Matematisk Fysik FöF4

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MATHEMATICAL PHYSICS FTF131

LECTURE 1

Ordinary differential equations

1 1^{st} order

(i) exact d.e. $A(x,y)dx + B(x,y)dy = 0$ is exact iff:

$$\frac{\partial A}{\partial y} = \frac{\partial B}{\partial x}.$$

The solution is

$$C = \int A(x,y)\,dx + \int B(x,y)\,dy$$

C: constant

proof: Act with $\frac{d}{dx} = \frac{\partial}{\partial x} + \frac{dy}{dx}\frac{\partial}{\partial y} \Rightarrow$

$$0 = A(x,y) + \int \frac{\partial B}{\partial x}\,dy + \frac{dy}{dx}\int \frac{\partial A}{\partial y}\,dx + \frac{dy}{dx}B(x,y) =$$

$$= \left\{\text{use } \frac{\partial A}{\partial y} = \frac{\partial B}{\partial x}\right\} = 2A(x,y) + 2\frac{dy}{dx}B(x,y) \qquad \square$$

(ii) linear d.e. $\frac{dy}{dx} + f(x)y = g(x)$

This d.e. becomes exact when multiplying by $e^{\int f(x)dx}$:

$$e^{\int f dx}\,dy + e^{\int f dx}\left[f(x)y - g(x)\right]dx = 0$$

(iii) Scaling form (a.k.a. isobaric): $A(x,y)dx + B(x,y)dy = 0$

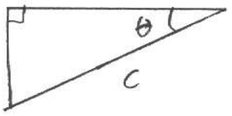
Assume that the scale of y varies as x^m, i.e. we assume that

$$A(\lambda x, \lambda^m y)\,d(\lambda x) = \lambda^r A(x,y)\,dx$$
$$B(\lambda x, \lambda^m y)\,d(\lambda^m y) = \lambda^r B(x,y)\,dy$$

The substitution $y = x^m z$ yields a seperable equation for dx and dz.

Appetizer: Prove Pythagoras theorem using scaling (dimensional) analysis.

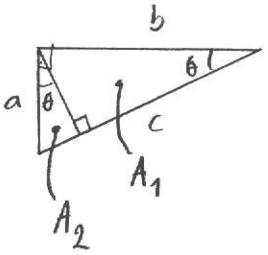
1)



area: $A = f(c, \theta) = c^2 g(\theta)$

smallest angle — dimensional analysis

2)



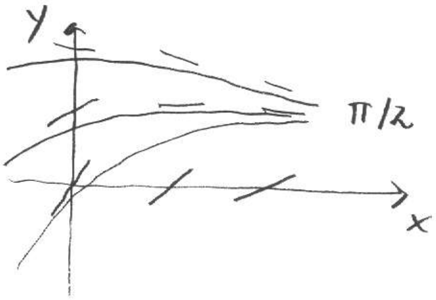
area: $A = A_1 + A_2 =$

$= b^2 g(\theta) + a^2 g(\theta) = c^2 g(\theta)$

$\therefore \quad a^2 + b^2 = c^2$

(iv) graphical qualitative analysis: $y' = f(x,y)$

e.g. $y' = \cos y + e^{-x}$



converges to $\frac{\pi}{2}$

($\exists$ solution that converges to $\frac{5\pi}{2}$)

2 2nd order equation

often yields special functions $\Rightarrow$ look it up!

3 Higher order

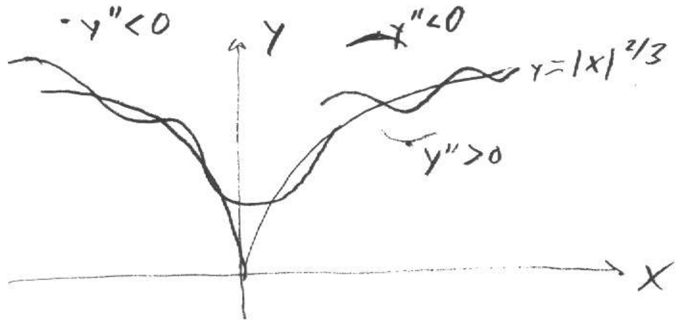
(i) constant coefficients: $y(x) = e^{\alpha x} \Rightarrow$ polynomial equation for α.

(ii) general strategies

- simplify by identifying small argument behavior (keeping only terms that dominate for small x)
- identify large x behavior

- iterative improvement

eg: $y'' = x^2 - y^3$



$\underbrace{\text{right hand side}}_{=\text{RHS}} = 0$ for $y = |x|^{2/3}$

$\Rightarrow x=0$ is rather singular, solution seems to oscillate around $y=|x|^{2/3}$

First iteration: let $y \approx (x^2)^{1/3}$, write $y^3 = x^2 - y''$,

substitute: $y = (x^2)^{1/3}$ on RHS: $y' = \frac{2}{3}x^{-1/3}$, $y'' = -\frac{2}{9}x^{-4/3}$

$$\Rightarrow y^3 = x^2 + \frac{2}{9}|x|^{-4/3} \approx x^2\left(1 + \frac{2}{9}|x|^{-10/3}\right)$$

$$\Rightarrow y \approx |x|^{2/3}\left(1+\frac{2}{9}|x|^{-10/3}\right)^{1/3} \underset{\substack{\uparrow \\ \text{Taylor expansion}}}{\approx} |x|^{2/3}\left(1+\frac{2}{27}|x|^{-10/3}\right)$$

Substitute this to the RHS, get next approximation.

Alternatively, let $y = |x|^{2/3} + \eta(x)$ and substitute this into equation, keep only linear terms of $\eta(x)$:

$$\Rightarrow \ldots \Rightarrow \quad \eta(x) \approx \frac{1}{|x|^{1/3}} \cos\left(\frac{3\sqrt{3}}{5}|x|^{5/3} + \theta_0\right)$$

(iii) power series solution:

expand $y(x) = \sum a_n x^n$

Appetizer: solve $x^3+ax^2+bx+c=0$ (1) (4)

set $z = x + a/3 \Rightarrow z^3 = x^3 + ax^2 + \dots \Rightarrow$ for z, the equation (1) becomes $z^3+pz+q=0$.

Then, set $z = u + \frac{\alpha}{u} \Rightarrow z^3 = u^3 + \underbrace{3\alpha u + 3\frac{\alpha^2}{u}}_{3\alpha(u+\frac{\alpha}{u}) = 3\alpha z} + \frac{\alpha^3}{u^3}$

$\Rightarrow u^3 + (3\alpha+p)z + q + \frac{\alpha^3}{u^3}$

choose $\alpha = -p/3$: $\quad u^3 + q + \frac{\alpha^3}{u^3} = 0$

$$(u^3)^2 + qu^3 + \alpha^3 = 0$$

2^{nd} order for $u^3 \Rightarrow$ obtain $u^3 \Rightarrow$ obtain $u \Rightarrow$ obtain $z \Rightarrow$ obtain x.

Another example:

Solve $2x^3y' = 1 + \sqrt{1+4x^2y}$

Substitute $u = \sqrt{1+4x^2y} \geq 0. \Rightarrow -u + xu' = 1$

separable! $\quad x\,du - (1+u)\,dx = 0$

$$\int \frac{dx}{x} - \int \frac{du}{1+u} = C' = \text{constant}$$

$$\Rightarrow \ln \frac{|x|}{1+u} = C'$$

$\Rightarrow u = E|x| - 1 \quad$ (note that $E|x| > 1$)

Insert this into original substitution

$$\Rightarrow y = \frac{k^2x^2 - 2kx}{4x^2}, \quad k > 0$$

lecture 2: elementary integration techniques

1 Partial fractions

$$\int dx \frac{1}{x^2-3x+2} = \int \frac{dx}{(x-2)(x-1)} = \int \frac{1}{x-2} - \frac{1}{x-1}\, dx =$$

$$= \ln|x-2| - \ln|x-1| = \ln\left|\frac{x-2}{x-1}\right|$$

2 derive a diff eq.

$$I = \int_0^\infty \frac{\sin x}{x}\, dx \qquad \text{study } I(\alpha) = \int_0^\infty e^{-\alpha x} \frac{\sin x}{x}\, dx$$

$$I'(\alpha) = -\int_0^\infty e^{-\alpha x} \sin x\, dx = -\mathrm{Im} \int_0^\infty e^{-\alpha x} e^{ix}\, dx =$$

$$= -\mathrm{Im}\left[\frac{1}{-\alpha+i} e^{(-\alpha+i)x}\right]_0^\infty = -\frac{1}{\alpha^2+1}$$

$$\Rightarrow I(\alpha) = -\int \frac{d\alpha}{\alpha^2+1} = -\arctan\alpha + C$$

We have $I(\infty) = 0 \Rightarrow C = \pi/2 \Rightarrow I(\alpha) = -\arctan\alpha + \frac{\pi}{2} =$

$$= \operatorname{arccotan} \alpha$$

$$\Rightarrow I(0) = \frac{\pi}{2}$$

3 Tricks

$$I_0(\alpha) = \int_{-\infty}^{\infty} e^{-\alpha x^2}\, dx$$

$$I_0^2(\alpha) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\alpha(x^2+y^2)}\, dx\, dy = \int_{r=0}^{\infty}\int_{\theta=0}^{2\pi} r e^{-\alpha r^2}\, dr\, d\theta =$$

$$= 2\pi \int_{r=0}^{\infty} (-2\alpha r) e^{-\alpha r^2}\, dr \frac{1}{-2\alpha} = \frac{\pi}{\alpha}$$

$$\Rightarrow I_0(\alpha) = \sqrt{\frac{\pi}{\alpha}}$$

$$I_2(\alpha) = \int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx = -\frac{\partial}{\partial\alpha} I_0(\alpha) = \frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}}$$

⑥

$$I_4(\alpha) = \int_{-\infty}^{\infty} x^4 e^{-\alpha x^2} dx = \frac{3}{4}\frac{1}{\alpha^2}\sqrt{\frac{\pi}{\alpha}} \quad \text{etc.}$$

(i) Approximation techniques: <u>saddle point method</u>

$$I = \int_{-\infty}^{\infty} e^{f(x)} dx, \quad f(x) \to -\infty, \ |x| \to \infty$$

find the maximum $x = x_0$ of $f(x)$, expand around the maximum: (note: $f'(x_0) = 0$)

$$f(x) = f(x_0) + \frac{1}{2}(x-x_0)^2 f''(x_0) + \frac{1}{6}(x-x_0)^3 f'''(x_0) + \dots$$

$$\Rightarrow I \approx \int_{-\infty}^{\infty} e^{f(x_0) + \frac{1}{2}(x-x_0)^2 f''(x_0) + \dots} dx =$$

$$= e^{f(x_0)} \int_{-\infty}^{\infty} e^{\frac{1}{2}(x-x_0)^2 f''(x_0) + \underbrace{\frac{1}{6}(x-x_0)^3 f'''(x_0) + \dots}_{\text{neglect these!}}} dx \approx$$

$$= e^{f(x_0)} \int_{-\infty}^{\infty} e^{\frac{1}{2} f''(x_0) x^2} dx = e^{f(x_0)} \sqrt{\frac{2\pi}{-f''(x_0)}} \quad (\text{note: } f''(x_0) < 0)$$

?

- further corrections: add more terms in the Taylor series (note: neglect odd exponents)

$$\Rightarrow I \approx e^{f(x_0)} \sqrt{\frac{2\pi}{-f''(x_0)}} \left\{ 1 + \frac{1}{8} \frac{f''''(x_0)}{[f''(x_0)]^2} \right\}$$

- method works even if f is complex. expand around maximum of $\mathrm{Re}\, f$
- works if the integration path is a curve in the complex plane (at least as long as contributions from path ends are small):

$$\to \gamma \quad I = \int_\gamma e^{f(z)} dz$$

holds for analytic functions with some modifications:

I_C is independent of path:

$I_C = I_{C'}$ since $I_{C-C'} = 0$

- $f(z)$, $z = x + iy$ is analytic if $f'(z) = \lim_{h \to 0} \frac{f(z+h) - f(z)}{h}$ $\exists$

- set $f(z) = u(x,y) + iv(x,y) \Rightarrow$ Cauchy-Riemann's eq:

$$\begin{cases} \dfrac{\partial u}{\partial x} = \dfrac{\partial v}{\partial y} \\ \dfrac{\partial u}{\partial y} = -\dfrac{\partial v}{\partial x} \end{cases} \Rightarrow \nabla^2 u = \nabla^2 v = 0$$

$\Rightarrow$ $u(x,y)$ and $v(x,y)$ have no extrema (max. or min), only saddle points

$\Rightarrow$ choose the path C so that it passes through a saddle point of u and v, and the region of large $u(x,y)$ is as small as possible

Near a saddle point $f(z) \simeq f(z_0) + \frac{1}{2} f''(z_0)(z - z_0)^2$

Set $z = z_0 + t(\cos\theta + i\sin\theta) \Rightarrow$

$$f(z) \approx f(z_0) + \frac{1}{2} f''(z_0) t^2 (\cos^2\theta - \sin^2\theta + 2i\cos\theta\sin\theta) =$$

$$= f(z_0) + \frac{1}{2} |f''(z_0)| e^{i\varphi} t^2 e^{i2\theta}$$

$$\Rightarrow \begin{cases} u(x,y) = u(x_0,y_0) + \frac{1}{2} t^2 |f''(z_0)| \cos(2\theta + \varphi) \\ v(x,y) = v(x_0,y_0) + \frac{1}{2} t^2 |f''(z_0)| \sin(2\theta + \varphi) \end{cases}$$

Choose path C is such that $2\theta + \varphi = \pi$ (cos-term largest)
$\Rightarrow$ our path goes where it is steepest = Method of steepest descent

- in this path, $v(x,y) =$ constant near z_0: stationary phase approximation

$$\therefore \quad I_c \approx \int_{-\infty}^{\infty} \underbrace{dt e^{-i(\varphi/2 \pm \pi/2)}}_{=dz} e^{iv(x_0,y_0)} e^{u(x_0,y_0) - \frac{1}{2}t^2|f''(z_0)|} dt =$$

only a phase change

$$= e^{iv(x_0,y_0) - i\varphi/2 \pm i\pi/2 + u(x_0,y_0)} \sqrt{\frac{2\pi}{|f''(z_0)|}}$$

use $e^{\pm i\pi/2} = \pm \frac{1}{\sqrt{-1}}$:

$$I_c = \pm e^{f(z_0)} \sqrt{\frac{2\pi}{-f''(z_0)}}$$

The sign is determined so that the expression, apart from $e^{f(z_0)}$, has the same phase as the path at z_0

5 Multidimensional integrals

(i) symmetry

example: $\vec{I}(\vec{E}) = \int d^3p \, \vec{p}\,(\vec{p}\cdot\vec{E})\, e^{-ap^2}$

$\vec{I}$ is a vector $\Rightarrow$ must have a direction. The only direction that is special is the direction of $\hat{E}$

$\Rightarrow \vec{I} \parallel \vec{E} \Rightarrow$ write $\vec{I} = \hat{E}(\vec{I}\cdot\hat{E})$

$$\vec{I}\cdot\hat{E} = E\int d^3p\,(\vec{p}\cdot\hat{E})^2 e^{-\alpha p^2}$$

choose a coord. system such that $\vec{E} = E\hat{x} \Rightarrow$

$$\vec{I}\cdot\hat{E} = E\int d^3p \; p_x^2 e^{-ap^2} = E\frac{1}{3}\int d^3p\,(p_x^2+p_y^2+p_z^2)e^{-ap^2}$$

$$= 4\pi E\frac{1}{3}\int_0^{\infty} dp\, p^2 p^2 e^{-ap^2} = E\frac{1}{2\alpha}\left(\frac{\pi}{\alpha}\right)^{3/2}$$

$$\Rightarrow \vec{I} = \vec{E}\frac{1}{2\alpha}\left(\frac{\pi}{a}\right)^{3/2}$$

