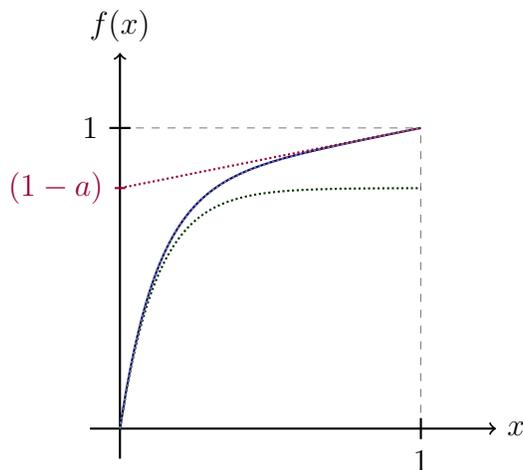


Figure 10.12. Comparison of inner, outer, and true solutions

conditions near $x = 0$ and the outer solution satisfies the solution well near $x = 1$. Again we had to subtract a value so that in the transition region, where both solutions are valid, this allowed us to get a matching solution. Now we could calculate the first order correction, but because it works so well, we see that there is little point for this problem. This method works quite well in general; you simply have to follow the steps of the recipe! This is known as the *van Dyke matching principle*.

Example: Electro-kinetics in a Cylindrical Capillary

We will now discuss a more difficult example that should clarify more on this solution technique. Here we will go into more detail to make the method more clear. Recall that when we discussed solving variable coefficient equations using variation of parameters, particularly when we know a homogeneous equation, we solved,

$$\frac{d^2 y}{dx^2} - \cosh(\Psi_0)y = \frac{d\Psi_0}{dx}, \quad (10.4.18)$$

where,

$$\Psi_0 = 2 \ln \left(\frac{1 + te^{-x}}{1 - te^{-x}} \right). \quad (10.4.19)$$

This is obviously not your usual equation. The equation was derived in a problem for microfluidics. In experiments on capillaries of diameters on the order of a few hundred nanometers, Gabriel Lopez wanted to know the fluid flow undergoing electrokinetic forces. We can

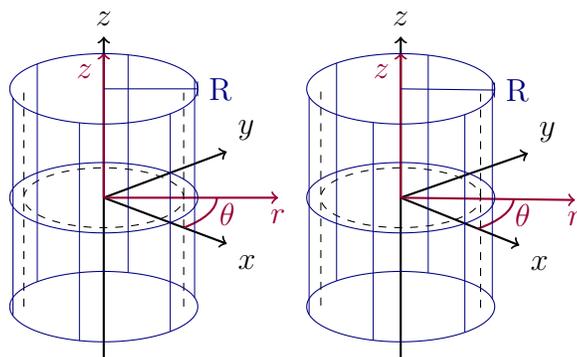


Figure 10.13. Capillary with electrokinetic effects (stereoscopic images)

calculate the flow using the distribution of the potential inside the capillary. Then the distribution of charged particles and the fluid velocities can be found. The equation that describes the electrostatic distribution is the Poisson equation;

$$\nabla^2 \Psi = -\frac{\rho_0}{\epsilon \epsilon_0}. \quad (10.4.20)$$

The right hand side is the charge density divided by the electric properties of the solution. The charge density is related to the potential itself. If we consider a binary electrolyte such as salt, the equation will look similar to,

$$\nabla^2 \Psi = \kappa^2 \sinh(\Psi). \quad (10.4.21)$$

here the potential, Ψ , is made dimensionless by the factor, $\frac{kt}{e} \approx 27$ mV. This is not important for the mathematics, but still useful to note.

Now we know that the following equation has an exact solution if we are solving for a flat surface,

$$\frac{d^2 \Psi}{dx^2} = \kappa^2 \sinh(\Psi). \quad (10.4.22)$$

Here we had to multiply both sides by $\kappa \frac{d\Psi}{dx}$, then consider. If we have cylindrical symmetry we need a different Laplace operator. Then the equation is,

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{d\Psi}{dr} \right) = \kappa^2 \sinh(\Psi). \quad (10.4.23)$$

This will make the problem more difficult to solve because we do not have the trick of the total differential. So this is not easily solved analytically. We may approach this by separating the domain into subdomains will be very useful. A common method of solution is to consider the potential to be relatively low throughout the domain. Then the right hand side is small and we can linearize the hyperbolic sine function. The form of the equation becomes,

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{d\Psi}{dr} \right) = \kappa^2 \Psi. \quad (10.4.24)$$

This is solved in terms of modified Bessel functions of the first kind, $I_0(\kappa r)$. This is popular, but not very natural; most materials have very high charges. Some common materials such as glass (quartz) will often give on the order of 50 to 70 mV. This however is two to three times the value at which the approximation remains reasonable. Then we cannot linearize the equation.

Let's use the trick of matched asymptotic expansions. Rewriting the equation into an equivalent form,

$$\frac{1}{\kappa^2} \frac{d^2\Psi}{dr^2} + \frac{1}{\kappa^2 r} \frac{d\Psi}{dr} = \sinh(\Psi). \quad (10.4.25)$$

The variable κ is known as the inverse screening parameter and has the dimensions of inverse length. The inverse of kappa, κ^{-1} , is often called the *Debye parameter* or *inverse Debye length*. This refers to Debye's study of electrolytes. The potential depends on the radial position in the form of $\frac{e^{-\kappa r}}{r}$. Thus the Debye parameter indicates how quickly the effect of screening will die off. We are more interested in the math, but we must understand this to be able to intelligently divide up the problem into subdomains. We define the inner variable as $x = \kappa(R - r)$. This is a dimensionless variable which starts at the wall and moves toward the interior of the capillary. Now if we consider the nature of the equation very near the edge of the capillary, the curvature of the capillary will have little effect on the equation. (Consider that when one walks on Earth's surface, we don't worry much about the curvature if we are only walking around Albuquerque!) We can assume that it is effectively flat provided that the potential drops very rapidly—as is the case in highly electrolytic solutions. Thus our two subdomains would be: a layer near the wall where the physics is approximately flat, and near the center where the curvature is significant. (This is similar to how near the space station, we will start to care about the curvature!) Now if we have a highly electrolytic solution, then the effect of the solution will have dropped sufficiently that the central approximation will only need the linear term. This will not introduce any unphysical inaccuracy. The inner variable must be such that it is much less than the dimensionless radius of the capillary, or $x \ll \kappa R$. On the other hand if we have a quickly declining right hand side, then $\kappa R \gg 1$ and $\frac{1}{\kappa R} = \varepsilon$ makes for a good small parameter.

Now let us consider that $dx = -\kappa dr$, then $dx^2 = \kappa^2 dr^2$. Also $\frac{1}{\kappa r} = \frac{1}{\kappa R - x}$ and with the small x condition is approximately $\frac{1}{\kappa R}$. This is all we need to replace the equation form for

the inner solution (which is the outer part of our physical problem),

$$\Psi_{\text{in}} = \Psi_{\text{in}}^{(0)} + \left(\frac{1}{\kappa R}\right) \Psi_{\text{in}}^{(1)} + \dots \quad (10.4.26)$$

We will only take the terms out to being linear with respect to $\frac{1}{\kappa R}$. Considering the expansion of the right hand side,

$$\sinh\left(\Psi_{\text{in}}^{(0)} + \left(\frac{1}{\kappa R}\right) \Psi_{\text{in}}^{(1)}\right) = \sinh\left(\Psi_{\text{in}}^{(0)}\right) + \frac{1}{\kappa R} \cosh\left(\Psi_{\text{in}}^{(0)}\right) \Psi_{\text{in}}^{(1)}. \quad (10.4.27)$$

This takes into account that $\left(\frac{1}{\kappa R}\right)$ is small by making a Taylor expansion around the first term and is our linear correction to the charge density function. The differential equation becomes in total,

$$\left(\frac{d^2}{dx^2} - \frac{1}{\kappa R} \frac{d}{dx}\right) \left(\Psi_{\text{in}}^{(0)} + \left(\frac{1}{\kappa R}\right) \Psi_{\text{in}}^{(1)}\right) = \sinh\left(\Psi_{\text{in}}^{(0)}\right) + \frac{1}{\kappa R} \cosh\left(\Psi_{\text{in}}^{(0)}\right) \Psi_{\text{in}}^{(1)}. \quad (10.4.28)$$

So expanding the parenthesis and ignoring super-linear terms, we can collect the terms and construct

$$\frac{d^2 \Psi_{\text{in}}^{(0)}}{dx^2} + \frac{1}{\kappa R} \frac{d^2 \Psi_{\text{in}}^{(1)}}{dx^2} - \frac{1}{\kappa R} \frac{d \Psi_{\text{in}}^{(0)}}{dx} = \sinh\left(\Psi_{\text{in}}^{(0)}\right) + \frac{1}{\kappa R} \cosh\left(\Psi_{\text{in}}^{(0)}\right) \Psi_{\text{in}}^{(1)}. \quad (10.4.29)$$

When we separate for terms of different order, the zeroth order is

$$\frac{d^2 \Psi_{\text{in}}^{(0)}}{dx^2} = \sinh\left(\Psi_{\text{in}}^{(0)}\right), \quad (10.4.30a)$$

and the first order is

$$\frac{d^2 \Psi_{\text{in}}^{(1)}}{dx^2} - \frac{d \Psi_{\text{in}}^{(0)}}{dx} = \cosh\left(\Psi_{\text{in}}^{(0)}\right) \Psi_{\text{in}}^{(1)}. \quad (10.4.30b)$$

What we have is a nonlinear equation in the zeroth order, but we have a known exact solution. The other equation is a non-homogeneous second order equation with variable coefficients. This is the hard problem to solve, but at least it is linear. We didn't get rid of the second order derivative (as in the previous example), but it does allow us to ignore the effect of the curvature. That is the main difficulty in solving this problem.