(ii) auxiliary integrals

· example: $I = \int_{S'} d^3k \frac{1}{1-\frac{1}{3}(\cos k_x + \cos k_y + \cos k_z)}$,

$$S': \begin{cases} -\pi < k_x < \pi \\ -\pi < k_y < \pi \\ -\pi < k_z < \pi \end{cases}$$

Use $\frac{1}{\alpha} = \int_0^\infty dz\, e^{-\alpha z} \Rightarrow I = \int_0^\infty dz \int_{S'} d^3k\, e^{-z[1-\frac{1}{3}(\cos k_x + \dots + \cos k_z)]}$

$$\Rightarrow I = \int_0^\infty dz\, e^{-z} \left(\int_{-\pi}^{\pi} dk\, e^{-\frac{z}{3}\cos k} \right)^3$$

It turns out that $f = \int_{-\pi}^{\pi} dk\, e^{\alpha \cos k}$ can be evaluated:

$$f'(\alpha) = \int_{-\pi}^{\pi} dk \cos k\, e^{-\alpha \cos k} = \int_{-\pi}^{\pi} dk \frac{\partial}{\partial k}\left(\sin k\, e^{\alpha \cos k}\right) + \alpha \sin^2 k\, e^{\alpha \cos k}$$

$$= \int_{-\pi}^{\pi} dk \sin^2 k\, e^{\alpha \cos k}$$

$$f''(\alpha) = \int_{-\pi}^{\pi} dk \cos^2 k\, e^{\alpha \cos k}$$

from book

$\Rightarrow f''(\alpha) + \frac{1}{\alpha} f'(\alpha) - f(\alpha) = 0$: Bessel equation for imaginary argument

solution: $f(\alpha) = A I_0(\alpha) + B K_0(\alpha)$

Now $f(0) = 2\pi$ (finite) $\Rightarrow B = 0 \Rightarrow A = 2\pi$

$\Rightarrow I = \int_0^\infty dz\, e^{-z} \left[I_0\left(\frac{z}{3}\right) 2\pi \right]^3$ (can't be evaluated analytically, by Jari)

$\approx 1.51639 \cdot (2\pi)^3$

6. Gradshteyn-Ryzhik

7. ~~Not~~ Mathematica

LECTURE 3:

Review: Integrals - elementary ways to evaluate them

Today: Integrals - advanced methods (complex analysis)

$f(z)$ is analytic if $f'(z) \; \exists = \lim_{h\to 0} \frac{f(z+h)-f(z)}{h}$, i.e. the limit is finite and independent of how $h \to 0$.

Two paths: 1) $h \in \mathbb{R}$: $f(z) = u(x,y) + i v(x,y)$, $z = x+iy$

$$\Rightarrow \quad f'(z) = \frac{\partial u}{\partial x} + i \frac{\partial v}{\partial x}$$

2) $h \in i\mathbb{R}$. $f'(z) = \frac{\partial u}{i\partial y} + i \frac{\partial v}{i \partial y}$

1) & 2) $\Rightarrow$ Cauchy-Riemann eq: $\begin{cases} \frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \\ \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x} \end{cases}$

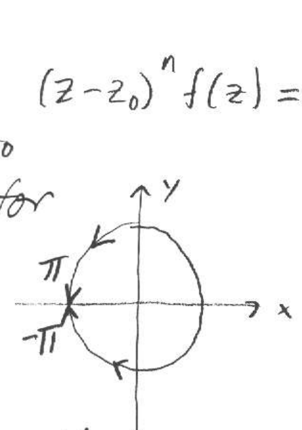
$$\Rightarrow \nabla^2 u = \nabla^2 v = 0$$

Nonanalycities:

1) poles: n^{th} order pole at z_0 if $\lim_{z\to z_0} (z-z_0)^n f(z) = \text{const.} \neq 0$

2) branch cut: eg: $\ln z$ has a branch for

$\operatorname{Im} z = 0$, $\operatorname{Re} z < 0$



3) essential singularity: $\lim_{z\to z_0} (z-z_0)^n f(z) = \infty \;\; \forall n \in \mathbb{N}$

eg: $e^{1/z}$, $z_0 = 0$.

Laurent series:

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n$$

Integrate along a closed contour, encircling z_0 (a circle):

$$\oint_C dz\, f(z) = \{ z = z_0 + re^{i\theta} \;,\; dz = ire^{i\theta}\, d\theta \} =$$

$$= \int_0^{2\pi} d\theta\, ire^{i\theta} \sum_{-\infty}^{\infty} a_n (re^{i\theta})^n \underset{\substack{\uparrow \\ \text{uniform} \\ \text{convergence}}}{=} \sum_{-\infty}^{\infty} a_n i r^{n+1} \underbrace{\int_0^{2\pi} d\theta\, e^{i(n+1)\theta}}_{= 2\pi \delta(n-1)} =$$

$$= 2\pi i\, a_{-1}$$

$\Rightarrow$ for an arbitrary closed contour we have

$$\oint_C dz\, f(z) = 2\pi i \sum_{\substack{\text{isolated} \\ \text{singularities}}} a_{-1}$$

provided that the region bounded by C only contains isolated singularities (ie no branch cuts). This is the Residue Theorem. a_{-1} is called the residue at the singularity.

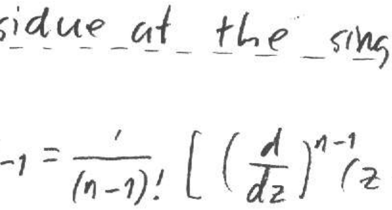
- at n^{th} order pole: $a_{-1} = \frac{1}{(n-1)!} \left[\left(\frac{d}{dz} \right)^{n-1} (z - z_0)^n f(z) \right]_{z = z_0}$

Examples:

1) Standard:

$$I = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \underbrace{\frac{\omega^2}{L^2(\omega^2 - \omega_0^2)^2 + R^2 \omega^2}}_{\substack{\propto \frac{1}{\omega^2},\ \omega \text{ large} \\ \Rightarrow \text{convergence}}}$$

Choose a contour:

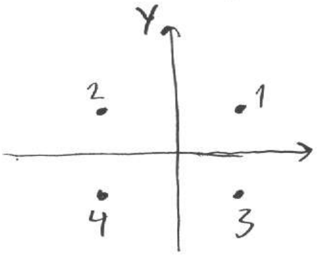


integral along the arc: $\Omega \cdot \frac{1}{\Omega^2} \to 0$

$$\Rightarrow I = \oint_C \frac{d\omega}{2\pi} \frac{\omega^2}{L^2(\omega^2 - \omega_0^2)^2 + R^2 \omega^2}$$

$\rightarrow$

Find the poles: $L^2(\omega^2-\omega_0^2)^2 + R^2\omega^2 = 0 \Rightarrow \omega_1, \omega_2, \omega_3, \omega_4$ (12)



$$\omega = \pm\sqrt{\omega_0^2 - \left(\frac{R}{2L}\right)^2} \pm i\frac{R}{2L}$$

$$\omega_1 = -\omega_4, \quad \omega_3 = \omega_1^*, \quad \omega_2 = -\omega_1^*$$

$$\Rightarrow I = \oint_C \frac{d\omega}{2\pi} \frac{\omega^2/L^2}{(\omega-\omega_1)(\omega-\omega_2)(\omega-\omega_3)(\omega-\omega_4)}$$

Only poles inside C are no. 1 and 2. Residues:

$$\omega=\omega_1: \quad \frac{\omega_1^2}{(\omega_1-\omega_2)(\omega_1-\omega_3)(\omega_1-\omega_4)} = \frac{\omega_1}{2}\frac{1}{\omega_1^2-(\omega_1^*)^2}$$

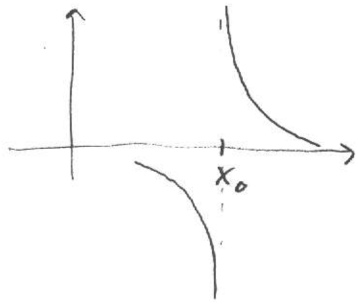
$$\omega=\omega_2: \quad \frac{\omega_1^*}{2}\frac{1}{\omega_1^2-(\omega_1^*)^2}$$

$$\Rightarrow I = \frac{1}{L^2}\frac{1}{2\pi}\underset{\substack{\uparrow \\ \text{from} \\ \text{Residue} \\ \text{theorem}}}{2\pi i}\,\frac{1}{2}\frac{\omega_1+\omega_1^*}{\omega_1^2-(\omega_1^*)^2} = \frac{i}{2L^2}\frac{1}{\omega_1-\omega_1^*} = \frac{1}{L^2}\frac{1}{4\,\mathrm{Im}\,\omega_1} = \frac{1}{2RL}$$

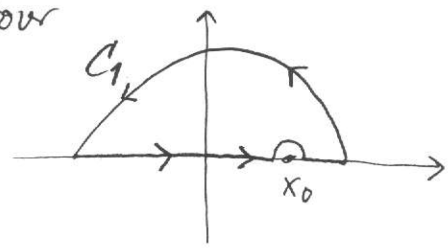
2) Common:

$$I = \int_{-\infty}^{\infty} \frac{f(x)}{x-x_0}\,dx$$

Strictly speaking, this does not converge:



We'll use the contour



$$I_{C_1} = \oint_{C_1} \frac{f(x)}{x-x_0}\,dx = \lim_{\varepsilon\to 0^+}\left[\int_{-\infty}^{x_0-\varepsilon} \frac{f(x)}{x-x_0}\,dx + \int_{x_0+\varepsilon}^{\infty} \frac{f(x)}{x-x_0}\,dx + \int_{\pi}^{0} d(\varepsilon e^{i\theta})\frac{f(x_0+\varepsilon e^{i\theta})}{\varepsilon e^{i\theta}}\right]$$

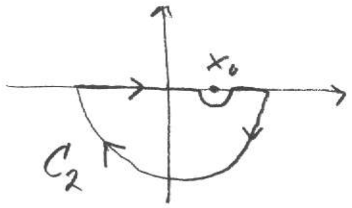
$$+ \lim_{R\to\infty}\int_0^{\pi} d(Re^{i\theta})\frac{f(Re^{i\theta})}{Re^{i\theta}-x_0}$$

Assume • $f(|z|) \Rightarrow 0, \ |z| \to \infty$: last term $\to 0$

• $f(z)$ is analytic at $z = z_0$: The third term $\to -i\pi f(x_0)$

$$\Rightarrow I_{C_1} = i\pi f(x_0) + \underbrace{\lim_{\varepsilon \to 0^+} \left[\int_{-\infty}^{x_0 - \varepsilon} \frac{f(x)}{x - x_0} dx + \int_{x_0+\varepsilon}^{\infty} \frac{f(x)}{x - x_0} dx \right]}_{\equiv \mathcal{P} \int_{-\infty}^{\infty} dx \frac{f(x)}{x - x_0} \ = \text{ Cauchy principal value}}$$

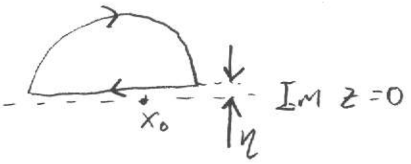
For a contour

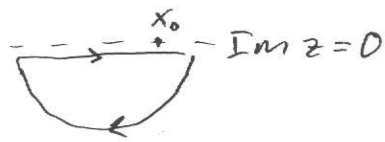


$$I_{C_2} = + i\pi f(x_0) + \mathcal{P} \int_{-\infty}^{\infty} dx \frac{f(x)}{x - x_0}$$

$\uparrow$ note!

The contours C_1 and C_2 can be modified:

$C_1 \to$ 

; $C_2 \to$ 

$$\oint_{C_1} \frac{dz\, f(z)}{z - z_0} = \lim_{\eta \to 0^+} \int_{-\infty}^{\infty} dx \frac{f(x)}{x - x_0 + i\eta} = -i\pi f(x_0) + \mathcal{P} \int_{-\infty}^{\infty} dx \frac{f(x)}{x - x_0}$$

$$\oint_{C_2} dz \frac{f(z)}{z - z_0} = \lim_{\eta \to 0^+} \int_{-\infty}^{\infty} dx \frac{f(x)}{x - x_0 - i\eta} = i\pi f(x) + \mathcal{P} \int_{-\infty}^{\infty} dx \frac{f(x)}{x - x_0}$$

$$\Rightarrow \text{Operationally, } \lim_{\eta \to 0^+} \frac{1}{x - x_0 \pm i\eta} = \mathcal{P} \frac{1}{x - x_0} \mp i\pi \delta(x - x_0)$$

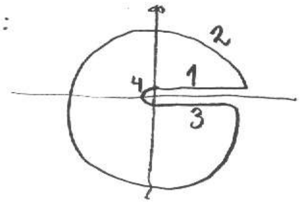
3) Semi-infinite

$$I = \int_0^{\infty} dt\, f(t)$$

Assume • $\lim_{z \to \infty} |z f(z)| = 0$

• $f(z)$ has no singularities on the pos real axis

Consider $\tilde{I} = \oint_C \ln z \, f(z) \, dz$, take branch of $\ln z$ such that $\operatorname{Im} \ln z \in [0, 2\pi[$. Choose C:



$$\tilde{I} = \tilde{I}_1 + \tilde{I}_2 + \tilde{I}_3 + \tilde{I}_4 =$$

$\tilde{I}_4 \to \lim_{\varepsilon \to 0} \varepsilon \ln \varepsilon \, f(\varepsilon) = 0$

$\tilde{I}_2 \to 0$ since we have assumed $R f(Re^{i\theta}) \to 0$, $R \to \infty$

$$= \int_0^\infty dt \, (\ln t) f(t) + \int_\infty^0 dt \left[\ln (t e^{2\pi i})\right] f(t) =$$

$$= \int_0^\infty dt \, \ln t \, f(t) + \int_\infty^0 dt \, (\ln t + 2\pi i) f(t) =$$

$$= -2\pi i \int_0^\infty dt \, f(t) = -2\pi i \, I$$

but $\tilde{I} = 2\pi i \sum_i \operatorname{Res}_{z_i} \left[f(z_i) \ln z_i \right] \Rightarrow I = -\sum_i \operatorname{Res}_{z_i} \left[f(z_i) \ln z \right]$

Example: $\int_0^\infty \frac{dt}{t^3+1}$: poles $t = e^{i\frac{\pi}{3}}, e^{i\frac{3\pi}{3}}, e^{i\frac{5\pi}{3}}$

$$\Rightarrow I = -\left[i\frac{\pi}{3} \frac{1}{(e^{i\pi/3} - e^{i3\pi/3})(e^{i\pi/3} - e^{i5\pi/3})} + \right.$$

$$+ i\frac{3\pi}{3} \frac{1}{(e^{3\pi/3} - e^{i\pi/3})(e^{3\pi/3} - e^{i5\pi/3})} +$$

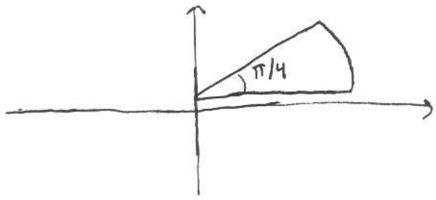
$$\left. + i\frac{5\pi}{3} \frac{1}{(e^{i5\pi/3} - e^{i\pi/3})(e^{5\pi/3} - e^{i3\pi/3})} \right] =$$

$$= \frac{2\sqrt{3}}{9}\pi$$

4) Transformation

Choose a path that transforms the integral to the s-g known

e.g. $I = \int_0^\infty dx\, e^{i\alpha x^2}$, $\alpha > 0$



$I_C = 0$ (no poles inside C) =

$$= \int_0^\infty dx\, e^{i\alpha x^2} + \int_{\theta=0}^{\pi/4} d(Re^{i\theta})\, e^{i\alpha R^2 e^{i2\theta}} +$$

$$+ \int_\infty^0 d(xe^{i\pi/4})\, e^{i\alpha x^2 e^{i\pi/2}} =$$

$$= I + iR \int_0^{\pi/4} d\theta\, e^{i\theta + i\alpha R^2(\cos 2\theta + i\sin 2\theta)} - e^{i\pi/4}\int_0^\infty dx\, e^{-\alpha x^2} =$$

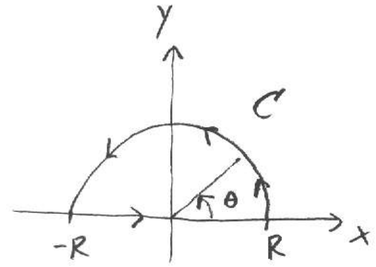
$$= I + \underbrace{iR \int_0^{\pi/4} d\theta\, e^{-\alpha R^2 \sin 2\theta + i(\theta + \alpha R^2 \cos 2\theta)}}_{\to 0,\ R \to \infty} - e^{i\pi/4}\frac{1}{2}\sqrt{\frac{\pi}{\alpha}}$$

$$\therefore\ 0 = I - e^{i\pi/4}\frac{1}{2}\sqrt{\frac{\pi}{\alpha}} \Rightarrow I = \frac{1}{2}e^{i\pi/4}\sqrt{\frac{\pi}{\alpha}} = \frac{1}{2}\sqrt{\frac{\pi}{2\alpha}}(1+i)$$

example:

$$I = \int_{-\infty}^{\infty} \frac{x^2\,dx}{(x^2+a^2)^2}$$

Consider $\quad \tilde{I} = \oint_C \frac{z^2\,dz}{(z^2+a^2)^2}$, $\quad C:$



we can write $\quad \tilde{I} = \underbrace{\int_{-R}^{R} \frac{x^2\,dx}{(x^2+a^2)^2}}_{\to I} + \underbrace{\int_0^{\pi} \frac{R^2 e^{i2\theta}\,d\theta}{(R^2 e^{i2\theta}+a^2)^2}}_{\to 0}$ if $R \to \infty$

$\tilde{I}$ has poles in $z = \pm ia$ (poles of order 2), since

$$\frac{z^2}{(z^2+a^2)^2} = \frac{z^2}{(z+ia)^2(z-ia)^2}$$

the only pole inside C is $z = ia$, where we have

$$a_{-1} = \frac{1}{(2-1)!}\left[\frac{d}{dz}\,\frac{(z-ia)^2 z^2}{(z^2+a^2)^2}\right]_{z=ia} =$$

$$= \left.\frac{2z(z+ia)^2 + z^2 \cdot 2(z+ia)}{(z+ia)^4}\right|_{z=ia} =$$

$$= \ldots = \frac{1}{4ia}$$

Using the theorem of residues, we have

$$I = 2\pi i \, \frac{1}{4ia} = \frac{\pi}{2a}$$

LECTURE 4

Review: Residue theorem and its applications

today: complex analysis, sums, meromorphic functions

Powerseries $\sum_{n=1}^{\infty} a_n (z-z_0)^n$ converge for $|z-z_0| < R$
diverge for $|z-z_0| > R$

Summing series:

(i) Recognize Taylor series e.g. $\sum_{n=1}^{\infty} \frac{x^n}{n} =$

$$= -\sum_{n=0}^{\infty} \frac{1}{n!} \left[\frac{\partial^n}{\partial x^n} \left(\ln(1-x) \right) \right]_{x=0} x^n =$$

$$= -\ln(1-x) \qquad \text{if } |x| < 1$$

(ii) Recognize Riemann sums (integral representation)

e.g: $\frac{2\pi}{N} \sum_{n=0}^{N} f\left(\frac{2\pi}{N} n \right) \approx \int_{x_0}^{x_N} dx\, f(x) = \int_0^{2\pi} dx\, f(x)$

exact for $N \to \infty$, keeping higher powers at N^{-1} yields Euler summation formula

$$\Delta x \sum_{n=0}^{N} f(x_N) \approx \int_{x_0}^{x_N} dx\, f(x) + \frac{(\Delta x)^2}{12} \left[f'(x_N) - f'(x_0) \right] + \dots$$

(iii) Recognize as sum of residues

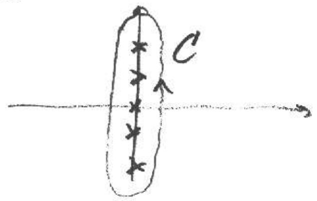
e.g. $\sum_{-\infty}^{\infty} F\left(in \frac{2\pi}{\beta} \right) = \sum_{z_n} (z_n)$

$\Rightarrow$ poles of $n_\beta(z) = \frac{1}{e^{\beta z} - 1}$ residues at these poles

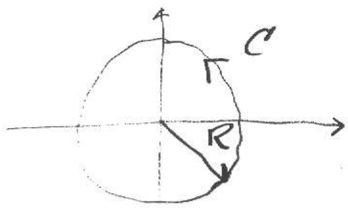
$$n_\beta(z) = \frac{1}{e^{\beta(z - z_n + z_n)} - 1} = \frac{1}{e^{\beta(z-z_n)} - 1} \approx \frac{1}{\beta} \frac{1}{z - z_n}$$

$$\Rightarrow \sum_{n=0}^{\infty} F\left(i n \frac{2\pi}{\beta}\right) = \beta \sum_{z_n} \text{Res}\left\{ n_B(z) F(z) \right\} = \frac{\beta}{2\pi i} \oint_C dz\, F(z)\, n_B(z)$$

where C must enclose all poles:



2^{nd} example: $S = \sum_{-\infty}^{\infty} (-1)^n f(n)$



Consider $I = \oint_C \frac{dz}{2\pi i} \frac{\pi}{\sin \pi z} f(z)$

if: $|z f(z)| \to 0$, $|z| \to \infty \Rightarrow I = 0$

else: $I = \sum_{\text{poles}} \text{Res}\left[\frac{\pi}{\sin \pi z} f(z)\right]$

poles: if $\sin \pi z = 0$: residues are $\frac{1}{\pi}(-1)^n f(n)$

and/or poles of $f(z) \Rightarrow$

$$0 = \sum_{-\infty}^{\infty} (-1)^n f(n) + \sum_{\substack{\text{poles of}\\ f(z)}} \text{Res}\left[\frac{\pi}{\sin \pi z} f(z)\right]$$

$$\Rightarrow \sum_{-\infty}^{\infty} (-1)^n f(n) = - \sum_{\text{poles}} \text{Res}\left[\frac{\pi}{\sin \pi z} f(z)\right]$$

e.g. $$\sum (-1)^n / (a+n)^2 = \sum_{\substack{\text{poles of}\\ (n+1)^{-2}}} \text{Res}\left[\frac{\pi}{\sin \pi z} \frac{1}{(a+z)^2}\right] =$$

$$= -\frac{1}{(2-1)!} \frac{\partial}{\partial z}\left(\frac{\pi}{\sin \pi z}\right)\Bigg|_{z=-a} = \pi^2 \frac{\cos \pi a}{\sin^2 \pi a}$$

for $\sum_{-\infty}^{\infty} f(n)$, use $\pi \cot \pi z$ instead of $\frac{\pi}{\sin \pi z}$

could be tan

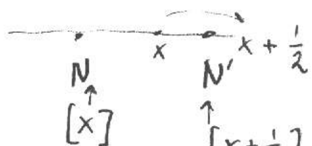
Approximate methods

(i) Use integral approximation as above

(ii) Identify the largest term, and proceed from there

e.g. $f(x) = \sum_{-\infty}^{\infty} e^{-\alpha(n-x)^2}$. If α is very large, only terms with $n \approx x$ are important; define $[x]$ = largest integer not larger than x

$\Rightarrow [x+\frac{1}{2}]$ = integer nearest to x:



$$\Rightarrow f(x) \approx e^{-\alpha([x+\frac{1}{2}]-x)^2}$$

(similar to saddlepoint method).

(iii) If many terms are of equal importance, transform to a convenient form: Poisson summation formula:

$$\sum_{n=-\infty}^{\infty} \varphi(2\pi n) = \frac{1}{2\pi}\sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} d\tau\, \varphi(\tau) e^{-ik\tau}$$

e.g. $\underset{\substack{\uparrow \\ \text{same as in (ii)}}}{f(x)} = \sum_{-\infty}^{\infty} e^{-\alpha(\frac{2\pi n}{2\pi}-x)^2} = \frac{1}{2\pi}\sum_{k=-\infty}^{\infty} \underbrace{\int_{-\infty}^{\infty} d\tau\, e^{-\alpha(\frac{\tau}{2\pi}-x)^2} e^{-ik\tau}}$

$$= \int_{-\infty}^{\infty} d\tau \exp\left[-\frac{\alpha}{4\pi^2}\tau^2 + \left(\frac{\alpha x}{\pi} - ik\right)\tau - \alpha x\right.$$

$$= \int_{-\infty}^{\infty} d\tau \exp\left[-\frac{\alpha}{4\pi^2}\left(\tau - \frac{1}{2}\frac{4\pi^2}{\alpha}\left(\frac{\alpha x}{\pi} - ik\right)\right)^2 + \right.$$

$$+ \frac{\alpha}{4\pi^2}\frac{4\pi^4}{\alpha^2}\left(\frac{\alpha x}{\pi} - ik\right)^2 - \alpha x$$

$$= \sqrt{\frac{\pi}{\alpha}} \sum_{-\infty}^{\infty} \exp\left[-\frac{\pi^2}{\alpha}k^2 - 2\pi i x k\right]$$

if $\alpha \ll 1$, $k=0$ dominates $\Rightarrow f(x) = \sqrt{\frac{\pi}{\alpha}}\left\{\underset{\substack{\uparrow \\ \text{from } k=0}}{1} + \underset{\substack{\uparrow \\ \text{from } k=\pm 1}}{e^{-\frac{\pi^2}{\alpha}} 2\cos(2\pi x)}\right\}$

Meromorphic function = a fcn with a finite number of simple poles
=fcn. and no other singularities

Expressible as a sum over residues:

$$f(z) = f(0) + \sum_{\substack{\text{poles}\\ z_j}} R_j \left(\frac{1}{z - z_j} + \frac{1}{z_j} \right)$$

(assuming $z=0$ is not a pole and $f(z)$ does not diverge as $z \to \infty$)

R_j = Residues at z_j

e.g: $f(z) = \dfrac{1}{\sin z} - \dfrac{1}{z}$

(i) $f(0) = 0$

(ii) poles $z_j = j\pi$, $j \neq 0$

(iii) Residues are $\lim\limits_{z \to j\pi} \dfrac{z - j\pi}{\sin z} \overset{\text{l'Hopital}}{=} \lim \dfrac{1}{\cos z} = (-1)^j = R_j$

$$\Rightarrow \frac{1}{\sin z} = \frac{1}{z} + \sum_{j \neq 0} (-1)^j \left(\frac{1}{z - j\pi} + \frac{1}{j\pi} \right) =$$

$$= \frac{1}{z} + \sum_{j \neq 0} (-1)^j \frac{1}{z - j\pi} + \underbrace{\sum_{j \neq 0} (-1)^j \frac{1}{j\pi}}_{=\text{odd}} =$$

$\Rightarrow = 0$

$$= \sum_{j=-\infty}^{\infty} \frac{(-1)^j}{z - j\pi}$$

Why all this? Sometimes it's useful;

e.g: $\coth z = \dfrac{1}{z} + 2 \sum\limits_{j=1}^{\infty} \dfrac{z}{z^2 + (j\pi)^2}$

$$\Rightarrow I = \int_0^\infty dz \, \sin kz \, \coth z =$$

$$= \underbrace{\int_0^\infty dz \frac{\sin kz}{z}}_{\text{from earlier lectures}} + 2 \sum_1^\infty \underbrace{\int_0^\infty dz \frac{z \sin kz}{z^2 + (j\pi)^2}}_{=\text{tabulated} = \frac{\pi}{2} e^{-jk\pi},\ k>0} =$$

$$= \text{sgn}(k) \left[\frac{\pi}{2} + \pi \underbrace{\sum_1^\infty e^{-j|k|\pi}}_{=\text{geom. series}} \right] =$$

$$= \text{sgn}(k)\, \pi \left(\frac{1}{2} + \frac{1}{1 - e^{-\pi|k|}} - 1 \right) = \frac{\pi}{2} \coth \frac{\pi k}{2}$$

Strictly: Consider $I(\alpha) = \int_0^\infty e^{-\alpha z} \sin kz \coth z \, dz$, $I(\alpha) \to I$, $\alpha \to 0$

Analytic continuation:

Consider two regions S_1 och S_2 $S_1 \cap S_2 \neq \emptyset$ and functions $f_1(z)$ and $f_2(z)$ such that $f_j(z)$ is analytic for $z \in S_j$.
If $f_1(z) = f_2(z)$ for $z \in S_1 \cap S_2$, then the function $f(z)$:

$$f(z) = \begin{cases} f_1(z), & z \in S_1 \\ f_2(z), & z \in S_2 \end{cases}$$

is the <u>analytic continuation</u> of f_1 and f_2 to $S_1 \cap S_2$.

Example. Riemann zeta-fcn $\zeta(s) = \sum_{n=1}^{\infty} n^{-s}$, for $\mathrm{Re}\, s > 1$

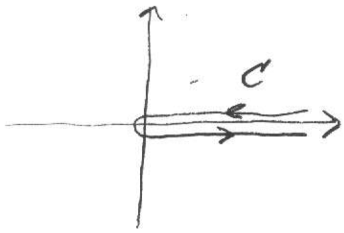
$$\Gamma(s) = \int_0^\infty dx\, x^{s-1} e^{-x}$$

Note: $\int_0^\infty dx\, e^{-nx} x^{s-1} = n^{-s}\Gamma(s)$

$$\Rightarrow \int_0^\infty dx\, x^{s-1} \sum_{n=1}^{\infty} e^{-nx} = \Gamma(s)\zeta(s)$$

$$\Rightarrow \zeta(s) = \frac{1}{\Gamma(s)} \int_0^\infty dx\, \frac{x^{s-1}}{e^x - 1}, \quad \mathrm{Re}\, s > 1$$

Consider $I_C = \int_C dz\, \frac{(-z)^{s-1}}{e^z - 1}$



branch $-z \equiv e^{-i\pi} z$

$\arg(z) \in [0, 2\pi[$

$(-z)^{s-1} = e^{(s-1)\ln|z| + (s-1)(-i\pi + i\arg(z))}$

$$\Rightarrow I_C = \int_\infty^0 dx\, \frac{x^{s-1}}{e^x - 1} e^{-(s-1)i\pi} + \int_0^\infty dx\, \frac{x^{s-1}}{e^x-1} e^{+(s-1)i\pi} =$$

$$= -\left(e^{is\pi} - e^{-is\pi}\right) \int_0^\infty dx\, \frac{x^{s-1}}{e^x - 1}$$

$$\Rightarrow \zeta(s) = \underbrace{\frac{i}{2\sin(i\pi)\Gamma(s)} \int_C dz\, \frac{(-z)^{s-1}}{e^z - 1} = \frac{-\Gamma(1-s)}{2\pi i} \int_C \frac{(-z)^{s-1}}{e^z - 1} dz}_{\text{analytic for all } s \in \mathbb{C} \neq +1, \text{ where it has a simple pole}}$$

$$\Rightarrow \zeta(-1) = -\frac{\Gamma(2)}{2\pi i}\int_{C} dz \, \frac{(-z)^{-n}}{e^{z}-1} = \quad C: \quad \rightarrow C'$$

$$= -\frac{\Gamma(2)}{2\pi i} 2\pi i \operatorname*{Res}_{z=0}\left[\frac{1}{z^2}\frac{1}{e^z-1}\right] = -\Gamma(2)\frac{1}{2!}\frac{\partial^2}{\partial z^2}\left(\frac{z}{e^z-1}\right)_{z=0} = -\frac{1}{12}$$

Note: $\zeta(s) = 0$ for $s = -2, -4, -6, \ldots$

Riemann's hypothesis. $\zeta(s) = 0 \Rightarrow \begin{cases} s = -2, -4, -6, \ldots \\ s = \frac{1}{2} + it, \quad t \in \mathbb{R} \end{cases}$

Proof $\Rightarrow 10^6$ USD!!