So rewriting the differential equation for the first order,

$$\frac{d^2 \Psi_{\text{in}}^{(1)}}{dx^2} - \cosh\left(\Psi_{\text{in}}^{(0)}\right) \Psi_{\text{in}}^{(1)} = \frac{d \Psi_{\text{in}}^{(0)}}{dx}. \quad (10.4.31)$$

The non-homogeneous and non-constant coefficient terms are both known from the zeroth order solution.

If we have the Dirichlet problem of a known potential at the boundary, we can say that $\Psi(r=R) = \Psi(x=0) = \zeta$. To make use of the zeroth solution, we must assume that the solution will go to zero as the solution goes to infinity. Now in this problem we can only go as far as the center of the cylinder, but our approximations will still work as long as

the function drops down close to zero significantly before reaching the center. So we may set the second boundary condition at an arbitrary radius. Now in the zeroth order solution $t = \tanh(\zeta)$ from the boundary condition.

We must now solve the first order correction. Using varying parameters we will first need to solve the homogeneous equation by finding the second solution and using a linear combination of the two, then we will vary the parameters. The homogeneous equation that we will start with is,

$$\frac{d^2\Psi_{\text{in}}^{(1)}}{dx^2} - \cosh\left(\Psi_{\text{in}}^{(0)}\right)\Psi_{\text{in}}^{(1)} = 0. \quad (10.4.32)$$

As long as we know one particular solution to this equation, we can find the universal solution by finding the second solution and using a linear combination. In these matched asymptotic solutions, usually we can guess one of the higher order solutions from other forms of the lower order solutions. For the first solution, it will help by observing both equations. We realize that by differentiating the zeroth order equation another time, we get,

$$\frac{d^3\Psi_{\text{in}}^{(0)}}{dx^3} - \cosh\left(\Psi_{\text{in}}^{(0)}\right)\frac{d\Psi_{\text{in}}^{(0)}}{dx} = 0. \quad (10.4.33)$$

What happens when we compare the equations, is we notice that $\Psi_1 = \frac{d\Psi_{\text{in}}^{(0)}}{dx}$ then we can quickly go from the first order homogeneous equation to the differentiated zeroth order equation. (This trivial idea was not easy to come by!) Thus a first homogeneous solution is actually the non-homogeneous term! Now if we find one, we know the other term as well.

$$\Psi_1 = \frac{d\Psi_{\text{in}}^{(0)}}{dx}, \quad (10.4.34a)$$

$$= \frac{4te^x}{t^2 - e^{2x}}. \quad (10.4.34b)$$

Again this is a particular solution to the homogeneous equation. The second solution is

$$\Psi_2 = \Psi_1 \int \frac{1}{\Psi_1^2} dx, \quad (10.4.35a)$$

$$= \frac{e^{2x} + t^2}{e^{2x} - t^2}. \quad (10.4.35b)$$

Finally, we must use variation of parameters to find the coefficients,

$$u_1(x) = \int \Psi_2 \frac{d\Psi_{\text{in}}^{(0)}}{dx} dx + C_1, \quad (10.4.36a)$$

$$= \int \Psi_2 \Psi_1 dx + C_1, \quad (10.4.36b)$$

$$u_2(x) = \int \Psi_1 \frac{d\Psi_{\text{in}}^{(0)}}{dx} dx + C_2, \quad (10.4.36c)$$

$$= \int \Psi_1 \Psi_1 dx + C_2. \quad (10.4.36d)$$

Coincidentally this simplified greatly—this is a very problem specific and lucky thing! With this we may construct the solution as,

$$\Psi_{\text{in}}^{(1)} = u_1(x)\Psi_1 + u_2(x)\Psi_2. \quad (10.4.37)$$

The constants are limited by the requirement that the first order correction to the inner solution must vanish both at zero and infinity. This will avoid unphysical contributions at the boundary. Applying the conditions to find C_1 and C_2 ,

$$\Psi_{\text{in}}^{(1)}(x=0) = 0, \quad (10.4.38a)$$

$$\Psi_{\text{in}}^{(1)}(x \rightarrow \infty) = 0, \quad (10.4.38b)$$

we get the solution,

$$\Psi_{\text{in}}^{(1)}(x) = \frac{2t [xe^x - t^2 \sinh(x)]}{e^{2x} - t^2}. \quad (10.4.39)$$

Then the total inner solution is,

$$\Psi_{\text{in}} = \Psi_{\text{in}}^{(0)} + \frac{1}{\kappa R} \Psi_{\text{in}}^{(1)}, \quad (10.4.40a)$$

$$= 2 \ln \left(\frac{1 + te^{-x}}{1 - te^{-x}} \right) + \left(\frac{1}{\kappa R} \right) \frac{2t [xe^x - t^2 \sinh(x)]}{e^{2x} - t^2}. \quad (10.4.40b)$$

This tells us what is happening to the solution in the small region near the wall. The region near the wall is the more difficult part to solve.

The outer solution will be easier because we will have a much smaller potential in the region. When we plot the potential, we observe that the potential drops down from ζ at faster than exponential. So everywhere above a certain point we will not be able to linearize



Figure 10.14. Plot of potential with x in capillary

the density dependence. We see that there is a small contribution in the outer solution that is due to the curvature (the $\sinh(x)$ term). Further beyond the point, the curvature becomes

very important, but simultaneously the potential becomes less than one $\Psi(x) < 1$. Around 1 the approximations will be the least accurate, but that is a price that we have to pay.

So now we must solve a different equation for the outer problem (middle of the pore). Here we must account explicitly for the curvature;

$$\frac{d^2\Psi_{\text{out}}}{dr^2} + \frac{1}{r} \frac{d\Psi_{\text{out}}}{dr} = \kappa\Psi. \quad (10.4.41)$$

The second term of the left hand side is the term that gives the curvature in the equation. At the same time the potential is low enough that we may approximate the right hand side by a simple linear approximation of the potential. This is due to the Taylor expansion of the hyperbolic sine,

$$\sinh(y) = y + \frac{y^3}{3!} + \dots. \quad (10.4.42)$$

We may stop at the first term, which is sufficiently accurate because the error is only $\mathcal{O}(\Psi^3)$. This is actually quite good as long as $y < 1$; otherwise the series diverges. In this case, for $\Psi < 1$ this is a good approximation. The problem we deal with now is something which has been solved by the modified Bessel functions. The first and second order solutions will be very similar, so we can separate the solutions. In the inner solutions the two terms were different, but in the outer they will end up being the same. So, using the modified Bessel functions of first kind (zero order) we have the known solutions

$$\Psi_{\text{out}}^{(0)} = A I_0(\kappa r), \quad (10.4.43)$$

and the first correction,

$$\Psi_{\text{out}}^{(1)} = B I_0(\kappa r). \quad (10.4.44)$$

We need to match these functions to the inner solution.

We will do this procedure next time; next class will be our final lecture. We will not hold class next Wednesday.

10.5 Lecture 30: December 2, 2013

We will next be doing the final. Dr. Petsev will try to send out the final Thursday. (Thursday was considered as an option.) The final is due Friday of next week at 2 PM in his office.

We return to the example from last time where we were solving the electrokinetic capillary problem.

Example: Electro-kinetics in a Cylindrical Capillary (cont.)

Note that this approach could be useful if we wanted to solve for on the outside of a cylinder as well. Here we would need to change the sign in front of the $-\frac{1}{\kappa r} \frac{d\Psi}{dr}$ term.