LECTURE 5

Review: Complex variables

Analytic continuation: $f_1(x) = \sum_0^\infty x^n$ converge for $|x|<1$

$$= \frac{1}{1-x}$$

$$f_2(x) = \frac{1}{1-x} \quad \text{analytic } \forall x \neq 1$$

Today: Linear Algebra!

- vector: $\vec{a}$ has a magnitude and a direction
- vectors $\{\vec{a}_i\}_{i=1}^n$ are linearly independent iff $\sum_i \lambda_i a_i = 0$ $\Rightarrow \lambda_i = 0$.
- The maximum number of linearly independent vectors in a vector space equals the dimension of the space
- Any set of N linearly dependent vectors $\{\vec{e}_i\}_{i=1}^N$ in an N-dimensional space forms a basis for the space, and every vector in the space can be uniquely written as a linear combination of the basis vectors.

- if any vector $\vec{x}$ in a vector space can be written as $\vec{x} = \sum_{i=1}^{M} \xi_i \vec{y}_i$, then the set $\{y_i\}_{i=1}^{M}$ is complete; if the coefficients ξ_i are not uniquely determined, then $\{y_i\}_{i=1}^{M}$ is over-complete. $\Rightarrow$ a basis is complete.

- a function $\vec{\phi}(\vec{x})$ is called a linear function, if
$$\vec{\phi}(\lambda \vec{a} + \mu \vec{b}) = \lambda \vec{\phi}(\vec{a}) + \mu \vec{\phi}(\vec{b}) \quad \forall \lambda, \mu, \vec{a}, \vec{b}$$

- the vectors $\vec{x}$ and $\vec{\phi}(\vec{x})$ may belong to different vector spaces, e.g. $\vec{x} = \sum_{i=1}^{N} x_i \vec{e}_i$ and $\vec{\phi}(\vec{x}) = \sum_{i=1}^{M} \phi_i \vec{f}_i$.
If $\vec{\phi}$ is linear, then
$$\vec{\phi}(\vec{x}) = \vec{\phi}\left(\sum_{1}^{N} x_i \vec{e}_i\right) = \sum_{i=1}^{N} x_i \underbrace{\vec{\phi}(\vec{e}_i)}_{= \sum_{j=1}^{M} A_{ji} \vec{f}_j} =$$
$$= \sum_{j=1}^{M} \underbrace{\left(\sum_{i=1}^{N} A_{ji} x_i\right)}_{= \phi_j} \vec{f}_j \quad \Rightarrow \quad \phi_j = \sum_{i=1}^{N} A_{ji} x_i, \quad j = 1, \dots, M$$
$$\Leftrightarrow \quad \vec{\phi} = A \vec{x}$$

- define A as a matrix with elements A_{ji}, $j = 1, \dots, M$ and $i = 1, \dots, N$. If B is a matrix such that $B(A\vec{x}) = \vec{x} \;\; \forall \vec{x}$, then B is the inverse matrix of A. If, for a given A, no such exists, A is called singular.

- Matrices related to A:

  transpose: A^T: $(A^T)_{ij} = A_{ji}$

  complex conjugate: A^*: $(A^*)_{ij} = (A_{ij})^*$

  Hermitian conjugate: A^+: $(A^+)_{ij} = (A_{ji})^*$

- Matrix A is Hermitian if $A = A^+$
- A is unitary if $A^{-1} = A^+$

  real $A = A^*$

  symmetric $A = A^T$

  orthogonal $A^{-1} = A^T$

- Transformations between two coordinate systems, or two basis: $\{\vec{e}_i\}$ $\{\vec{e}_i'\}$ are given by matrices

$$\vec{x} = \sum_i x_i \vec{e}_i = \sum_i x_i' \vec{e}_i'$$

If $\vec{e}_j' = \sum_i \gamma_{ij} \vec{e}_i \Rightarrow x_i = \sum_j \gamma_{ij} x_j' \Leftrightarrow x = \gamma x'$

Effect of a basis transformation on linear function:

$\vec{y} = A\vec{x}$: coordinate system $\{\vec{e}_i\}$: $y = Ax$

$\{\vec{e}_i'\}$: $y' = A'x'$

but $x = \gamma x'$, $y = \gamma y' \Rightarrow \gamma x' = A\gamma y' \Rightarrow x' = \gamma^{-1} A \gamma y'$

$\Rightarrow A' = \gamma^{-1} A \gamma$

- Two important quantities that are invariant under coordinate transformations:

trace (or spur): $\mathrm{Tr}\, A = \sum_i A_{ii}$

$\det A = \sum_P (-1)^P \prod_i A_{i,\,Pi}$

$$(-1)^P = \begin{cases} 1 & \text{if the permutation can be generated by an even number of transpositions} \\ -1 & \text{if the number is odd} \end{cases}$$

- the trace and the determinant are cyclically invariant:
$\mathrm{Tr}\,(AB) = \mathrm{Tr}\,(BA)$ and $\det\,(AB) = \det\,(BA)$

- the scalar product $\vec{a}\cdot\vec{b} = \sum_i a_i^* b_i$ is invariant under coordinate transformations if the transformation is unitary, i.e. $\gamma^+ = \gamma^{-1}$

Eigenvalue problem: $A\vec{x} = \lambda\vec{x}$, $\vec{x} \neq 0$, $\lambda \in \mathbb{C}$

In a given coordinate system this becomes

$\sum_j A_{ij} x_j = \lambda x_i \quad \forall i$

- the eigenvalue λ is determined by the secular equation:
$\det(A - \lambda I) = 0 \qquad I$ = unit matrix, $I_{ij} = \delta_{ij}$

- If A is Hermitian, then $\lambda_i \in \mathbb{R}$, and $\vec{x}_i \cdot \vec{x}_j = 0$ if $\lambda_i \neq \lambda_j$

- A Hermitian matrix can be diagonalised by a unitary transformation S such that $A' = S'^{-1} A S$, $(A')_{ij} = \delta_{ij}\lambda_i$.

- In terms of eigenvalues, $\mathrm{Tr}\, A = \sum_i \lambda_i$ and $\det A = \prod_i \lambda_i$

Functions of matrices

- a function $f(A)$, A is a square matrix, is defined through a power series expansion.

e.g.
$$e^A = I + A + \frac{1}{2!}A^2 + \dots$$
$$\sin A = A - \frac{1}{6}A^3 - \frac{1}{20}A^5 + \dots$$

- (Often) the functions are easiest to evaluate in the basis in which A is diagonal; to return to the original basis we note

$$(S'^{-1}AS')^n = S'^{-1}A\underbrace{S'S'^{-1}}_{I}AS' \cdots S'S'^{-1}AS' = S'^{-1}A^nS'$$

$$\Rightarrow S'^{-1}f(A)S' = f(S'^{-1}AS') \Rightarrow f(A) = S'f(S'^{-1}AS')S'^{-1}$$

choose S', $S'^{-1}AS'$ is diagonal $\Rightarrow$ easy.

- Particularly useful identity
$$\mathrm{Tr}(\ln A) = \ln(\det A)$$

- Due to the fact that $AB \neq BA$ for matrices in general, quite a few things become trickier.

e.g. $e^{A+B} \neq e^A e^B$ (corrections: Baker Hausdorff theory)

$X^2 + AX + B = 0$ much harder if A, B, X are matrices.

On a lighter side: How to evaluate determinants?

(i) from the definition $\det A = \sum_P' (-1)^P \prod_i A_{i P_i}$

number of permutations $= N! \Rightarrow$ extremely slow $N! \sim \left(\frac{N}{e}\right)^N$

(ii) by computer LU-composition $A = LU = \,$.

fast $T(N) \sim N^3$ but too much bookkeeping for manual use

$\uparrow_{\text{time}}$

(iii) small determinants

2×2: $a_{11}a_{22} - a_{12}a_{21}$

3×3: $a_{11}a_{22}a_{33} + a_{21}a_{32}a_{13} + a_{31}a_{12}a_{23} -$

$- a_{13}a_{22}a_{31} - a_{23}a_{32}a_{11} - a_{33}a_{12}a_{21}$

4×4: ??

(iv) a trick from the wonderland [Rev. C.L. Dodgson Proc. Royal Society, London 1866]

5·6−2·3

$$A = \begin{pmatrix} 5 & 2 & 1 & 1 & 0 \\ 3 & 6 & 2 & 1 & 4 \\ 1 & 2 & 2 & 1 & 4 \\ 0 & 1 & 3 & 3 & 5 \\ 2 & 1 & 1 & 0 & 2 \end{pmatrix} \to \begin{pmatrix} 24 & -2 & -1 & 4 \\ 0 & 8 & 0^{(\varepsilon)} & 0 \\ 1 & 4 & 3 & -7 \\ -2 & -2 & -3 & 6 \end{pmatrix} \to$$

$\frac{1}{6}(24\cdot 8 + 2\cdot 0) = 32$

$\frac{1}{8}(32\cdot 12 + 4\cdot 4) = 50$ $\quad\frac{1}{0}(4\cdot 0 - 12\cdot($

$$\begin{pmatrix} 32 & 4 & 0 \\ -4 & 12 & 0 \\ 6 & -2 & 1 \end{pmatrix} \to \begin{pmatrix} 50 & ? \\ -16 & -4 \end{pmatrix}$$

Replace problemat element with ε

Instead:
$$\begin{pmatrix} -2 & -1 & 4 \\ 8 & \varepsilon & 0 \\ 4 & 3 & -7 \end{pmatrix} \to \begin{pmatrix} 4-\varepsilon & -4\varepsilon \\ 12-2\varepsilon & -7\varepsilon \end{pmatrix} = \frac{1}{\varepsilon}(-28\varepsilon + 7\varepsilon^2 + 48\varepsilon - ($$

$$= 20 - \varepsilon \to 20 \text{ as } \varepsilon \to 0$$

$\therefore$ Replace "?" with 20: $\begin{pmatrix} 50 & 20 \\ -16 & -4 \end{pmatrix} \to \frac{1}{12}(-200 + 320) = 1($

time $T(N) = T(N-1) + (N-1)^2 \Rightarrow T(N) \sim N^3$.

This method "preserves integrity" - if all numbers are integers only integers appear in the calculation.

LECTURE 6

Review: Linear Algebra

Today: eigenvalue problems
Green's functions

Eigenvalue problems can be defined for a general linear operator $\mathcal{L} u = \lambda u$

linearity: $\mathcal{L}(\alpha u + \beta v) = \alpha \mathcal{L} u + \beta \mathcal{L} v$

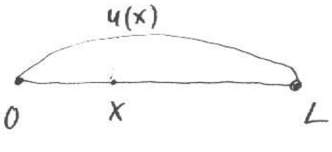
e.g. $\mathcal{L} u = \frac{d^2}{dx^2} u + p(x) \frac{d}{dx} u + q(x) u \qquad (u = u(x))$

$$\mathcal{L} u = \int_{-\infty}^{\infty} dy \, K(x,y) \, u(y)$$

$\mathcal{L}$ is Hermitian if $\underbrace{\int dx \, v^*(x) \, \mathcal{L} u(x)}_{= \langle v | \mathcal{L} | u \rangle} = \left[\int dx \, u^*(x) \, \mathcal{L} v(x) \right]^*$

if $\mathcal{L}$ is Hermitian, then $\lambda \in \mathbb{R}$, and $\langle u_m | u_n \rangle = \delta_{m,n}$

e.g. one dimensional string:



$$-T \frac{\partial^2 u}{\partial x^2} + \rho \frac{\partial^2 u}{\partial t^2} = 0$$

T = tension
ρ = density

Look for solutions $u(x,t) = e^{i\omega t} u(x,0)$

$\Rightarrow \left(\rho \omega^2 + T \frac{\partial}{\partial x^2} \right) u(x,0) = 0 \qquad \leftarrow$ eigenvalue problem!

Boundary conditions: $u(0,t) = u(L,t) = 0$

$\Rightarrow u(0,0) = u(L,0) = 0$

$\Rightarrow u(x,0) = \sum_{n=1}^{\infty} a_n \sin \frac{n\pi x}{L}$

Substitute into eig. probl:

$$\sum_{n=1}^{\infty} a_n \left[\rho\omega^2 - T\left(\frac{\pi n}{L}\right)^2\right] \sin\frac{n\pi x}{L} = 0$$

multiply by $\sin\frac{m\pi x}{L}$ and integrate $\int_0^L dx$

$$\Rightarrow \; 0 = a_m\left[\rho\omega^2 - T\left(\frac{\pi m}{L}\right)^2\right] \quad \Rightarrow \text{eigenvalue } \omega_m = m\frac{\pi}{L}\sqrt{\frac{T}{\rho}}$$

- eigenfunctions of Hermitian operator form a basis of the relevant space: all sufficiently well-behaved functions can be written as $\sum_{n=1}^{\infty} a_n u_n(x)$
- inhomogenous eigenvalue problems:

$$\mathcal{L}u(x) - \lambda u(x) = f(x)$$

Assume $\mathcal{L}$ Hermitian and let the solution of the homogenous problem $\mathcal{L}u - \lambda u = 0$ be known as $\{\lambda_n, u_n(x)\}$

Write $u(x) = \sum_n a_n u_n(x)$

$$f(x) = \sum_n b_n u_n(x)$$

$$\Rightarrow \sum_n a_n\left[\mathcal{L}u_n(x) - \lambda u_n(x)\right] = \sum_n f_n u_n(x)$$

$$\Rightarrow \sum_n a_n u_n(x)(\lambda_n - \lambda) = \sum_n f_n u_n(x)$$

Now, integrate:

$$\int dx\, u_m^*(x) \Rightarrow \sum_n \delta_{n,m}(\lambda_n - \lambda) = \sum_n f_n \delta_{n,m}$$

$$\Rightarrow a_m = \frac{f_m}{\lambda_n - \lambda}$$

$$\Rightarrow u(x) = \sum_n \frac{u_n(x)}{\lambda_n - \lambda} f_n$$

but $f_n = \langle u_n | f\rangle = \int dx'\, u_n^*(x) f(x')$

$$\Rightarrow u(x) = \int dx' \underbrace{\sum_n \frac{u_n(x)\, u_n^*(x')}{\lambda_n - \lambda}}_{= G(x,x')} f(x') = \int dx'\, \underset{\substack{\uparrow \\ \text{Green's function}}}{G(x,x')}\, f(x')$$

Summing over eigenfunctions is usually quite difficult. We need another way to obtain $G(x,x')$.

The solution of $\mathcal{L}u - \lambda u = f$ is $u(x) = \int dx'\, G(x,x') f(x')$

If $f(x') = \delta(x')$, then $u(x) = G(x,0)$.

$\Rightarrow$ $G(x,0)$ satisfies $\mathcal{L}\, G(x,0) - \lambda G(x,0) = \delta(x)$.