Figure 10.15. Capillary with electrokinetic effects

Now the equation for the potential is the Poisson–Boltzmann equation,

$$\nabla^2 \Psi = \kappa^2 \sinh(\Psi). \quad (10.5.1)$$

We consider a region near to the wall where the potential is especially high and the curvature is relatively insignificant. The radius is much greater and as we get near to the center the potential will be less than one and the hyperbolic sine term can be linearized. On the wall we made use of the fact that the equation

$$\frac{d^2 \Psi}{dx^2} = \kappa^2 \sinh(\Psi) \quad (10.5.2)$$

may be solved exactly. Far from the wall, we needed to solve

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{d\Psi}{dr} \right) = \kappa^2 \Psi. \quad (10.5.3)$$

We first had to identify the two separate regions in the physical problem. Then we related these regions to length scales and the small parameter ($\frac{1}{\kappa R}$). Since κR is large, the boundary region is very small; thus we identified the two regions. Presenting the solutions in the form of the inner variables and expansion around small parameter; $\Psi_{\text{in}} = \Psi_{\text{in}}^{(0)} + \frac{1}{\kappa R} \Psi_{\text{in}}^{(1)} + \dots$. In total we will get four different differential equations; this is reduced to three because the outer solutions (near the middle) will have exactly the same mathematical forms. We have

zeroth and first order equations for the inner and outer zones. In the general case we would have something unsolvable, but now we can solve for these effects. We have previously solved the equations;

$$\Psi_{\text{in}}^{(0)} = 2 \ln \left(\frac{1 + te^{-x}}{1 - te^{-x}} \right). \quad (10.5.4)$$

This is exactly what was found by solving the flat equation. The outer solution is the solution of the linearized equation,

$$\Psi_{\text{out}}^{(0)} = A I_0(\kappa r). \quad (10.5.5)$$

This one does not satisfy the boundary on the edge of the cylinder, so it is hard to know the value of the constant.

Zeroth order solution matching

Now let's find A by matching the two solutions. Observing the zeroth order equation near the surface, consider the asymptotics of the function,

$$\frac{1 + y}{1 - y} \approx 1 + 2y, \quad (10.5.6a)$$

$$2 \ln \left(\frac{1 + y}{1 - y} \right) \approx 2 \ln(1 + 2y), \quad (10.5.6b)$$

$$\approx 2(2y), \quad (10.5.6c)$$

$$= 4y. \quad (10.5.6d)$$

In general from the asymptotics the solution tends to

$$\Psi_{\text{in}}^{(0)}(r) \rightarrow 4te^{-\kappa(R-r)}. \quad (10.5.7)$$

where we substituted for $x = \kappa(R - r)$ to return to the outer variable form. Extrapolating the outer solution near the wall, from tables on asymptotics of Bessel functions

$$\Psi_{\text{out}}^{(0)} \approx \frac{Ae^{\kappa r}}{\sqrt{2\pi\kappa R}}. \quad (10.5.8)$$

If we take our solution and look at asymptotic behavior, the two asymptotics must become the same to match the solution. We get from this,

$$4te^{-\kappa R}e^{\kappa r} = \frac{Ae^{\kappa r}}{\sqrt{2\pi\kappa R}}, \quad (10.5.9a)$$

$$A = 4te^{-\kappa R}\sqrt{2\pi\kappa R}. \quad (10.5.9b)$$

Recall that $t = \tanh(\zeta/2)$. Now we can completely write our zero order solution;

$$\Psi^{(0)}(r) = 2 \ln \left(\frac{1 + te^{-x}}{1 - te^{-x}} \right) + 4te^{-\kappa R}\sqrt{2\pi\kappa R} I_0(\kappa r) + C \quad (10.5.10)$$

This applies to the whole region. This is not all because we have matched the two solutions so that the solutions are matched where the both are contributing to the system. That's

why we solved for A . We must subtract one of the two asymptotic solutions to get the right value; so we select from the second term,

$$\boxed{\Psi^{(0)}(r) = 2 \ln \left(\frac{1 + te^{-x}}{1 - te^{-x}} \right) + 4te^{-\kappa R} \sqrt{2\pi\kappa R} I_0(\kappa r) - 4te^{-\kappa(R-r)}}. \quad (10.5.11)$$

First order solution matching

Moving on to the first order correction of the solutions, we would like to match the first order inner and outer. The first order inner solution is,

$$\Psi_{\text{in}}^{(1)} = \frac{2t [\kappa(R-r)e^{\kappa(R-r)} - t^2 \sinh(\kappa(R-r))]}{e^{2\kappa(R-r)} - t^2}. \quad (10.5.12)$$

For large x the asymptotic form of the expression is $-t^3 e^{-\kappa(R-r)}$. This is for near the wall. For near the center we have the first order equation is similar to the zeroth, but with a different constant;

$$\Psi_{\text{out}}^{(1)} = B I_0(\kappa r). \quad (10.5.13a)$$

This will have the same asymptotics as the zeroth order,

$$\Psi_{\text{out}}^{(1)} \approx \frac{B e^{\kappa r}}{\sqrt{2\pi\kappa R}}. \quad (10.5.13b)$$

Requiring that the two expressions be the same in their asymptotic form,

$$-t^3 e^{-\kappa(R-r)} = \frac{B e^{\kappa r}}{\sqrt{2\pi\kappa R}}, \quad (10.5.14a)$$

$$B = -t^3 \sqrt{2\pi\kappa R} e^{-\kappa R}. \quad (10.5.14b)$$

So the complete first order solution with inner and outer solutions is;

$$\boxed{\Psi^{(1)}(r) = \frac{2t [\kappa(R-r)e^{\kappa(R-r)} - t^2 \sinh(\kappa(R-r))]}{e^{2\kappa(R-r)} - t^2} - t^3 \sqrt{2\pi\kappa R} e^{-\kappa R} I_0(\kappa r) + t^3 e^{-\kappa(R-r)}}. \quad (10.5.15)$$

The complete solution will be $\Psi(r) = \Psi^{(0)} + \frac{1}{\kappa R} \Psi^{(1)}$,

$$\begin{aligned} \Psi(r) = & 2 \ln \left(\frac{1 + te^{-x}}{1 - te^{-x}} \right) + 4te^{-\kappa R} \sqrt{2\pi\kappa R} I_0(\kappa r) - 4te^{-\kappa(R-r)} \\ & + \frac{1}{\kappa R} \left[\frac{2t [\kappa(R-r)e^{\kappa(R-r)} - t^2 \sinh(\kappa(R-r))]}{e^{2\kappa(R-r)} - t^2} - t^3 \sqrt{2\pi\kappa R} e^{-\kappa R} I_0(\kappa r) + t^3 e^{-\kappa(R-r)} \right] \end{aligned} \quad (10.5.16)$$

Now consider if we wanted the charge of the surface. The charge is,

$$\sigma = \varepsilon \varepsilon_0 \left[\frac{d\Psi}{dr} \right]_{r=R}. \quad (10.5.17)$$

We would effectively be finding the charge by taking the derivative of the potential and evaluating it at the surface. Then we would only care about the inner solution contributions Ψ_{in} . The resulting charge is,

$$\sigma = 2\kappa\epsilon\epsilon_0 \left[\sinh\left(\frac{\zeta}{2}\right) - \frac{1}{\kappa R} \tanh\left(\frac{\zeta}{4}\right) \right]. \quad (10.5.18)$$

The first term comes from the flat solution which is the zero order, the second term comes from the correction for the curvature. This is interesting because this equation was previously derived semi-empirically. The asymptotic analysis now can tell us what the meaning of each of the two terms is from a theoretical standpoint. If the problem outside the cylinder was being solved, the only difference is that we would have a plus sign in front of the second term.

For a charged capillary filled with electrolyte solution where an electric field is applied on both sides, the fluid will move. It has been shown early in the 1900s, that the fluid flow



Figure 10.16. Capillary fluids driven by electric fields

is given by the equation

$$\nabla^2 \mathbf{v} = \frac{\epsilon\epsilon_0}{\eta} \mathbf{E} \nabla^2 \Psi. \quad (10.5.19)$$

Thus the potential distribution inside determines the fluid flow profile. Previously this was alluded to as when we know the potential we can know many things about what is going on in the capillary.

In the cylindrical symmetry we are looking for a solution for the velocity in the form of,

$$\mathbf{v} = \mathbf{v}^{(0)} + \frac{1}{\kappa R} \mathbf{v}^{(1)}. \quad (10.5.20)$$

Clearly we may show that there is a similarity between these two equations such that the form of the potential directly gives us the form of the velocity solution. For the inner part

(close to the wall), we can substitute for the expansions

$$\begin{aligned} \frac{d^2}{dx^2} \left(\mathbf{v}_{\text{in}}^{(0)} + \frac{1}{\kappa R} \mathbf{v}_{\text{in}}^{(1)} \right) - \frac{1}{\kappa R} \frac{d}{dx} \left(\mathbf{v}_{\text{in}}^{(0)} + \frac{1}{\kappa R} \mathbf{v}_{\text{in}}^{(1)} \right) \\ = \frac{\varepsilon \varepsilon_0}{\eta} \mathbf{E} \left[\frac{d^2}{dx^2} \left(\Psi_{\text{in}}^{(0)} + \frac{1}{\kappa R} \Psi_{\text{in}}^{(1)} \right) - \frac{1}{\kappa R} \frac{d}{dx} \left(\Psi_{\text{in}}^{(0)} + \frac{1}{\kappa R} \Psi_{\text{in}}^{(1)} \right) \right] \end{aligned} \quad (10.5.21)$$

Then we can apply the operators and ignore terms greater than first order and collect the terms. For the zero order,

$$\frac{d^2 \mathbf{v}^{(0)}}{dx^2} = \frac{\varepsilon \varepsilon_0}{\eta} \mathbf{E} \frac{d^2 \Psi_{\text{in}}^{(0)}}{dx^2}, \quad (10.5.22)$$

and for the first order,

$$\frac{d^2 \mathbf{v}^{(1)}}{dx^2} - \frac{d \mathbf{v}^{(1)}}{dx} = \frac{\varepsilon \varepsilon_0}{\eta} \mathbf{E} \left(\frac{d^2 \Psi_{\text{in}}^{(1)}}{dx^2} - \frac{d \Psi_{\text{in}}^{(0)}}{dx} \right). \quad (10.5.23)$$

The solution to the zeroth order term is a known one;

$$\mathbf{v}_{\text{in}}^{(0)} = \frac{\varepsilon \varepsilon_0}{\eta} \mathbf{E} \left[\zeta - \Psi_{\text{in}}^{(0)}(x) \right]. \quad (10.5.24)$$

The boundary conditions to obtain this;

$$\mathbf{v}(r=R) = \mathbf{0}, \quad (10.5.25a)$$

$$\Psi(r=R) = \zeta. \quad (10.5.25b)$$

Also the velocity reaches steady state far away, and the potential goes to zero far away. So we are looking at a solution that behaves properly near the wall, but does not satisfy the boundary condition in the center. The other solution is the following,

$$\mathbf{v}_{\text{in}}^{(1)} = \frac{\varepsilon \varepsilon_0}{\eta} \mathbf{E} \Psi_{\text{in}}^{(1)}. \quad (10.5.26)$$

This is from the constraints,

$$\mathbf{v}(r=R) = \mathbf{0}, \quad (10.5.27a)$$

$$\Psi(r=R) = 0. \quad (10.5.27b)$$

So we have the first order and zeroth order corrections. Combining the inner velocity is found,

$$\mathbf{v}_{\text{in}} = \mathbf{v}_{\text{in}}^{(0)} + \frac{1}{\kappa R} \mathbf{v}_{\text{in}}^{(1)}, \quad (10.5.28a)$$

$$= \frac{\varepsilon \varepsilon_0}{\eta} \mathbf{E} \left[\zeta - \Psi_{\text{in}}(x) \right]. \quad (10.5.28b)$$

This is what we generally observe in solving this kind of potential problem; the velocity flow profile follows exactly the shape of the potential. The same thing will come out when we solve for the outer solution. In the end we end up with the result;

$$\mathbf{v} = \mathbf{v}^{(0)} + \frac{1}{\kappa R} \mathbf{v}^{(1)}, \quad (10.5.29a)$$

$$= \frac{\varepsilon \varepsilon_0}{\eta} \mathbf{E} \left[\zeta - \left(\Psi^{(0)} + \frac{1}{\kappa R} \Psi^{(1)} \right) \right]. \quad (10.5.29b)$$

This concludes this problem.

We will not have asymptotics problems on the final since there were no homework's on the concepts. This unit was to give you an idea and feeling for how these methods work. Any other material may be on the final.

UNIT 11

Chapters 21 & 22—Probability and Statistics

11.1 Lecture 30: November 26, 2014

Probability and Stochastic Processes

We will primarily be covering concepts in this lecture. In particular we will cover discrete random variables. Bernoulli was one of the pioneers of statistics. He was motivated by gambling and wrote a long article called *The Art of Conjecture* which deals with coin tosses and probabilities.

So let us define a space of possible outcomes, then pick one randomly. In a coin toss we only have two possibilities with heads and tails. A dice has six outcomes, and others can be much more complicated. In general, we have a probability of an event,

$$p\{E_j\} = \lim_{N \rightarrow \infty} \frac{N_j}{N}. \quad (11.1.1)$$

$j = 1, 2, \dots, n$ which gives the dimensionality of the sample space (*e.g.* 2 for coin, 6 for dice). If each attempt always gives you the same outcome, then

$$N_j = N \rightarrow p(E_j) = 1. \quad (11.1.2)$$

Probabilities are normalized. If you have many different probabilities, the sum is one;

$$\sum_{j=1}^n p(E_j) = 1. \quad (11.1.3)$$

This property may be used for normalization.

If we have a *joint probability distribution*, where outcomes are occurring simultaneously, Both may occur, and there is the probability that only one of them will occur. Then,

$$p(i \text{ or } j) = p(E_i) + p(E_j). \quad (11.1.4)$$

To define the overlapping region, we use the symbol $A \cap B$. To define the connection of both regions, we use the symbol $A \cup B$.

The theory of probability is based on a few axioms. For all possible outcomes, Ω ,

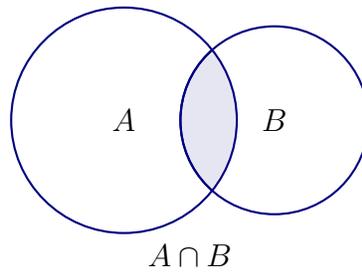


Figure 11.1. Venn diagram of related sets

1. $p(A) \geq 0$
2. $p(\Omega) = 1$
3. for $A \cap B = \emptyset$ then $p(A \cup B) = p(A) + p(B)$
4. given $p(A)$ (probability for A) then for anything but A is $1 - p(A)$
5. The probability for the empty set is zero: $p(\emptyset) = 0$

Conditional Probability

We have different types of probability based on our system. An important one is the *conditional probability*. What is the probability of being on a particular spot in a lattice. This will require the knowledge of the probabilities of being at the neighbors. This is represented by

$$p(A|B) p(B) = p(A \cap B). \tag{11.1.5}$$

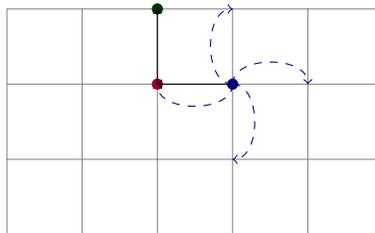


Figure 11.2. Brownian particle on a lattice

This is a useful simplified representation of a Brownian particle. Clearly present position is a result of previous positions, and future locations will branch from there.

If we have independent outcomes,

$$p(A, B) = p(A)p(B). \tag{11.1.6}$$

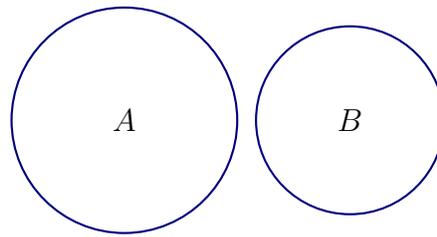


Figure 11.3. Independent outcomes

for heads or tails the probability is $1/2$ each. What now is the chance to get heads twice in a row is

$$P(H, H) = \frac{1}{2} \frac{1}{2}, \quad (11.1.7a)$$

$$= \frac{1}{4}. \quad (11.1.7b)$$

in general we will have repeated probabilities of the form of $1/2^n$, or

$$P(H, H, \dots, H) = \frac{1}{2^n}. \quad (11.1.8)$$

Mean Values (Expected value)

For a set X with values x_i for $i = 1, \dots, n$, then the mean is expressed,

$$\mu = \sum_{i=1}^n x_i P(x_i). \quad (11.1.9)$$

We may also represent the mean with $\langle X \rangle$ or \bar{X} . $x_i = f(x_i)$ for $f(x)$

$$E \{f(x)\} = \langle f(x) \rangle, \quad (11.1.10a)$$

$$= \sum_{i=1}^n f(x_i) p(x_i). \quad (11.1.10b)$$

$$f(x) = X^m$$

The moment:

$$E \{X^m\} = \sum_{i=1}^n x_i^m \phi(x_i). \quad (11.1.11)$$

gives the m^{th} moment. Usually this is not equivalent:

$$E \{X^2\} \neq E \{X\}^2. \quad (11.1.12)$$

Now considering $E \{(X - \mu)^m\} = \langle (X - \mu)^m \rangle$ is the m^{th} central moment (relative to the mean).