In general $G(x,x')$ satisfies $\mathcal{L} G(x,x') - \lambda G(x,x') = \delta(x-x')$

<u>example</u>: $\mathcal{L} = \frac{d^2}{dx^2}$, set $\lambda = -k^2$, boundary conditions: $u(0)=u(L)=0$

$$\Rightarrow \quad \frac{d^2 G(x,x')}{dx^2} + k^2 G(x,x') = \delta(x-x')$$

(i) $x \neq x'$: $\quad \frac{d^2 G}{dx^2} + k^2 G = 0$

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

(ii) near $x = x'$:

- $G(x,x')$ must be continous: if it weren't $\frac{d^2 G}{dx^2} \propto \delta'(x-x')$

- $G'(x,x')$ must be discontinous, so that $\frac{d^2 G}{dx^2} \propto \delta(x-x')$. The magnitude of the discontinuity must be such that

$$G'(x,x')\big|_{x=x'+\varepsilon} - G'(x,x')\big|_{x=x'-\varepsilon} = 1 \qquad (*)$$

$$\Rightarrow \quad \begin{cases} a \sin kx' = b \sin k(x'-L) \\ ka \cos kx' = kb \cos k(x'-L) - 1 \end{cases}$$

↑ from (*)

$$\Leftrightarrow \begin{cases} a = \dfrac{\sin k(x'-L)}{k \sin kL} \\[2ex] b = \dfrac{\sin kx'}{k \sin kL} \end{cases}$$

Hence:

$$G(x,x') = \begin{cases} \dfrac{\sin k(x'-L) \sin kx}{k \sin kL} & , \quad x < x' \\[2ex] \dfrac{\sin kx' \sin k(x'-L)}{k \sin kL} & , \quad x > x' \end{cases} =$$

$$= \frac{\sin k(x_> - L) \sin k x_<}{k \sin kL} \quad , \quad \begin{array}{l} x_> = \max(x,x') \\ x_< = \min(x,x') \end{array}$$

In higher dimensions, it is often convenient to write

$$G(x,x') = u(x,x') + v(x,x')$$

where $u(x,x')$ satisfies $\mathcal{L}u - \lambda u = \delta(\vec{x} - \vec{x}')$, but does not satisfy boundary conditions, whereas v satisfies $\mathcal{L}v - \lambda v = 0$ and obey BC's such that $u + v$ satisfy the BC's required for G.

boundary conditions

$\Rightarrow$ solve first for $u(x,x')$ (fundamental solution), then for $v(x,x')$ — the BC's for $\mathcal{L}v - \lambda v = 0$ depend on the choice of $u(x,x')$.

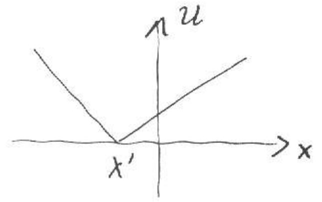
Fundamental solutions:

Poisson equation: $\nabla^2 u(\vec{x}, \vec{x}') = \delta(\vec{x} - \vec{x}')$

1) One dimension: $\dfrac{d^2}{dx^2} u(x,x') = \delta(x - x')$

$\Rightarrow$ $u(x,x')$ is continous

$u'(x,x')$ jumps by 1



$\Rightarrow u(x,x') = \frac{1}{2}|x-x'|$

2) two dimensions: set $\vec{r}\,' = 0$, Note that $u(\vec{r},\vec{r}\,')$ depend only on $\vec{r}-\vec{r}\,'$ due to symmetry:

$$\nabla^2 u(\vec{r},0) = \delta^{(2)}(\vec{r})$$

Symmetry (again): $u(\vec{r},0)$ depend only on $r = |\vec{r}|$

- Use Gauss's theorem: $\int_{\partial\Omega} \nabla u \cdot d\hat{n} = \iint_{\Omega} \underbrace{\nabla^2 u}_{\text{known}}\, d^2r =$

$$= \iint_{\Omega} \delta^{(2)}(\vec{r})\, d^2 r = 1$$

Choose Ω to be a disc with radius R.

$\Rightarrow$ $d\hat{n} = \hat{e}_r$ = unit vector in radial direction

$$\Rightarrow 1 = R\int_0^{2\pi} d\theta\, (\nabla u)_{\hat{r}} = R \cdot 2\pi \cdot \left(\frac{\partial u}{\partial r}\right)_{r=R}$$

$$\Rightarrow \left(\frac{\partial u}{\partial r}\right)_{r=R} = \frac{1}{2\pi R} \Rightarrow \frac{\partial u}{\partial r} = \frac{1}{2\pi r} \Rightarrow u(\vec{r},0) = \frac{1}{2\pi}\ln r$$

3) Three dimensions: $\nabla^2 u(\vec{r},0) = \delta^{(3)}(\vec{r})$

Ω = ball with radius R

$$\iint_{\partial\Omega} \nabla u \cdot d\hat{n} = \iiint_{\Omega} \underbrace{\nabla^2 u}_{\text{known}}\, d^3 r = 1$$

$$\Rightarrow 4\pi R^2 \left(\frac{\partial u}{\partial r}\right)_R = 1 \Rightarrow \frac{\partial u}{\partial r} = \frac{1}{4\pi r^2} \Rightarrow u(\vec{r},0) = -\frac{1}{4\pi r}$$

$$\Leftrightarrow u(\vec{r},\vec{r}\,') = -\frac{1}{4\pi|\vec{r}-\vec{r}\,'|}$$

Retarded vs advanced G.

Consider the wave equation $\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\Phi(x,t) = F(x,t)$

Green's function: $\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right) G(x,t,x',t') = \delta(x-x')\,\delta(t-t')$

Symmetry: $G = G(x-x', t-t')$

$\Rightarrow \Phi(x,t) = \int d^d x \int_{-\infty}^{\infty} dt\; G(x-x', t-t')\, F(x',t')$

d = dimension

Causality: $G^R(x,t) = 0$ for $t<0$

R = "retarded" = response is delayed

Note: $G^A(x,t) = 0$ for $t>0$

A = "advanced"

Fourier transform the equation:

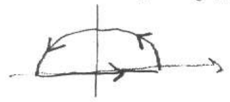
$$\left(-k^2 + \frac{\omega^2}{c^2}\right) G(k,\omega) = 1 \Rightarrow G(k,\omega) = \frac{c^2}{\omega^2 - k^2c^2}$$

$$\Rightarrow G(x,t) = \int \frac{d^d k}{(2\pi)^d} \int \frac{d\omega}{2\pi}\, e^{i(\vec{k}\cdot\vec{x} - \omega t)}\, G(\vec{k},\omega)$$

- implication of causality: $f(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, e^{-i\omega t} f(\omega)$

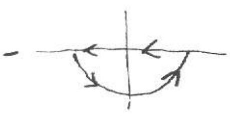
(i) $t<0$

$e^{-i\omega t} \to 0$ if $\mathrm{Im}(\omega) \to +\infty$ $\Rightarrow$ close contour in the upper half plane



(ii) $t>0$

$e^{-i\omega t} \to 0$ if $\mathrm{Im}(\omega) \to -\infty$ $\Rightarrow$ close contour in the lower half plane



$\Rightarrow$ if $f(\omega)$ only has poles in the lower half plane (LHP) then $f(t<0)=0$ and causality is guaranteed.

$\Rightarrow$ we can enforce causality by giving ω a small imaginary part in $G(k,\omega)$:

$$G^R(k,\omega) = G(k, \omega + i\eta) \quad , \quad \eta > 0$$
$$= \frac{c^2}{(\omega+i\eta)^2 - k^2c^2}$$

$\Rightarrow$ $G(x,t)$ can be determined $\Rightarrow$ $\Phi(x,t)$.

LECTURE 7

Review: Eigenvalue problems, Green's functions

Today: perturbation theory

1. Volume perturbations

(i) non-degenerate

Assume Hermitian.

eigenvalue problem: $\mathcal{L}u = \lambda u$ (hard)

we want solutions $\{\lambda_n, u_n(x)\}$. Consider another, easier, problem $\mathcal{L}^0 u^0 = \lambda^0 u^0$ (easy), with the solutions $\{\lambda_n^0, u_n^0(x)\}$.

If $\mathcal{L} \simeq \mathcal{L}^0$, in some sense, we can write the hard problem as

$$(\mathcal{L}^0 + \underbrace{\delta\mathcal{L}^0}_{=\mathcal{L}-\mathcal{L}^0})u = \lambda u$$

indices (no exponents on λ)

Write $\lambda_n = \lambda_n^0 + \underbrace{\lambda_n^1}_{\sim \delta L} + \lambda_n^2 + \cdots$

$$u_n(x) = u_n^0(x) + \sum_m a_{mn}^{(1)} u_m^0(x) + \sum_m a_{mn}^{(2)} u_m^0(x) + \ldots$$

where $a_{mn}^{(j)} \sim (\delta\mathcal{L})^j$

$$\Rightarrow \left(\mathcal{L}^0 + \delta\mathcal{L}^0\right)\left[u_n^0(x) + \sum_M a_{mn}^{(1)} u_m^0(x) + \dots\right] =$$

$$= \left(\lambda_n^0 + \lambda_n^1 + \dots\right)\left[u_n^0(x) + \sum_M a_{mn}^{(1)} u_m^0(x) + \dots\right]$$

Seperate powers $(\delta\mathcal{L})^j$, $j = 1, \dots$

$j=0$: $\quad \mathcal{L}^0 u_n^0(x) = \lambda_n^0 u_n^0(x)$

$j=1$: $\quad \mathcal{L}^0 \sum_m a_{mn}^{(1)} u_m^0(x) + \delta\mathcal{L}\, u_n^0(x) =$

$$= \lambda_n^0 \sum_m a_{mn}^{(1)} u_m^0(x) + \lambda_n^1 u_n^0(x)$$

$j=2$: $\quad$ Simile...

Order $j=0$: $\quad \sum_M a_{mn}^{(1)} \lambda_m^0 u_m^0(x) + \delta\mathcal{L}\, u_n^0(x) =$

$$= \lambda_n^0 \sum_M a_{mn}^{(1)} u_m^0(x) + \lambda_n^1 u_n^0(x)$$

Form the scalar product with $u_n^0(x)$, and use $u_m^0 u_n^0 = \delta_{mn}$

$\Rightarrow \quad a_{nn}^{(1)} \lambda_n^0 + u_n^0 \cdot \delta\mathcal{L}\, u_n^0 = \lambda_n^0 a_{nn}^{(1)} + \lambda_n^1$

Hence $\quad \lambda^1 = u_n^0 \cdot \delta\mathcal{L}\, u_n^0 \quad \leftarrow$ first order correction of λ

Take a scalar product with $u_{m \neq n}^0$

$\Rightarrow \quad a_{mn}^{(1)} \lambda_m^0 + u_m^0 \cdot \delta\mathcal{L}\, u_n^0 = \lambda_m^0 a_{mn}^{(1)}$

Hence $\quad a_{mn}^{(1)} = \dfrac{u_m^0 \cdot \delta\mathcal{L}\, u_n^0}{\lambda_n^0 - \lambda_m^0} \quad \leftarrow$ first order corr. of a

$\therefore \quad u_n = u_n^0 + \sum_m \dfrac{u_m^0 \cdot \delta\mathcal{L}\, u_n^0}{\lambda_n^0 - \lambda_m^0} u_m^0 + \dots$

$\Rightarrow \delta\mathcal{L}$ is small if $|u_m^0 \cdot \delta\mathcal{L}\, u_n^0| \ll |\lambda_n^0 - \lambda_m^0|$.

Note that $a_{nn}^{(1)}$ is undetermined thus far: it must be fixed by requiring $u_n \cdot u_m = \delta_{nm} \underset{\text{some algebra}}{\Rightarrow} \mathrm{Re}\, a_{nn}^{(1)} = 0$

Example: $L^0 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $L = L^0 + \frac{\varepsilon}{2}\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$

the easy problem: $\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} u = \lambda u \Rightarrow \left\{\frac{1}{2}, \begin{pmatrix} 1 \\ 0 \end{pmatrix}\right\}_1, \left\{-\frac{1}{2}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right\}_2$

$$\Rightarrow \begin{cases} \lambda_1^1 = (1\ 0)\,\frac{\varepsilon}{2}\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\varepsilon}{2}(1\ 0)\begin{pmatrix} 0 \\ -i \end{pmatrix} = 0 \\ \lambda_2^1 = (0\ 1)\,\frac{\varepsilon}{2}\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0 \end{cases}$$

$a_{12}^{(1)} = -i\frac{\varepsilon}{2}$ and $a_{21}^{(1)} = -i\frac{\varepsilon}{2}$

$$\therefore \begin{cases} u_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} - i\frac{\varepsilon}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ u_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} - i\frac{\varepsilon}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{cases}$$

Example: Mathieu eq.

$$\frac{d^2\psi}{d\theta^2} + (b - s\cos^2\theta)\psi(\theta) = 0, \quad \psi(0) = \psi(2\pi)$$

Consider $-s\cos^2\theta$ as a perturbation.

$\Rightarrow$ unperturbed eq. $\psi''(\theta) + b\psi(\theta) = 0$

$\Rightarrow b_n^0 = n^2 \qquad u_n^{0+}(\theta) = \sqrt{\frac{1}{\pi}}\cos n\theta$ (even solution)

$\qquad\qquad\qquad u_n^{0-}(\theta) = \sqrt{\frac{1}{\pi}}\sin n\theta$ (odd solution)

(for $n=0$, the normalization of u_0^{0+} is $\sqrt{\frac{1}{2\pi}}$)

- the perturbation $s\cos^2\theta$ has even parity $(\cos^2\theta = \cos^2(-\theta))$
  $\Rightarrow$ it does not mix states of even and odd parity.

- $b_n = n^2 - \langle u_n^{0+} | -s\cos^2\theta | u_n^{0+} \rangle = n^2 + \frac{s}{\pi}\frac{1}{4}\int_0^{2\pi} d\theta \cos^2 n\theta \cos\theta$

$= n^2 + \frac{1}{2}s$

$$a_{mn}^{(1)} = \frac{\langle u_m^0 | -s\cos^2\theta | u_n^0 \rangle}{-b_n^2 + b_m^2} = -\frac{1}{\pi}\frac{s}{m^2-n^2}\int_0^{2\pi} d\theta \cos n\theta \cos^2\theta \cos n\theta =$$

$$= -\frac{1}{4}\frac{s}{m^2-n^2}\left(\delta_{n,m+2} + \delta_{n,m-2}\right)$$

- in <u>degenerate case</u>, i.e. if two eigenvalues are equal, we'd have

$$a_{mn}^{(1)} = \frac{u_m^0 \cdot \delta\mathcal{L}\, u_n^0}{\lambda_n^0 - \lambda_m^0}$$

which gives a problem (since $\lambda_m = \lambda_n$).