If $m = 2$ this is known as the *variance* of x and is denoted with

$$E \{(X - \mu)^2\} = \text{Var} \{X\} = \sigma^2. \tag{11.1.13}$$

Now

$$\sigma^2 \geq 0, \tag{11.1.14a}$$

$$\sigma^2 = E \{X^2\} - E \{X\}^2. \tag{11.1.14b}$$

We will prove this identity by going through the definitions.

$$E \{(X - \mu)^2\} = E \{X^2 - 2X\mu + \mu^2\}. \tag{11.1.15a}$$

Determining an expected value is a linear operation, meaning in particular that,

$$E \{x + y + z\} = \sum_{i=1}^n (x + y + z)P(x)P(y)P(z), \tag{11.1.16a}$$

$$= \sum_{i=1}^n x \underbrace{P(x)P(y)P(z)}_{\mathbb{P}(x)} + \sum_{i=1}^n y \underbrace{P(x)P(y)P(z)}_{\mathbb{P}(y)} + \sum_{i=1}^n z \underbrace{P(x)P(y)P(z)}_{\mathbb{P}(z)}. \tag{11.1.16b}$$

so returning to the derivation,

$$= E \{X^2\} - 2\mu E \{X\} + E \{\mu\}, \tag{11.1.17a}$$

$$= \sum_{i=1}^n x_i^2 P(x_i) - 2\mu \sum_{i=1}^n x_i P(x_i) + \sum_{i=1}^n P(x_i), \tag{11.1.17b}$$

$$\sum_{i=1}^n P(x_i) = 1 \text{ and } \sum_{i=1}^n x_i P(x_i) = \mu$$

$$= E \{X^2\} - 2\mu^2 + \mu^2, \tag{11.1.17c}$$

$$= E \{X^2\} - \mu^2, \tag{11.1.17d}$$

$$= E \{X^2\} - E \{X\}^2. \tag{11.1.17e}$$

For a cumulative distribution

$$p(x_i) \rightarrow X = x_i, P(x_i) \rightarrow X \leq x_i. \tag{11.1.18}$$

where

$$P(x_i) = \sum_{x_i \leq x} p(x_i). \tag{11.1.19}$$

We can have joint probabilities or joint cumulative probabilities

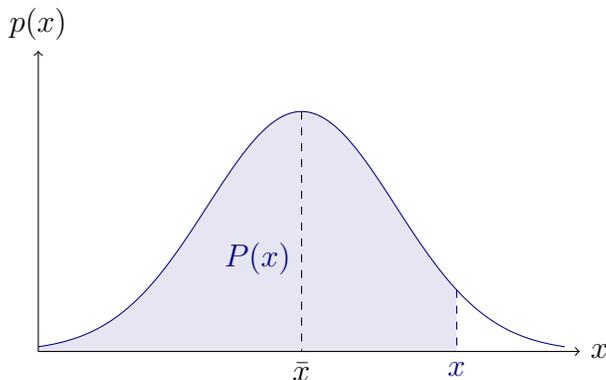


Figure 11.4. Cumulative distribution

$$P(x_i, y_j) = \sum_{x \leq x_i} \sum_{y \leq y_j} p(x_i)p(y_j). \tag{11.1.20}$$

$$E \{f(x, y)\} = \sum_{x \leq x_i} \sum_{y \leq y_j} f(x_i, y_j)p(x_i, y_j). \tag{11.1.21}$$

See example 3 in the book. then

$$E \{(X - \mu_x)(Y - \mu_y)\} = \text{Cov}(X, Y) \tag{11.1.22}$$

This is referred to as the *covariance* and gives how related the two random events are. This is not the same as $E \{(X - \mu_x)\} E \{(Y - \mu_y)\}$. Also $\text{Cov}(X, Y) = 0$ is a necessary, but not sufficient condition for them to be independent.

Coin Toss

Returning to the coin toss. If we want to have the probability of doing exactly m times in n tosses ($n \geq m$). For each toss we have the probability of one half. The number of possible outcomes for n tosses is 2^n , but we only want to know one. So how many ways can we get this? This is the same problem as with the lattice with n cells and we want to arrange m objects on the lattice. This can be done many ways. Say we want to arrange 6 objects in a

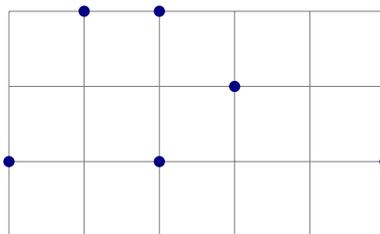


Figure 11.5. Several occupied states on a lattice

lattices of 24 sites; we can arrange this many ways.

Now considering problems of statistical mechanics, if we have a total of n options. For trial 1 we have n possible options, for trial 2 we have only $n - 1$ choices. Moving on to trial 3 we have been reduced to only $n - 2$ we have fewer down to $n - m + 1$ possibilities if we have done m trials. The resulting probabilities,

$$n(n - 1)(n - 2) \cdots (n - m + 1) = \frac{n!}{m!(n - m)!}. \tag{11.1.23}$$

In this way we can arrange m objects over n places. It does not really matter which item we put in each place, so long as the places themselves are equivalently filled. To correct for this we could rearrange it $m!$ times. This gives the total number of configurations that conform to the requirement. This is the fraction of outcomes that corresponds to the requirement;

$$\text{probability to have } m \text{ heads} = \frac{n!}{m!(n - m)!} \frac{1}{2^n}. \tag{11.1.24}$$

and gives the probability to have m heads.

$$\frac{n!}{m!(n - m)!} \tag{11.1.25}$$

gives m objects that are indistinguishable on n locations for $n \geq m$. $n = m$ gives only one possibility.

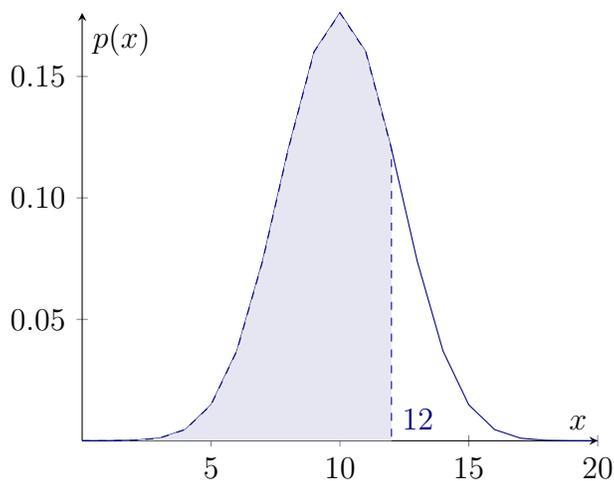


Figure 11.6. Binomial distribution for $n = 20$ trials; cumulative probability of twelve or fewer heads

The peak probability is at $1/2$. We want to find the maximum of the function using differentiation. Derivatives of factorial functions is difficult, but we may use the Stirling approximation (where n , m and $(n - m)$ are large), then

$$\ln x! \approx x \ln x - x. \tag{11.1.26}$$

This formula significantly simplifies the function. To find the maximum,

$$\frac{\partial}{\partial m} \left(\frac{n!}{m!(n-m)!} \right) = 0. \quad (11.1.27a)$$

all we need for minimization is

$$\frac{\partial}{\partial m} \left(\frac{1}{m!(n-m)!} \right) \approx -m \ln m + m - (n-m) \ln(n-m) + (n-m). \quad (11.1.28a)$$

For a peaking function, the logarithm of the function will also peak at that point. The

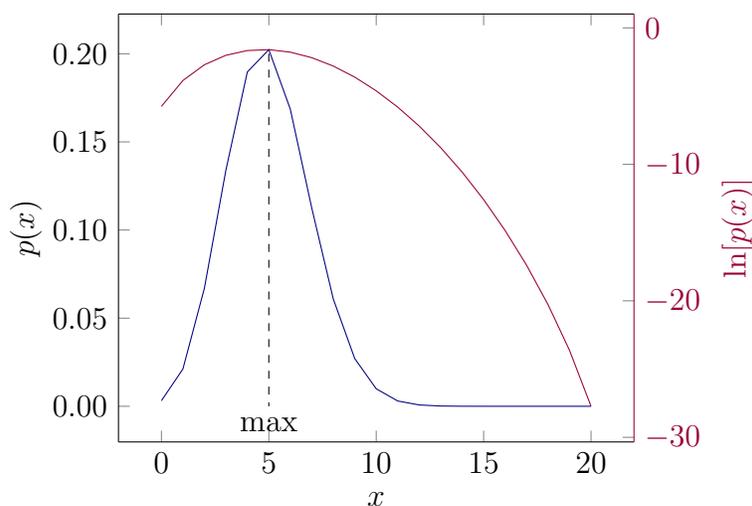


Figure 11.7. Binomial and log of binomial distribution for $n = 20$ and $p = 0.25$

approximation will further simplify

$$\frac{\partial}{\partial m} \left(\frac{1}{m!(n-m)!} \right) \approx \ln \left(\frac{n-m}{m} \right) = 0. \quad (11.1.29a)$$

Thus $\frac{n-m}{m} = 1$ gives the solution of the minimum,

$$m = \frac{n}{2}. \quad (11.1.30)$$

Now when we have either one or another possibility to occur p or q with $p+q=1$. Then,

$$p(m) = \frac{n!}{m!(n-m)!} p^m q^{n-m}. \quad (11.1.31)$$

if $p = 1/2$ then $q = 1/2$ and the second part of the right hand side will be $1/2^n$ as seen previously. For molecules on the lattice we are dealing with numbers on the order of $n \approx 10^{23}$. For such values the graph is nearly the delta function with a very high accuracy of the Stirling formula;

$$x! = x \ln x - x. \quad (11.1.32)$$

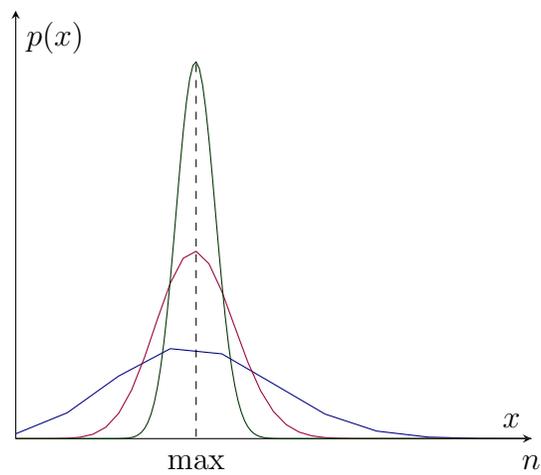


Figure 11.8. Probability narrowing toward δ -function with increasing sample size n . Binomial distribution with $p = 0.35$ for changing n while graphing with equal areas: $n = 10$ (blue), $n = 40$ (red), and $n = 160$ (green).