Consider the degenerate subspace seperately:

let $\lambda_n = \lambda_m$, relabel states $u_{n,j}$, $j = 1,2$.

$$(\mathcal{L}^0 + \delta\mathcal{L})\, u_n = \lambda_n u_n$$

$$\mathcal{L}^0 u_{n,1} = \lambda_n^0 u_{n,1}$$

$$\mathcal{L}^0 u_{n,2} = \lambda_n^0 u_{n,2}$$

Write $u_n^0 = \alpha u_{n,1}^0 + \beta u_{n,2}^0$. $\qquad u_n = u_n^0 + u_n^1$

$$\lambda_n = \lambda_n^0 + \lambda_n^1$$

$$\Rightarrow \mathcal{L}^0 u_n^1 + \alpha\,\delta\mathcal{L}\, u_{n,1}^0 + \beta\,\delta\mathcal{L}\, u_{n,2}^0 =$$

$$= \lambda_n^1 \alpha u_{n,1}^0 + \lambda_n^1 \beta u_{n,2} + \lambda_n^0 u_n^1$$

now $u_{n,1}^0 \cdot | \Rightarrow$

$$u_{n,1}^0 \cdot \mathcal{L} u_n^1 + \alpha u_{n,1}^0 \cdot \delta\mathcal{L}\, u_{n,1}^0 + \beta u_{n,1}^0 \cdot \delta\mathcal{L}\, u_{n,2}^0 =$$

$$= \lambda_n^1 \alpha + \lambda_n^0 u_{n,1}^0 \cdot u_n^1$$

Write $\quad u_n^1 = \sum_m a^1_{mn} u^0_m$

$$\Rightarrow \quad a^{(1)}_{mn1}\lambda_n + \alpha u^0_{n,1}\cdot \delta\mathcal{L}\, u^0_{n,1} + \beta u^0_{n,1}\cdot \delta\mathcal{L}\, u^0_{n,1} =$$

$$= a^{(1)}_{mn1}\lambda^0_n + \alpha\lambda^1_n$$

Similar with $u^0_{n,2}$ yields

$$\lambda^1_n \begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \begin{pmatrix} u^0_{n,1}\cdot\delta\mathcal{L}\, u^0_{n,1} & u^0_{n,1}\cdot\delta\mathcal{L}\, u^0_{n,2} \\ u^0_{n,2}\cdot\delta\mathcal{L}\, u^0_{n,1} & u^0_{n,2}\cdot\delta\mathcal{L}\, u^0_{n,2}\end{pmatrix}$$

which is a 2×2 eigenvalue problem for α, β.

2. Boundary perturbations

(not in MW - but look in eg. Morse + Fehlbach)

example: $\quad (1) \quad \nabla^2\Psi(\vec r) - \lambda\Psi(\vec r) = 0, \quad \vec r \in \Omega$

$$\nabla\Psi\cdot\hat n + \underbrace{f(\vec r)\Psi(\vec r)}_{\text{boundary perturbation, assume small}} = 0, \quad \vec r \in \partial\Omega$$

unperturbed problem: $\quad (2) \quad \nabla^2\Psi^0(\vec r) - \lambda^0\Psi^0(\vec r) = 0, \quad \vec r \in \Omega$

$$\nabla\Psi^0\cdot\hat n = 0, \quad \vec r \in \partial\Omega$$

Green's functions. $G(\vec r, \vec r\,')$ of unperturbed problem

Note that the eigenfunctions of the easy problem (2) can be chosen to be real (since ∇^2 is Hermitian)

$$\Rightarrow \quad G(\vec r, \vec r\,') = \sum_n \frac{u_n(\vec r)\, u_n^*(\vec r\,')}{\lambda_n - \lambda} = G(\vec r\,', \vec r)$$

$\Rightarrow G$ satisfies $\quad (3) \quad \nabla'^2 G(\vec r, \vec r\,') - \lambda G(\vec r, \vec r\,') = \delta(\vec r - \vec r\,')$

$$\nabla' G(\vec r, \vec r\,')\cdot\hat n' = 0, \quad \vec r\,' \in \partial\Omega$$

Change $\vec r \to \vec r\,'$ in (1) and multiply by $G(\vec r, \vec r\,')$

$$\Rightarrow \quad G(\vec{r},\vec{r}')\,\nabla'^2\Psi(\vec{r}') - \lambda G(\vec{r},\vec{r}')\Psi(\vec{r}') = 0$$

Multiply (3) by $\Psi(\vec{r}')$

$$\Rightarrow \quad \Psi(\vec{r}')\,\nabla'^2 G(\vec{r},\vec{r}') - \lambda\Psi(\vec{r}')\,G(\vec{r},\vec{r}') = \Psi(\vec{r}')\,\delta(\vec{r}-\vec{r}')$$

Subtract and integrate over $\vec{r}'$:

$$\Rightarrow \quad \int_\Omega d^d r' \left[\Psi(\vec{r}')\,\nabla'^2 G(\vec{r},\vec{r}') - G(\vec{r},\vec{r}')\,\nabla'^2\Psi(\vec{r}')\right] = \Psi(\vec{r})$$

Use Green's theorem. $\int_\Omega dV\,(f\nabla^2 g - g\nabla^2 f) = \int_{\partial\Omega} dS\,(f\partial_n g - g\partial_n f)$

$$\Rightarrow \int_{\partial\Omega} d^{d-1}r' \Big[\Psi(\vec{r})\underbrace{\nabla' G(\vec{r},\vec{r}')\cdot\hat{n}}_{=0} - G(\vec{r},\vec{r}')\underbrace{\nabla'\Psi(\vec{r}')\cdot\hat{n}}_{=-f(\vec{r}')\Psi(\vec{r}')}\Big] = \Psi(\vec{r})$$

$$\Rightarrow \Psi(\vec{r}) = \int_{\partial\Omega} d^{d-1}r'\; f(\vec{r}')\,G(\vec{r},\vec{r}')\,\Psi(\vec{r}')$$

If we know $\Psi(\vec{r})$ on the surface, we know it everywhere. For

$\vec{r}\in\partial\Omega$

we have

$$\Psi(\vec{r}) = \int_{\partial\Omega} d^{d-1}r'\, f(\vec{r}')\,G(\vec{r},\vec{r}')\,\Psi(\vec{r}') \quad \leftarrow \text{integral eq.}$$

Set $\Psi(\vec{r}) = u_n^0(\vec{r}) + \sum_m a_{mn}^{(1)} u_m^c$

$$G(\vec{r},\vec{r}') = \sum_m \frac{u_m^c(\vec{r})\,u_m^c(\vec{r}')}{\lambda_m^c - \lambda}$$

$$\Rightarrow u_n^0(\vec{r}) + \sum_m a_{mn}^{(1)} u_m^0 = \sum_m u_m^0(\vec{r}) \int_{\partial\Omega} d^{d-1}r' \,\frac{f(\vec{r}')\,u_m^c(\vec{r}')\,u_n^0(\vec{r}')}{\lambda_m^c - \lambda}$$

Multiply by $u_n^0(\vec{r})$ and integrate $\int_\Omega d^d r$

$$\Rightarrow \quad 1 + a_{nn}^{(1)} = \frac{\int_{\partial\Omega} d^{d-1}r\, f(\vec{r})\, u_n(\vec{r})\, u_n(\vec{r})}{\lambda_n^0 - \lambda} = \frac{f_{nn}}{\lambda_n^0 - \lambda}$$

Multiply both sides by $(\lambda_n^0 - \lambda)$:

$$\underbrace{(\lambda_n^0 - \lambda)}_{\text{order } f}\,(1 + \underbrace{a_{nn}^{(1)}}_{\text{order } f}) = f_{nn}$$

$\Rightarrow$ to $\mathcal{O}(f)$: $\lambda = \lambda_n - f_{nn}$

or equivalently

$$\lambda_n^1 = - f_{nn} = - \int_{\partial\Omega} d^{d-1}r\; f(\vec{r})\, |u_n^0(\vec{r})|^2$$

- perturbations in the shape of the boundary can be treated similarly: Transform the problem to an integral equation.

LECTURE 8

<u>Review</u>: Perturbation theory

<u>today</u>: Integral equations

Linear integral equation:

$$h(x) f(x) = g(x) + \lambda \int_a^b K(x,y) f(y)\, dy$$

where h, g, K are known (K = kernel). λ, f unknown.
(λ often called an eigenvalue)

Fredholm eq: $h(x) = 0$ (Fredholm of the 1st kind)
$h(x) = 1$ (— 2nd —)

Volterra eq: $K(x,y) = 0$ for $y > x$

$$\Rightarrow h(x) f(x) = g(x) + \lambda \int_a^x K(x,y) f(y)\, dy$$

A Volterra eq. can be turned into a differential eq., eg:

$$u(x) = f(x) + \underbrace{\int_0^x dy\, e^{x^2-y^2} u(y)}_{= e^{x^2} g(x)}$$

$$\Rightarrow g'(x) = e^{-x^2} u(x) = e^{-x^2} f(x) + g(x)$$

boundary cond.: $g(0) = 0$

$$\Rightarrow g(x) = e^x \int_0^x dy\, e^{-y-y^2} f(y)$$

$$\Rightarrow u(x) = f(x) + e^{x+x^2} \int_0^x dy\, e^{-y-y^2} f(y)$$

Formally, write

$$hf = g + \lambda K f$$

cf. matrix eq: $\tilde{h}\vec{f} = \vec{g} + \lambda \tilde{K}\vec{f}$

diagonal matrix

<u>Degenerate kernel:</u>

If $K(x,y) = \lambda \sum_{i=1}^{n} \phi_i(x) \int_a^b dy\, \psi_i(y) f(y)$

$\Rightarrow$ int eq. is

$$\lambda \sum_i \frac{\phi_i(x)}{h(x)} \int_a^b dy\, \psi_i(y) f(y) + \frac{g(x)}{h(x)} = f(x)$$

Multiply by $\psi_j(x)$ and integrate $\int dx$:

$$\Rightarrow \lambda \sum_i \underbrace{\int_a^b dx\, \psi_j(x) \frac{\phi_i(x)}{h(x)}}_{=A_{ji}} \underbrace{\int_a^b dy\, \psi_i(y) f(y)}_{=f_i} + \underbrace{\int_a^b dx\, \psi_j(x) \frac{g(x)}{h(x)}}_{=b_j} =$$

$$= \underbrace{\int_a^b dx\, \psi_j(x) f(x)}_{=f_j}$$

$$\Rightarrow \lambda \sum_i A_{ji} f_i + b_j = f_j \qquad j = 1, \ldots, n$$

$$\Leftrightarrow \lambda \hat{A}\vec{f} + \vec{b} = \vec{f} \qquad \text{matrix equation.}$$

Note:

- if $(\lambda\tilde{A} - I)$ is singular, i.e. if λ^{-1} is an eigenvalue to $\tilde{A}$, no solution exists for a general $\vec{b}$

- if $(\lambda\tilde{A} - I)$ is not singular, a solution $\exists$ for $\vec{b} \neq 0$, but not for $\vec{b} = 0$. $\Rightarrow$ solve matrix eq. $\Rightarrow$ get f_i $\Rightarrow$ the original eq. then gives

$$f(x) = \frac{g(x)}{h(x)} + \lambda \sum_i \frac{\phi_i(x)}{h(x)} f_i$$

- each kernel can be approximated arbitrarily well with a degenerate one

<u>General Kernel:</u> Fredholms Theorems:

1/ <u>either</u> $f(x) = g(x) + \lambda \int_a^b dy\, K(x,y) f(y)$ has a unique solution for any $g(x)$, <u>or</u>

$$f(x) = \lambda \int_a^b K(x,y) f(y)\, dy$$

has at least one non-trivial solution (λ = eigenvalue).

2/ If λ is not an eigenvalue, then λ is not an eigenvalue of the transposed eq

$$f(x) = g(x) + \lambda \int_a^b dy\, K(y,x)\, f(y)$$

either. If λ is an eigenvalue, also

$$f(x) = \lambda \int_a^b dy\, K(y,x) f(y)$$

has at least one non-trivial solution.

3) If λ is an eigenvalue, the inhomogenous eq has a solution iff

$$\int_a^b \phi(x) g(x)\, dx = 0$$

$\forall$ solutions $\phi(x)$ of

$$\phi(x) = \int_a^b dy\, K(x,y)\,\phi(y)$$

Series solutions:

$$f(x) = g(x) + \lambda \int_a^b K(x,y) f(y)\, dy$$

iterate starting with $f(x) = g(x)$:

$$\Rightarrow f(x) \approx g(x) + \lambda \int_a^b K(x,y) g(y)\, dy + $$
$$+ \lambda^2 \int_a^b dy \int_a^b dy'\, K(x,y) K(y,y') g(y') + \dots$$

Neumann series:

Converges for small λ and bounded $K(x,y)$, eg:

$$\nabla^2 \psi - \frac{2m}{\hbar^2} V(r)\psi + k^2 \psi = 0 \quad [\text{hard}] \qquad (\psi = \psi(r)).$$

$$\nabla^2 \psi + k^2 \psi = 0 \quad [\text{easy}]$$

easy $\Rightarrow$ Green's functions $G_0(r, r')$. $\Rightarrow$ hard equation can be written as

$$\underset{\substack{\uparrow \\ \text{solution to the} \\ \text{easy problem}}}{\psi(r) = \psi_0(r)} - \frac{2m}{\hbar^2} \int G_0(r,r') V(r') \psi(r')\, d^d r'$$

Iterate: $\psi(r) \approx \psi_0(r) - \dfrac{2m}{\hbar^2} \displaystyle\int G_0(r,r') V(r') \psi_0(r')\, d^d r'$

This is known as the Born approximation.

<u>Another series solution</u> (Fredholm's series)

write

$$f(x) = g(x) + \lambda \int_a^b R(x,y,\lambda)\, g(y)\, dy$$

$\uparrow$

Resolvent kernel $= \dfrac{D(x,y,\lambda)}{D(\lambda)}$

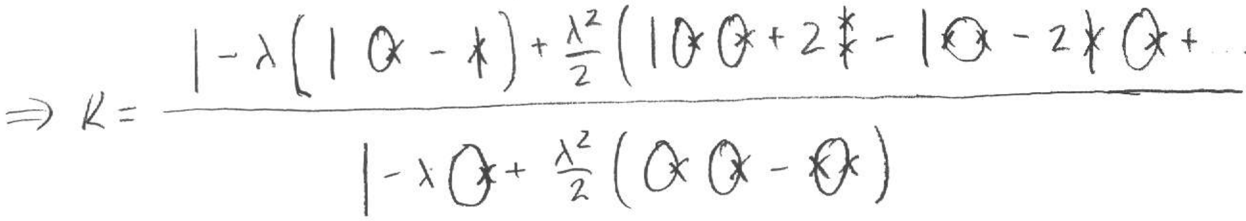
$$D(x,y,\lambda) = K(x,y) - \lambda \int \begin{vmatrix} K(x,y) & K(x,z) \\ K(z,y) & K(z,z) \end{vmatrix} dy + \frac{1}{2!}\lambda^2 \iint \begin{vmatrix} K(x,y) & K(x,z) & K(x,z') \\ K(z,y) & K(z,z) & K(z,z') \\ K(z',y) & K(z',z) & K(z',z') \end{vmatrix} dz'\, dz + \ldots$$

$$D(\lambda) = 1 - \lambda \int K(z,z)\, dz + \frac{1}{2!}\lambda^2 \iint \begin{vmatrix} K(z,z) & K(z,z') \\ K(z',z) & K(z',z') \end{vmatrix} dz'\, dz + \ldots$$

Graphically: $K(x,y) \longrightarrow |$

$\int K(x,z) K(z,y)\, dz \longrightarrow$

$\int K(z,z)\, dz \longrightarrow$



(converges for all λ).