11.2 Lecture 31: December 1, 2014

Binomial Distribution

Previously we had come up with the binomial distribution and want to look at some important results. We are considering randomly distributed objects in bins. If we have bins of size Δt with a total interval of t , then the probability is,

$$p = \frac{\Delta t}{t}, \quad (11.2.1)$$

and is related to the cumulative probability

$$P(m) = \frac{n!}{m!(n-m)!} p^m (1-p)^{n-m}. \quad (11.2.2)$$

Similarly,

$$P(m) = \frac{n!}{m!(n-m)!} \left(\frac{\Delta t}{t}\right)^m \left(1 - \frac{\Delta t}{t}\right)^{n-m}. \quad (11.2.3)$$

Now,

$$\mu = np = \frac{n\Delta t}{t} = \lambda t. \quad (11.2.4)$$

For small Δt and large n ,

$$p(m) \approx \frac{(\lambda \Delta t)^m}{m!} e^{-\lambda \Delta t}, \quad (11.2.5)$$

where $\lambda = n/t$ is the number of particles per bin. The above equation is known as the *Poisson distribution*. This is applicable to many things including chemical reactions, waiting times in restaurants, *etc.*

Continuous Random Variables

For *continuous random variables*, the values are no longer discrete but can take on any number. We will substitute summation with integration. Now a probability is expressed with $p(x) dx$ and gives us the probability of finding a particular realization of a random variable in an interval,

$$p(x) dx = \text{Prob} [x \leq X \leq x + dx]. \quad (11.2.6)$$

Then to find over the domain $[a, b]$,

$$\text{Prob} [a \leq X \leq b] = \int_a^b p(x) dx. \quad (11.2.7)$$

To normalize the system,

$$\int_{-\infty}^{\infty} p(x) dx = 1. \quad (11.2.8)$$

This is the continuous equivalent to the summation, $\sum_{j=1}^n p(E_j) = 1$.

We will also have the cumulative probability,

$$P(x) = \text{Prob} [X \leq x]. \quad (11.2.9a)$$

This gives us the probability to find X less than some value x .

$$= \int_{-\infty}^x p(X) dX. \quad (11.2.9b)$$

The two integrals are easily related as

$$\frac{dP(x)}{dx} = p(x). \quad (11.2.10)$$

In the literature, the cumulative probability is often called the *integral probability*, while the other probability is the *differential probability*.

As an interesting physical example we can consider the distribution of particle sizes in a suspension, you can measure the weight change with time on the balance. The large particles (few of them) will hit first, then the middle range will come (there will be the most of them), and finally the small ones will drop down.

Now say we have a function of the random variable $f(x)$, we may want the average,

$$E \{f(x)\} = \int_{-\infty}^{+\infty} p(x)f(x) dx. \quad (11.2.11)$$

The average is defined,

$$\mu = \int_{-\infty}^{+\infty} xp(x) dx. \quad (11.2.12)$$

The central moments are thus defined,

$$E \{(x - \mu)^m\} = \int_{-\infty}^{+\infty} (x - \mu)^m p(x) dx. \quad (11.2.13)$$

We may also have multi-variate functions, for example x and y may both be random with a function $f(x, y)$. Now if we have a particle on a lattice, the x and y jumps may be completely independent. To find the average, we must integrate the function over x and y independently. In analogue to the single variable system,

$$p(x, y) dx dy = \text{Prob} [x \leq X \leq x + dx; y \leq Y \leq y + dy]. \quad (11.2.14)$$

Consequently the average is,

$$E \{f(x, y)\} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(x, y)p(x, y) dx dy. \quad (11.2.15)$$

Now say we only integrate over one variable,

$$\int_{-\infty}^{+\infty} f(x, y)p(x, y) dy = p(x). \quad (11.2.16)$$

If the inputs for X and Y are independent then,

$$E \{X + Y\} = E \{X\} + E \{Y\}, \quad (11.2.17)$$

and

$$\text{Var} [X + Y] = \text{Var} [X] + \text{Var} [Y]. \quad (11.2.18)$$

While,

$$E \{XY\} = E \{X\} E \{Y\}, \quad (11.2.19)$$

If they are dependent we may find a correlation coefficient. Let

$$E \{X\} = \mu_x, \quad (11.2.20a)$$

$$E \{Y\} = \mu_y. \quad (11.2.20b)$$

Then,

$$E \{(X - \mu_x)^2\} = \sigma_x^2, \quad (11.2.21a)$$

$$E \{(Y - \mu_y)^2\} = \sigma_y^2. \quad (11.2.21b)$$

The co-variance is thus,

$$\text{Cov} [X, Y] = E \{(X - \mu_x)(Y - \mu_y)\}, \quad (11.2.22a)$$

$$= \rho_{xy} \sigma_x \sigma_y. \quad (11.2.22b)$$

if $\rho_{xy} \equiv 0$ then X, Y are independent. Then

$$-1 \leq \rho_{xy} \leq 1. \quad (11.2.23)$$

The Normal Distribution

The Gaussian or normal distribution is given with,

$$p(x) dx = \frac{1}{(2\pi\sigma^2)^{1/2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} dx \quad (11.2.24)$$

The normal distribution is not all that special, but it does arise in the parabolic PDEs. Examples include the heat equation, diffusion equation, Stokes equation. The Gaussian distribution gives the Greens function of these equations. *e.g.*,

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}. \quad (11.2.25)$$

Einstein used this for the diffusion of Brownian motion. He assumed that a particle can move in any direction completely independently (which is not always true). The central limit theorem also says that distributions of a random variable will have a normal distribution.

The cumulative distribution,

$$P(x) = \frac{1}{(2\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} e^{-\frac{z^2}{2}} dz, \quad (11.2.26a)$$

$$= \frac{1}{2} \left[1 + \text{erf} \frac{x}{\sqrt{2}} \right]. \quad (11.2.26b)$$

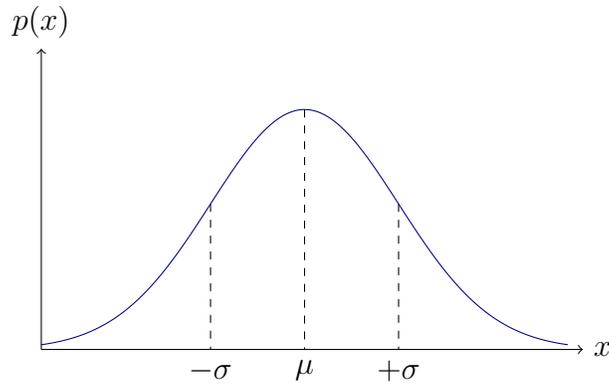


Figure 11.9. The normal distribution

If we tighten the variance the function will become more narrow. In the limit of small σ this is an excellent approximation of a delta function,

$$\lim_{\sigma \rightarrow 0} p(x) = \delta(x - \mu). \tag{11.2.27}$$

Further let's consider the generalization for two variables,

$$p(x, y) dx dy = \frac{1}{2\pi\sigma_x\sigma_y(1 - \rho_{xy}^2)^{1/2}} \exp\left(-\frac{\frac{x^2}{\sigma_x^2} + \frac{y^2}{\sigma_y^2} - \frac{2\rho_{xy}XY}{\sigma_x\sigma_y}}{2(1 - \rho_{xy}^2)}\right). \tag{11.2.28}$$

$$\rho_{xy}^2 = \frac{\sigma_{xy}^2}{\sigma_x\sigma_y}, \tag{11.2.29a}$$

$$\sigma_x^2 = E\{(X - \mu_x)^2\}, \tag{11.2.29b}$$

$$\sigma_y^2 = E\{(Y - \mu_y)^2\}, \tag{11.2.29c}$$

$$\sigma_{xy}^2 = E\{(X - \mu_x)(Y - \mu_y)\}. \tag{11.2.29d}$$

Characteristic Functions

if we are given $p(x)$,

$$\phi(s) = E\{e^{isx}\} = \int_{-\infty}^{+\infty} e^{isx} p(x) dx. \tag{11.2.30}$$

This is related to the Fourier Transform. We may use some special properties of characteristic function,

$$\phi^{(n)}(0) = i^n E\{X^n\}. \tag{11.2.31}$$

This allows you to calculate the moments of the system very easily with $\phi(s)$. If we take the Maclaurin series,

$$\phi(s) = \underbrace{\phi(0)}_{i^0 E\{x^0\}} + \underbrace{\phi'(0)}_{iE\{x\}} s + \frac{1}{2!} \underbrace{\phi''(0)}_{i^2 E\{x^2\}} s^2 + \dots. \tag{11.2.32}$$

Then,

$$p(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-isx} \phi(s) ds. \quad (11.2.33)$$

for $\mu \neq 0$.

$$\phi'(0) = i\mu, \quad (11.2.34a)$$

$$\phi''(0) = -\mu^2 - \sigma^2, \quad (11.2.34b)$$

$$\phi'''(0) = i^3 (\mu^3 + 3\mu\sigma^2). \quad (11.2.34c)$$

$$\Phi(s) = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} e^{is(x-\mu)} e^{-\frac{(x-\mu)^2}{2\sigma^2}} dx = e^{-\frac{\sigma^2 s^2}{2}}. \quad (11.2.35)$$

$$\Phi'(0) = 0, \quad (11.2.36a)$$

$$\Phi''(0) = \sigma^2, \quad (11.2.36b)$$

$$\Phi'''(0) = 0. \quad (11.2.36c)$$

Stochastic Processes

A good resource for literature on stochastic process include:

1. S. Chandrasekhar, Rev. Mod. Phys. 15 (1943) 1

Chandrasekhar won the Nobel for calculating the critical mass of a star. The article is a well cited review of the topic.

2. N. G. van Kampen *Stochastic Processes in Physics and Chemistry*, Elsevier.

The book has a chapter on stochastic processes in quantum systems.

3. C. Gardiner, *Handbook of Stochastic Methods*, Springer.

Gardiner was a post-doctoral assistant of Donald MacQuarrie. This book has good overview of Brownian motion and the physical motivations. Also the text includes a review on Langevin's paper.

Mathematical Statistics

This field allows us to analyze a system to find a distribution which represents the real population, with an estimate of error. We may use this for systems such as statistical mechanical systems. When we have, say, 10^{23} atoms it is impossible to find exactly the behavior of the system, however we may use the statistical effect of the parts of the system. Then all we need to know are things such as the temperature, pressure, volume, *etc.* to determine the behavior of the system. The probabilities associated with the system will be very accurate for such large quantities. The Gaussian distribution becomes much like a delta function.

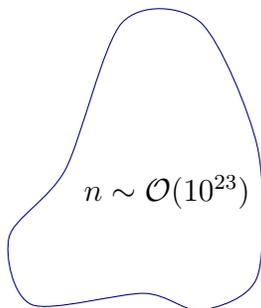


Figure 11.10. In a molecular system the size of n is large

Statistics and probability seem to be inherent to quantum mechanics, whereas in most other systems it appears as an emergent phenomenon. This brings the question of whether statistical systems are fundamental to nature.

In statistics, we will do the following. We will consider the probability distribution as the key function of the system, $f(x, \theta)$.

$$\hat{\theta} = \hat{\theta}(x_1, x_2, x_3, \dots, x_n). \quad (11.2.37)$$

We will always be limited to some sample. This is referred to as sample statistics. The average of the samples is defined,

$$\bar{x} = \frac{x_1 + x_2 + x_3 + \dots + x_n}{n} = \hat{\mu}. \quad (11.2.38)$$

This must be distinguished from the average since it is based on a small sample. So then we care about the error of the samples. This is illustrated in the fact that often the data is plotted with error bars. The variance is calculated;

$$\hat{s}^2 = \frac{(x_1 - \bar{x})^2 + (x_2 - \bar{x})^2 + \dots + (x_n - \bar{x})^2}{n - 1} \quad (11.2.39)$$

Here the variance is better estimated by deciding by $n - 1$ instead of n .

Next class is our last class, with finals afterward.

11.3 Lecture 32: December 3, 2014

Mathematical Statistics (cont.)

Consider a set of finite or large (or possibly infinite) possible values of a random variable. Since we may not handle all possible values, we will take a sample to use as the representative measure of the whole set. This sample allows us to find a parameter, $\hat{\theta} = \hat{\theta}(x_1, x_2, \dots, x_n)$, which is in some way a useful measurement of the set. Consider as an example the mean,

$$\bar{x} = \frac{x_1 + x_2 + \dots + x_n}{n} = \hat{\mu}. \quad (11.3.1)$$

We may consider doing an infinite number of measurements, but of course in the real world we would stop short at a smaller value. We may then be interested in the average, but we cannot consider it to be the true expected value so we indicate it with $\hat{\mu}$. It is based on the particular number of measurements you have done, and the more more measurements taken the better the resulting approximation of the expected value.

Now the average quality defined by the average may be used in the standard deviation (which is the root of the sum of the squared deviations, decided by the number of samples),

$$\hat{S}^2 = \frac{(x_1 - \bar{x})^2 + (x_2 - \bar{x})^2 + \dots + (x_n - \bar{x})^2}{n - 1}. \quad (11.3.2)$$

Note that for a sample, the standard deviation will usually be closer to the population standard deviation if we divide by $n - 1$ instead of n . This gives us a quantity similar to the population standard deviation;

$$\hat{S}^2 = \hat{\sigma}^2. \quad (11.3.3)$$

Thus a quantity in general,

$$\hat{\theta} = \hat{\theta}(x_1, x_2, \dots, x_n), \quad (11.3.4)$$

which is based on all random realizations of an event, is called an *estimator*, and it is an estimator for the particular parameter θ . Thus,

$$\hat{\mu} = \frac{X_1 + X_2 + \dots + X_n}{n}, \quad (11.3.5)$$

is an estimator of the mean, or

$$E\{\hat{\mu}\} = \frac{1}{n} [E\{X_1\} + E\{X_2\} + \dots + E\{X_n\}]. \quad (11.3.6a)$$

Recalling that $E\{X_i\} = \mu_i$, then

$$\frac{1}{n} \sum_i E\{X_i\} = \frac{1}{n} n\mu, \quad (11.3.6b)$$

$$= \mu. \quad (11.3.6c)$$

If the estimator for the quantity equals the quantity itself, or $E\{\theta\} = \theta$, then the estimator is said to be unbiased. There is an example in the text on page 1077, (Example 1), which deals with the issue of a biased estimator.

The estimator is expected to become better as the sample increases, or

$$\lim_{n \rightarrow \infty} E \left\{ \hat{\theta}_n \right\} = \theta. \quad (11.3.7)$$

If we look at the deviation,

$$\lim_{n \rightarrow \infty} \left[\left(\hat{\theta}_n - \theta \right)^2 \right] = 0. \quad (11.3.8)$$

In other words the greater the sample the better the accuracy.

Determination of Estimators

We discuss the *maximum likelihood method* (MLM) for the determination of estimators.

Let's now look into how the estimator is determined. If we have a function that depends on some random variables and gives a parameter of interest, $f(x; \theta)$, then if X_1, X_2, \dots, X_n are independent random variables we can define a function,

$$L(X_1, X_2, \dots, X_n; \theta) = f(X_1; \theta) f(X_2; \theta) \cdots f(X_n; \theta). \quad (11.3.9)$$

We have here considered that since the variables are independent then their probabilities will be a product. So each probability tells us how likely it is to have the variable to satisfy,

$$x_1 \leq X_1 \leq x_1 + dx_1. \quad (11.3.10)$$

So we can write these probabilities for all variables. Now, L is the likelihood function and we want to maximize it with respect to θ . We want to maximize the joint probability with respect to the parameter. The condition for an extremum is that the derivative must be zero; for maxima (not a minimum or inflection point) the second derivative must be less than zero. In equation form,

$$\frac{\partial L}{\partial \theta} = 0; \quad (11.3.11a)$$

$$\frac{\partial^2 L}{\partial \theta^2} < 0. \quad (11.3.11b)$$

Then we will have a maximum for $\theta = \hat{\theta}$. Now if the function L peaks at a particular point, then the logarithm of the product of $f(X_i; \theta)$ will also peak at that same point. This is because the logarithm is a monotonic function, so if we have a function $F(\theta)$ then $\ln(F(\theta))$ will peak at the same value of θ . Since we are not so much interested in the value of the function, but in where we exhibit the maximum in θ the logarithm of the function will suffice. This is a useful property that is often applied in statistical mechanics. Note that we cannot have a probability of zero if we are to do this because otherwise the log of zero is infinite and we have no solution. Now replacing $L(\theta)$ with $\ln(L(\theta))$,

$$\frac{\partial \ln(L)}{\partial \theta} = 0; \quad (11.3.12a)$$

$$\frac{\partial^2 \ln(L)}{\partial \theta^2} < 0. \quad (11.3.12b)$$

So we have similar equivalents.