<u>Schmidt - Hilbert series</u>

Consider Hermitian kernels $K(x,y) = K^*(y,x)$, start with the homogenous equation:

$$f(x) = \lambda \int dy\, K(x,y) f(y)$$

- This is an eigenvalue eq, solutions: $\{\lambda_i, u_i(x)\}$.
- K Hermitian $\Rightarrow$ $u_i(x)\cdot u_j(x) = \delta_{ij}$

$$\int dx\, u_i^* u_j(x) = \delta_{ij}$$

Theorem:

All functions $\phi(x)$ that can be written as

$$\phi(x) = \int dy\, K(x,y)\psi(y).$$

can be expanded as $\phi(x) = \sum_i c_i u_i(x)$

The coefficients are

$$c_i = \int dx\, u_i^*(x)\phi(x) = \int dx \int dy\, u_i^*(x) K(x,y)\psi(y) =$$

$$= \int dx \int dy\, \psi(y) K^*(y,x) u_i^*(x) = \int dy\, \psi(y) \lambda_i^{-1} u_i^*(y) =$$

$$= \lambda_i^{-1} \int dx\, u_i^*(x)\psi(x)$$

Consider now the inhomogenous equation:

$$f(x) = g(x) + \lambda \int dy\, K(x,y) f(y)$$

$$\Rightarrow f(x) - g(x) = \lambda \int dy\, K(x,y) f(y) = \sum_i c_i u_i(x)$$

$$c_i = \int dx\, u_i^*(x)\left[f(x) - g(x)\right] = \frac{\lambda}{\lambda_i} \underbrace{\int dx\, u_i^* f(x)}_{=f_i}$$

$$g_i = \int dx\, u_i^* g(x)$$

$$\Rightarrow f_i - g_i = \frac{\lambda}{\lambda_i} f_i \Rightarrow f_i = \frac{\lambda_i}{\lambda_i - \lambda} g_i \Rightarrow c_i = \frac{\lambda}{\lambda_i - \lambda} g_i$$

$$\Rightarrow f(x) = g(x) + \sum_i \frac{\lambda}{\lambda_i - \lambda} u_i(x) \int dy\, u_i^*(y) g(y)$$

cf. $f(x) = g(x) + \lambda \int dy\, R(x,y,\lambda) g(y)$

$$\Rightarrow R(x,y,\lambda) = \sum_i \frac{u_i(x) u_i^*(x)}{\lambda_i - \lambda}$$

$\Rightarrow$ If you can solve the homogenous equation for a Hermitian kernel, you can solve the inhomogenous case.

- For integral equations of the type
$$f(x) = g(x) + \int dy\, K(x,y)\, f(y)$$
an integral transformation is often convenient; which transform depends on the problem (often the Fourier transform)

- Occasionally, integral equations are more convenient than differential equations, since they can be easily iterated, they contain information about boundary conditions, and they are "smoother".

- Sometimes, integral equations can be used to evaluate complicated integrals

eg: $f(x) = e^{g(x)}$

$$\mathcal{F}[f(x)] = \int_{-\infty}^{\infty} dx\, e^{ikx} f(x) \quad \leftarrow \text{often difficult!}$$

calculate $\mathcal{F}[f'(x)] = \int_{-\infty}^{\infty} dx\, e^{ikx} f'(x) =$

$$= \int_{-\infty}^{\infty} dx \left\{ \frac{\partial}{\partial x}\left[e^{ikx} f(x)\right] - ike^{ikx} f(x) \right.$$

$$= -ik\, f(k)$$

but also: $\mathcal{F}[f'(x)] = \int_{-\infty}^{\infty} dx\, e^{ikx} g'(x) f(x) =$

$$= \mathcal{F}[\,g'(x) f(x)\,]$$

Convolution theorem $\Rightarrow$

$$\mathcal{F}[g'(x) f(x)] = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk' \left[-i(k-k')\, g(k-k')\right] f(k')$$

$$\Rightarrow \quad k f(k) = \int_{-\infty}^{\infty} \frac{dk'}{2\pi} (k-k') g(k-k') f(k')$$

Particulary useful if $g(x) = \int_0^{2\pi} \frac{dk}{2\pi} e^{-ikx} g(k)$

$\Rightarrow g(k) = 0$ for $k < 0$

$$\Rightarrow \quad k f(k) = \int_{-\infty}^{k} \frac{dk'}{2\pi} (k-k') g(k-k') f(k')$$

But now,

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} [g(x)]^n = \sum_{n=0}^{\infty} \frac{1}{n!} \int_0^{\infty} \frac{dk_1}{2\pi} \cdots \int_0^{\infty} \frac{dk_n}{2\pi} e^{-i(k_1 + \ldots + k_n)x} G(k_1) \cdots G(k_n)$$

$\Rightarrow f(k) = 0, \quad k < 0$

$$\Rightarrow \quad k f(k) = \int_0^k \frac{dk'}{2\pi} (k-k') g(k-k') f(k')$$

Now, if $k g(k) \approx g_0$ for small k, we have

$$k f(k) = \frac{g_0}{2\pi} \int_0^k dk' f(k')$$

Ansatz: $f(k) = C k^{\alpha} \Rightarrow C k^{\alpha+1} = C \frac{g_0}{2\pi} \frac{k^{\alpha+1}}{\alpha+1}$

$\Rightarrow \alpha = \frac{g_0}{2\pi} - 1 \Rightarrow f(k) \approx C k^{\frac{g_0}{2\pi} - 1}$ for small k

- Note that the constant C must be determined seperately, eg from

$$f(x=0) = \int_0^{\infty} \frac{dk}{2\pi} f(k)$$

- For $k g(k) \propto \beta k^{\Gamma}$, $0 < \Gamma < 1$, we get more complicated behaviour:

$$f(k) = k^q e^{r k^s}, \quad \begin{cases} q = -\frac{1}{2} \frac{\Gamma + 2}{\Gamma + 1} \\ r = \frac{\Gamma + 1}{\Gamma} \left[\beta \Gamma(\Gamma + 1) \frac{1}{2\pi} \right]^{\frac{1}{\Gamma + 1}} \\ s = \frac{\Gamma}{\Gamma + 1} \end{cases}$$

Another example (seperable kernels, but also easy with Neumann series)

$$f(x) = x + \lambda \int_{-1}^{1} dy\, (y-x) f(y)$$

let $A = \int_{-1}^{1} dy\, y f(y)$, $B = \int_{-1}^{1} dy\, f(y)$

$$\Rightarrow \quad f(x) = x + \lambda A - \lambda x B$$

Insert this into A:

$$A = \int_{-1}^{1} dy\, y(y + \lambda A - \lambda y B) = \ldots = \frac{2}{3}(1 - \lambda B)$$

and into B:

$$B = \int_{-1}^{1} dy\, y + \lambda A - \lambda y B = \ldots = 2\lambda A$$

Hence

$$A = \frac{2}{3}(1 - \lambda B) = \frac{2}{3}(1 - 2\lambda^2 A)$$

$$\Rightarrow A = \frac{2}{3 + 4\lambda^2}$$

This gives us

$$B = 2\lambda A = \frac{4\lambda}{3 + 4\lambda^2}$$

Therefore, the solution is

$$f(x) = x + \frac{2\lambda - 4\lambda^2 x}{3 + 4\lambda^2} = \frac{3x + 2\lambda}{3 + 4\lambda^2}$$

LECTURE 4

Review: Integral eqs. & matrix eqs: Fredholm

Volterra $\xrightarrow[\text{often}]{}$ diff. eq.

Series solutions

today: Functional derivatives

Calculus of variations (unconstrained)

function $f: x \to y$ maps a number to another number, $y = y(x)$

functional $\mathcal{A}: f \to y$ maps a function to a number $\mathcal{A}[f]$

e.g: $I = \int_{-\infty}^{\infty} dx\, f(x)$

$I(x_0) = \int_{-\infty}^{x_0} dx\, f(x)$ function of x_0 and functional of f

derivative: how does the value of a function change if we change its argument a little?

$$f(x+\delta x) = f(x) + \delta x \frac{df}{dx} + o(\delta x)$$

[Recall that $\mathcal{O}(x)$ = "of order x": $\lim_{x\to 0} \frac{\mathcal{O}(x)}{x}$ = finite $\neq 0$

$o(x)$ = "smaller than x": $\lim_{x\to 0} \frac{o(x)}{x} = 0$

functional derivative: how does the value of a functional change as we change its argument slightly?

$$\mathcal{A}[f+\delta f] = \mathcal{A}[f] + \delta f \underbrace{\frac{\delta \mathcal{A}}{\delta f}}_{\text{What does this mean?}} + o(\delta f)$$

More carefully: write $\mathcal{A}[f+\delta f] = \mathcal{A}[f] + \mathcal{L}[\delta f] + o(\delta f)$, where $\mathcal{L}[\delta f]$ is a linear functional

$\mathcal{A}[f]$ is <u>differentiable</u> if there exists a linear functional $\mathcal{L}[f]$ such that

$$\| \mathcal{A}[f+\delta f] - \mathcal{A}[f] - \mathcal{L}[\delta f] \| \leq \|\delta f\| \cdot \varepsilon(\|\delta f\|)$$

for all $\|\delta f\| < \delta$. Here $\varepsilon(x)$ is a function such that $\varepsilon(x) \to 0$ as we let $x \to 0$.

Write $\mathcal{L}[\delta f] = \int dx \, \frac{\delta \mathcal{A}}{\delta f(x)} \delta f(x)$, where $\frac{\delta \mathcal{A}}{\delta f(x)}$ is the "functional derivative of $\mathcal{A}$."

<u>Examples</u>:

1. $\mathcal{A}[f] = \int_{-\infty}^{\infty} dx \, f(x)$

$$\delta\mathcal{A} = \mathcal{A}[f+\delta f] - \mathcal{A}[\delta f] = \int_{-\infty}^{\infty} dx \, \delta f(x)$$

$$\Rightarrow \quad \frac{\delta \mathcal{A}}{\delta f(x)} = 1$$

2. $\mathcal{A}_n[f] = \int_{-\infty}^{\infty} dx \, [f(x)]^n$

$$\delta\mathcal{A}_n = \int_{-\infty}^{\infty} dx \, \{ [f(x) + \delta f(x)]^n - [\delta f(x)]^n \} \approx$$

$$\approx \int_{-\infty}^{\infty} dx \left\{ [f(x)]^n + n [f(x)]^{n-1} \delta f(x) - [f(x)]^n \right\} =$$

$$= \int_{-\infty}^{\infty} dx \, n [f(x)]^{n-1} \delta f(x)$$

$$\Rightarrow \quad \frac{\delta \mathcal{A}_n}{\delta f(x)} = n [f(x)]^{n-1} \qquad \text{(cf. ordinary derivatives)}$$

3. $$\mathcal{A}[f] = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx'\, f(x)\, K(x,x')\, f(x')$$

$$\delta\mathcal{A} = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \left\{ \left[\delta f(x) K(x,x') f(x') + f(x) K(x,x') \delta f(x') \right] + o(\delta f) \right.$$

$$= \int_{-\infty}^{\infty} dx\, \delta f(x) \int_{-\infty}^{\infty} dx' \underbrace{\left[K(x,x') f(x') + f(x') K(x',x) \right]}_{= \frac{\delta \mathcal{A}}{\delta f(x)}}$$

4. $$\mathcal{A}[f] = \int_{-\infty}^{\infty} dx \left(\frac{\partial f}{\partial x} \right)^2$$

$$\delta\mathcal{A} = 2 \int_{-\infty}^{\infty} dx\, \frac{\partial f}{\partial x} \frac{\partial \delta f}{\partial x} + o(\delta f) =$$

$$= 2 \int_{-\infty}^{\infty} dx \left\{ \frac{\partial}{\partial x} \left[\frac{\partial f}{\partial x} \delta f(x) \right] - \frac{\partial^2 f}{\partial x^2} \delta f(x) \right\} =$$

$$= 2 \left[f'(\infty) \delta f(\infty) - f'(-\infty) \delta f(-\infty) \right] + \int_{-\infty}^{\infty} dx \left[-2 f''(x)\, \delta f(x) \right]$$

Usually, the class of relevant functions is restricted so that $\delta f(\infty) = \delta f(-\infty) = 0$.

$$\Rightarrow \quad \frac{\delta \mathcal{A}}{\delta f(x)} = -2 f''(x)$$

5. $$\mathcal{A}_{x_0}[f] = f(x_0)$$

$$\delta \mathcal{A}_{x_0} = \delta f(x_0) = \int_{-\infty}^{\infty} dx\, \delta(x - x_0)\, \delta f(x)$$

$$\Rightarrow \quad \frac{\delta \mathcal{A}}{\delta f(x)} = \delta(x - x_0)$$ (somewhat trivial...)

Chain rule: $\left(\frac{df}{dx} = \frac{df}{dy} \frac{dy}{dx} \right)$

$$\mathcal{A}[\underbrace{B_y[f]}] \quad \Rightarrow \quad \delta \mathcal{A}[B_y[\delta f]] = \mathcal{A}[B_y[f+\delta f]] - \mathcal{A}[B_y[f]] =$$

functional of f and function of y

$$= \mathcal{A}\left[B_y[f] + \int_{-\infty}^{\infty} dx \, \frac{\delta B_y}{\delta f(x)} \, \delta f(x) \right] - \mathcal{A}[B_y[f]] =$$

$$= \int_{-\infty}^{\infty} dy \, \frac{\delta \mathcal{A}}{\delta B_y} \int_{-\infty}^{\infty} dx \, \frac{\delta B_y}{\delta f(x)} \, \delta f(x)$$

$$\Rightarrow \quad \frac{\delta \mathcal{A}}{\delta f(x)} = \int_{-\infty}^{\infty} dy \, \frac{\delta \mathcal{A}}{\delta B_y} \, \frac{\delta B_y}{\delta f(x)}$$

e.g. $\mathcal{A}[f] = \int_{-\infty}^{\infty} dx \, [f(x)]^2$

$$B_y[f] = f'(y) \quad \Rightarrow \quad \delta B_y = \int_{-\infty}^{\infty} dx \, \delta(x-y) \delta f'(x) = \int_{-\infty}^{\infty} dx \, [-\delta'(x-y)] \delta f(x)$$

$$\Rightarrow \quad \frac{\delta \mathcal{A}[B_y[f]]}{\delta f(x)} = \int_{-\infty}^{\infty} dy \; 2 B_y[f] [-\delta'(x-y)] =$$

$$= \int_{-\infty}^{\infty} dy \; 2 f'(y) [-\delta'(x-y)] =$$

$$= -2 f''(x)$$ (compare with example 4)

<u>Variational calculus</u>:

which function f yields the minimal / maximal value of the functional $\mathcal{A}[f]$?

functions: if $f(x)$ has a minimum, then it occurs at a point x_0 such that $f'(x_0) = 0$

functionals: if $\mathcal{A}[f]$ has a min., then it occurs for a function $f_0(x)$ such that $\frac{\delta \mathcal{A}}{\delta f(x_0)} = 0$.

Many physical problems can be formulated as variational problems, eg

principle of minimal action = Hamilton's principle:

A particle follows a trajectory $\vec{r}(t)$ that minimizes the action $S[f] = \int_{-\infty}^{\infty} dt \; L(t, \vec{r}(t), \dot{\vec{r}}(t))$, where $L = T - V$ = the Lagrangian.

T ↑ kinetic energy, V ↑ potential energy

$$\delta S = \int_{-\infty}^{\infty} dt \left\{ \frac{\partial L}{\partial \vec{r}(t)} \delta \vec{r}(t) + \frac{\partial L}{\partial \dot{\vec{r}}(t)} \delta \dot{\vec{r}}(t) \right\} =$$

$$= \int_{-\infty}^{\infty} dt \sum_{\alpha = x,y,z} \left[\frac{\partial L}{\partial r_\alpha} \delta r_\alpha(t) + \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{r}_\alpha} \delta r_\alpha(t) \right) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{r}_\alpha} \right) \delta r_\alpha(t) \right]$$

$\delta S = 0 \Rightarrow$

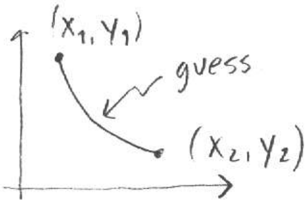
$$\frac{\partial L}{\partial r_\alpha} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{r}_\alpha} \right) = 0, \quad \alpha = x, y, z \quad \leftarrow \text{Euler-Lagrange eq.}$$

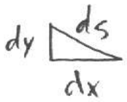
example: free particle: $V = 0$, $T = \frac{1}{2} m \dot{\vec{r}}^2 \Rightarrow L = \frac{1}{2} m \dot{\vec{r}}^2$

$$\Rightarrow 0 - \frac{d}{dt}(m\dot{\vec{r}}) = 0 \Rightarrow m\dot{\vec{r}} = \text{constant}$$

example: Find the curve (in the xy-plane), $y = y(x)$ that minimizes the time it takes a point mass to move from a initial point (x_1, y_1) to (x_2, y_2) under the influence of gravity.