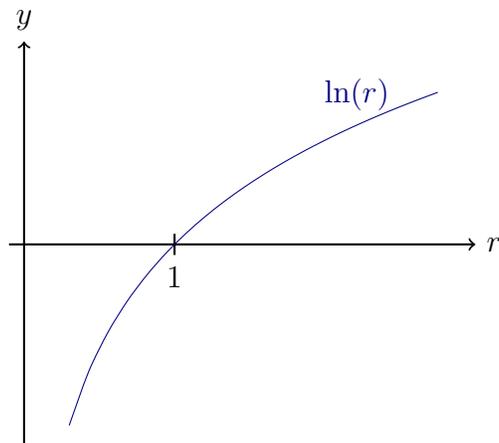


Figure 11.11. Logarithmic function

Poisson Distribution

As a case study, we may look at the *Poisson distribution*. The parameter of interest is λ , where we define a function,

$$L(\lambda) = \frac{\lambda^{X_1} e^{-\lambda}}{X_1!} \frac{\lambda^{X_2} e^{-\lambda}}{X_2!} \cdots \frac{\lambda^{X_n} e^{-\lambda}}{X_n!}. \quad (11.3.13)$$

These probabilities on the right hand side correspond to each of the $f(X_i; \theta)$ functions given above. Taking the logarithm, the products are reduced to sums;

$$\ln(L(\lambda)) = \left(\sum_{i=1}^n X_i \right) \ln(\lambda) - n\lambda - \sum_{i=1}^n \ln(X_i!). \quad (11.3.14)$$

Now we will take derivatives with respect to λ , so we may ignore the intimidating term with the factorials.

$$\frac{\partial \ln(L(\hat{\lambda}))}{\partial \hat{\lambda}} = \left(\sum_{i=1}^n X_i \right) \frac{1}{\hat{\lambda}} - n = 0. \quad (11.3.15)$$

This must be zero to be an extrema. Rearranging,

$$\hat{\lambda} = \frac{X_1 + X_2 + \cdots + X_n}{n}. \quad (11.3.16)$$

In other words we obtained the fact that λ is the mean. Nevertheless, it is the parameter of interest.

Now the question is is the second derivative criterion fulfilled? Taking the second derivative at the location of λ or the mean,

$$\left[\frac{\partial^2 \ln(L)}{\partial \lambda^2} \right]_{\lambda=\bar{x}} = -\frac{n}{\bar{X}} < 0. \quad (11.3.17)$$

This may be extended for other population parameters, with several examples in the text book.

Normal Distribution

Returning to the normal distribution we will look at several important properties. Defining,

$$p(x) dx = \frac{1}{(2\pi\sigma^2)^{1/2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} dx \quad (11.3.18)$$

The first term is from the normalization. If we define,

$$z = \frac{x - \mu}{\sigma}, \quad (11.3.19)$$

when we replace the variables, we rescale such that the mean is at the origin and the z axis

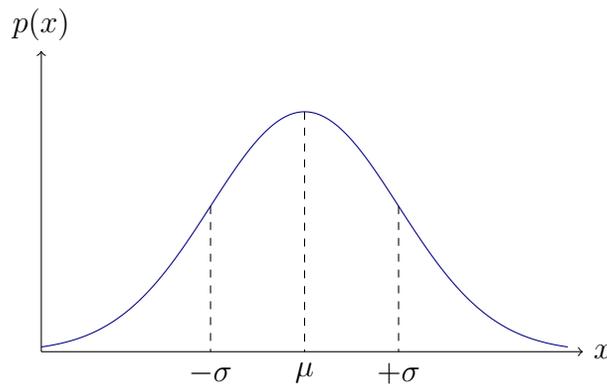


Figure 11.12. The normal distribution

is scaled with the standard deviation. This simplifies our expression significantly;

$$p(z) dz = \frac{1}{(2\pi)^{1/2}} e^{-\frac{z^2}{2}} dz. \quad (11.3.20)$$

This is important to generate random numbers which are normally distributed, which is useful in Brownian dynamics and Monte Carlo. Recall that this the function expression is a natural solution for diffusive systems. Due to the collisions between particles, the particles move around similarly to a normal distribution. In other words it is less likely for a particle to move a large distance than a small one (though it is usually not forbidden). We can simulate this with gaussian random noise by taking the randomly generated numbers from the computer language that we are working with and reforming it using the gaussian distribution. In these methods and algorithms they usually use the formulation with z and then the program (or you the user) may translate it back into the form of your specific problem with x . This is called the standardized distribution.

Now say we have a variable X with a given μ_x and σ_x^2 , with another variable $Y = C_1X + C_2$. How will the variable Y behave? If X is itself normal, then Y will also have a normal distribution. Then the expected value for Y ,

$$\mu_y = C_1\mu_x + C_2, \quad (11.3.21a)$$

$$\sigma_y^2 = C_1^2\sigma_x^2. \quad (11.3.21b)$$

These properties may be shown by substitution of the definition of Y into the equation of the Gaussian distribution and simplifying. We may also have a possible more complicated situation of many variables; then

$$X = X_1 + X_2 + \cdots + X_n, \quad (11.3.22)$$

and the expected value is similarly a sum of the expected values,

$$\mu = \mu_1 + \mu_2 + \cdots + \mu_n, \quad (11.3.23a)$$

$$\sigma^2 = \sigma_1^2 + \sigma_2^2 + \cdots + \sigma_n^2. \quad (11.3.23b)$$

Now consider that the average of a sample may be a sum,

$$\bar{X} = \frac{X_1 + X_2 + \cdots + X_n}{n}, \quad (11.3.24)$$

where each X_i has its own mean, μ_i , and variance σ_i^2 . Then, X will have a mean $\bar{X} = n$ and variance $\frac{\sigma^2}{n}$. So here we again arrive at a conclusion that as we increase the number of measurements, the variance will decrease and give a better approximation of the mean for finite number of measurements.

Confidence Intervals

The final thing we will discuss is confidence intervals. A confidence interval is intended to answer the question: What is the probability to find our variable within certain limits? With a given distribution (such as the normal distribution), we may look at how this may be found. So say we have a parameter θ and we want to know,

$$\eta = \text{Prob}[\theta_1 \leq \theta \leq \theta_2]. \quad (11.3.25)$$

Here η is called the *confidence level*. The bracketed area between $[\theta_1, \theta_2]$ is the *confidence interval*. So how do we find these?

Say for example, we have $\theta_1 = +a$ and $\theta_2 = -a$. We decide to have a mean of 0 and a symmetric confidence interval. So what is the probability in this area? Clearly this is an integral and is easy to find. In other words going from a given value of a to find η is very clear, but the inverse problem is more difficult. Now if instead we want to find a when given a value of η , in other words we want to know what the probability of events happening are. The probability to find the variable within the limit is the integral,

$$\text{Prob}[-a \leq x \leq a] = \frac{1}{(2\pi)^{1/2}} \int_{-a}^a e^{-\frac{x^2}{2}} dx = \eta. \quad (11.3.26)$$

Hence the integral can give the value of η . So it is a problem that will have to be inverse of what you may expect. Now the values of a for a given η is tabulated for several common confidence values such as 95% and 99%. These may be found instead by iteration or trial and error if desired.

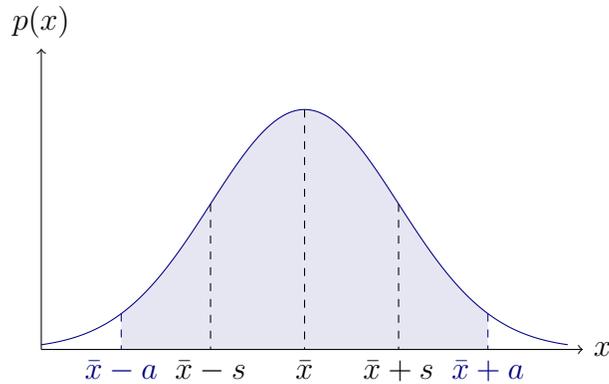


Figure 11.13. Determination of a confidence interval

So say we select a sample of n measurements, $x_1, x_2, x_3, \dots, x_n$ and we determine the mean and variance,

$$\bar{x} = \frac{x_1 + x_2 + x_3 + \dots + x_n}{n}, \quad (11.3.27a)$$

$$s^2 = \frac{\sum_{i=1}^n (x_i - \bar{x})^2}{n - 1}. \quad (11.3.27b)$$

Then we may decide what we want as the value of the confidence interval to be (such also 95%). Finally, we may find the value of a by trial and error or writing a numerical program to compute it iteratively. It may also be in tables. In steps we may list this as:

1. Gather n samples
2. Find the mean
3. Find the variance
4. Decide on η
5. Find a

This concludes the lecture materials for this course.

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