Note: $y_1 > y_2$





$ds^2 = dx^2 + dy^2 =$ (ds = small element on the curve)

$= dx \sqrt{1 + (y')^2}$

speed: $mg(y_1 - y) = \frac{1}{2} m v^2 \Rightarrow v = \sqrt{2g(y_1 - y)}$

$$T = \frac{1}{\sqrt{2g}} \int_{x_1}^{x_2} dx \frac{\sqrt{1 + [y'(x)]^2}}{\sqrt{y_1 - y}} \longrightarrow$$

Euler - Lagrange:

$$0 = \frac{\partial}{\partial y}\left[\sqrt{\frac{1+(y')^2}{y_1-y}}\right] - \frac{d}{dx}\left\{\frac{\partial}{\partial y'}\left[\sqrt{\frac{1+(y')^2}{y_1-y}}\right]\right\} = \dots =$$

$$= \frac{1}{2}\left\{1+[y'(x)]^2\right\} - y''(x)\left[y_1 - y(x)\right]$$

$$\Leftrightarrow \quad \frac{1}{y_1-y} = \frac{2y''}{1+(y')^2}$$

Multiply by y':

$$\underbrace{\frac{y'}{y_1-y}}_{=-\frac{d}{dx}\ln[y_1-y(x)]} = \underbrace{\frac{2y'y''}{1+(y')^2}}_{=\frac{d}{dx}\ln[1+y'(x)^2]}$$

$$\Rightarrow [1+(y')^2](y_1-y) = e^c$$

$$\Rightarrow \quad y' = \pm\sqrt{\frac{e^c}{y_1-y}-1} \quad \Leftrightarrow \quad dx = \pm\frac{dy}{\sqrt{\frac{e^c}{y_1-y}-1}} \qquad \text{Int: } \int_{x_1}^{x} \text{ and } \int_{y_1}^{y}$$

$$\Rightarrow \quad x - x_1 = \pm\sqrt{-(y_1-y)^2 + a(y_1-y)} \mp \frac{1}{2} a \arccos\left[1 - \frac{2}{a}(y_1-y)\right], \quad a = e^c$$

Let $\frac{a}{2}\cos\theta = \frac{a}{2} - (y_1-y) \Rightarrow x - x_1 = \mp\frac{a}{2}(\theta - \sin\theta)$

$$\Rightarrow \begin{cases} x = x_1 \mp \frac{a}{2}(\theta - \sin\theta) \\ y = y_1 - \frac{a}{2}(1-\cos\theta) \end{cases} \quad \leftarrow \text{cycloid}$$

Brachistochrone problem solved.

Trajectory starts at $\theta = 0$, ends at $(x_2, y_2) \Rightarrow a, \theta_{end}$.

LECTURE 10

Review: functional dervates
variational calculus

Today: — " — with constraints
applications to diff. eq.
functional integrals [path integrals]

Find $u(x)$ such that $I[u]$ is minimized subject to the constraint $J[u]=0$. $\Rightarrow$ Lagrange multipliers.

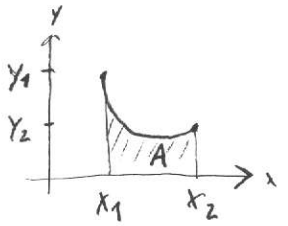
Cf. minimize $f(x,y) = x^4 - x^2 + y^2$
subject to $0 = x^3 - y + 1$
define $f(x,y,\lambda) = f(x,y) - \lambda(x^3 - y + 1)$
with $\frac{\partial f}{\partial x} = 0$, $\frac{\partial f}{\partial y} = 0$ $\Rightarrow$ $\begin{cases} y = -\frac{\lambda}{2} \\ x \in \{0, \frac{3\lambda \pm \sqrt{9\lambda^2+32}}{6}\} \end{cases}$

$\Rightarrow$ either $x = 0$, $y = 1$
or $x = \frac{1}{6}(3\lambda \pm \sqrt{9\lambda^2+32})$, $y = -\frac{\lambda}{2}$

Determine λ such that the constraint is satisfied.

E.g. $I[u] = \int_a^b dx\, F(u,u',x)$
$J[u] = \int_a^b dx\, G(u,u',x)$
$\Rightarrow$ minimize $I_\lambda[u] = \int_a^b dx\, [F(u,u',x) - \lambda G(u,u',x)]$ $\Rightarrow$ $u = u_\lambda(x)$
Choose λ such that $J[u_\lambda(x)] = 0$

example: find the shortest curve $y = y(x)$ such that $y(x_1) = y_1$, $y(x_2) = y_2$ and that the area between the curve and the x-axis is equal to A.



A line segment: dy $(dx^2+dy^2)^{1/2} = dx\,(1+(y')^2)^{1/2}$ dx

$$\Rightarrow I[y] = \int_{x_1}^{x_2} dx \sqrt{1+(y')^2}$$

$$J[y] = \int_{x_1}^{x_2} dx\, y - A$$

$$\Rightarrow \text{minimize} \int_{x_1}^{x_2} dx \left[\sqrt{1+(y')^2} - \lambda y(x)\right] \qquad (A \text{ can be skipped})$$

$$\text{EL:} \quad -\lambda - \frac{d}{dx}\frac{y'}{\sqrt{1+(y')^2}} = 0 \Rightarrow \frac{y'}{\sqrt{1+(y')^2}} = -\lambda x + C_1$$

$$\Rightarrow y' = -\frac{\lambda x - C_1}{\sqrt{1-(\lambda x - C_1)^2}} \Rightarrow y(x) = \frac{1}{\lambda}\sqrt{1-(\lambda x - C_1)^2} + C_2$$

$$\Rightarrow (y - C_2)^2 + \left(x - \frac{C_1}{\lambda}\right)^2 = \frac{1}{\lambda^2}$$

$\therefore$ part of a circle, constants C_1, C_2, λ are determined such that $y(x_{1,2}) = y_{1,2}$, and area $= A$.

This is a isoperimetric problem.

Consider now a minimization problem

$$\min_{u(x)} I[u] = \int_a^b dx \left[p(x)\,(u'(x))^2 + q(x)(u(x))^2\right]$$

subject to

$$J[u] = \int_a^b dx\, \rho(x)\,(u(x))^2 = \text{constant} \qquad (\text{a normalization condition})$$

Note: Since $J[u] = $ constant, minimizing $I[u]$ is equivalent to minimizing $K[u] = \dfrac{I[u]}{J[u]}$.

$$\text{EL:} \quad 2q(x)u(x) - 2\lambda\rho(x)u(x) - \frac{d}{dx}\left[2p(x)u'(x)\right] = 0$$

Multiply EL by $u(x)$, and integrate $\int_a^b dx$

$$\int_a^b dx\,[q(x) - \lambda\varrho(x)](u(x))^2 = \int_a^b dx\,\frac{d}{dx}[p(x)u'(x)]\,u(x) =$$

$$= \int_a^b dx\,\frac{d}{dx}[p(x)u'(x)u(x)] - p(x)(u'(x))^2 =$$

$$= -\int_a^b p(x)(u'(x))^2$$

$$\Rightarrow \int_a^b dx\,[p(x)(u'(x))^2 + q(x)(u(x))^2] = \lambda\int_a^b dx\,\varrho(x)(u(x))^2$$

$$\Rightarrow \quad K[u] = \lambda .$$

- The equation EL i an eigenvalue problem,

$$\frac{d}{dx}[p(x)u'(x)] - q(x)u(x) = -\lambda\varrho(x)u(x)$$

a <u>Sturm-Liouville problem</u>, and its eigenvalues λ_n have the properties

(i) a smallest eigenvalue λ_0 $\exists$

(ii) for large n, $\lambda_n \sim n^2$

$\Rightarrow$ the minimal value of $K[u]$ = the smallest eigenvalue of the equation

$$\frac{d}{dx}[p(x)u'(x)] - q(x)u(x) = \lambda\varrho(x)u(x)$$

$\Rightarrow$ A practical way of estimating the lowest eigenvalue λ_0 is to search for functions that minimize

$$\frac{\int_a^b dx\,[p(x)(u'(x))^2 + q(x)(u(x))^2]}{\int_a^b dx\,\varrho(x)(u(x))^2} \qquad \text{(Rayleigh quotient)}$$

e.g.

$$H\psi = E\psi$$

$$H\psi = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + Cx^\alpha\psi(x) = \frac{d}{dx}\left[-\frac{\hbar^2}{2m}\psi'(x)\right] - (Cx^\alpha)\psi(x) = -(-1)E\psi(x)$$

$$\Rightarrow \quad p(x) = -\frac{\hbar^2}{2m}, \quad q(x) = -Cx^\alpha, \quad \rho(x) = -1, \quad \lambda = E$$

$$\Rightarrow \quad \min_u K[u] = \frac{\int_{-\infty}^{\infty} dx \left[\frac{\hbar^2}{2m}(u'(x))^2 + Cx^\alpha (u(x))^2\right]}{\int_{-\infty}^{\infty} dx\,[u(x)]^2}$$

choose ansatz:

$$u(x) = e^{-\frac{1}{2}\gamma x^2}$$

$$u'(x) = -\gamma x e^{-\frac{1}{2}\gamma x^2}$$

$$\Rightarrow \quad K[u] = K[\gamma] = \frac{\int_{-\infty}^{\infty} dx \left[\frac{\hbar^2}{2m}\gamma^2 x^2 + Cx^\alpha\right] e^{-\gamma x^2}}{\int_{-\infty}^{\infty} dx\, e^{-\gamma x^2}} = \dots =$$

$$= \frac{\hbar^2}{4m}\gamma + C\,\frac{1+(-1)^\alpha}{2}\,\gamma^{-\frac{1}{2}\alpha}\,\Gamma\left(\frac{1+\alpha}{2}\right)$$

Minimize $K[\gamma]$ for $\alpha = 2n \Rightarrow \gamma = \left[\frac{1}{2nC}\frac{\hbar^2}{2m}\frac{2^n}{(2n-1)!!}\right]^{-\frac{1}{n+1}}$

gives an (upper) estimate for E_0.

for $n=1 \Rightarrow \gamma = \sqrt{\frac{2m}{\hbar^2}C}, \quad K[\gamma] = \sqrt{\frac{\hbar^2}{2m}C}$

Cf. exact: $C = \frac{1}{2}m\omega_0^2 \rightarrow E = \frac{1}{2}\hbar\omega_0$. We have

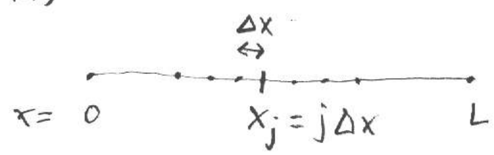
$\sqrt{\frac{2m}{\hbar}C} = \frac{1}{2}\hbar\omega_0$ (good ansatz to the first order)

<u>Functional integration</u>

$$\underbrace{\int D[f(x)]}_{\text{"sum over all functions } f(x)\text{"}} A[f]$$

- usually, the functions $f(x)$ must satisfy some boundary conditions, eg $f(0) = f(L) = 0$ or $f(x) = f(x+L)$.

- Consider the integral over $f(x)$ such that $f(0)=f_0$, and $f(L)=f_L$. Divide the interval $x=0,\dots,L$ into subintervals (small):



$$, \quad \Delta x = \frac{L}{N+1} \quad , \quad x_0 = 0 \, , \quad x_{N+1} = L$$

- values of the function: $f(x_j) = f_j$

$$f(x_0) = f_0$$

$$f(x_{N+1}) = f_L$$

$$\Rightarrow \int_{f(0)=f_0}^{f(L)=f_L} D[f(x)] = \lim_{N\to\infty} \int df_1 \int df_2 \cdots \int df_N$$

Note. $\{x_j, f(x_j)\}$ form a path

- only one kind of path integral can be done: let the integrand be

$$e^{-\frac{1}{2}\sum_{i,j} f_i^* M_{ij} f_j}$$

$$\Rightarrow I = \int_{-\infty}^{\infty} \cdot \int_{-\infty}^{\infty} df_1 \cdots df_N \, e^{-\frac{1}{2}\sum_{i,j} f_i^* M_{ij} f_j}$$

Assume that M_{ij} is Hermitian.

Regard $(f_1, \dots, f_N)$ as a vector in N-dimensional space. Change basis to eigenvectors of M: unitary transformation, Jacobian $= |\det U| = 1$.

$$I = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} du_1 \, du_N \, e^{-\frac{1}{2}\sum_{k,k'} u_{k'}^* \underbrace{\sum_{ij} U_{k'i}^* M_{ij} U_{jk}}_{=\lambda_k \delta_{k,k'} \text{ diagonal}} u_k}$$

$\uparrow$ eigenvalue of M

$$\Rightarrow I = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} du_1 \cdots du_N \, e^{-\frac{1}{2}\sum_k \lambda_k |u_k|^2} =$$

$$= \prod_{k=1}^{N} \sqrt{\frac{2\pi}{\lambda_k}} = \frac{(2\pi)^{N/2}}{\left(\prod_{k=1}^{N} \lambda_k\right)^{N/2}} = \frac{(2\pi)^{N/2}}{\sqrt{\mathrm{Det}(M)}}$$

example:

$$\beta F_{LG}[\psi] = \int dx \left(\tfrac{1}{2} K |\nabla\psi|^2 + \tfrac{1}{2} a |\psi|^2 \right)$$

$\psi \in \mathbb{C}$: order parameter

Averages: $$\langle A \rangle = \frac{\int D[\psi(x)] \, e^{-\beta F_{LG}[\psi]} A[\psi]}{\int D[\psi(x)] \, e^{-\beta F_{LG}[\psi]}}$$

Calculate $A = \psi^*(x_1)\psi(x_2)$. Easier in $\mathcal{F}$-space:

$$\psi(x) = \frac{1}{\sqrt{V}} \sum_k e^{i\vec{k}\cdot\vec{r}} \psi_k$$

$$\Rightarrow \begin{cases} \int dx \, |\nabla\psi|^2 = \sum_k k^2 |\psi_k|^2 \\ \int dx \, |\psi|^2 = \sum_k |\psi_k|^2 \end{cases}$$

Observable: $$A = \frac{1}{V} \sum_{k,k'} e^{i(kx_1 - k'x_2)} \psi_k^* \psi_{k'}$$

Note $$\frac{\delta^2}{\delta\lambda^*_{k_1} \delta\lambda_{k_2}} \Big| \underbrace{\int D[\psi_k] \, e^{-\beta F_{LG}[\psi] + \sum_k (\lambda_k^* \psi_k + \psi_k^* \lambda_k)}}_{= Z[\lambda]} =$$

$$= \int D[\psi_k] \, \psi^*_{k_2} \psi_{k_1} e^{-\beta F_{LG}[\psi_k]}$$

Now: $$\langle \psi^*_{k'} \psi_k \rangle = \frac{1}{Z[0]} \frac{\delta^2}{\delta\lambda_k \delta\lambda^*_{k'}} Z[\lambda] \Big|_{\lambda=0}$$

$$Z[\lambda] = \int D[\psi_k] \, e^{-\sum_k \underbrace{\left[(\frac{1}{2}Kk^2 + a)\psi_k^* \psi_k - \lambda_k^* \psi_k - \psi_k^* \lambda_k \right]}_{\text{complete square:}}}$$

$$\left(\tfrac{1}{2}Kk^2 + a\right)\left(\psi_k^* - \frac{\lambda_k^*}{\frac{1}{2}Kk^2 + a}\right)\left(\psi_k - \frac{\lambda_k}{\frac{1}{2}Kk^2 + a}\right) - \frac{1}{\frac{1}{2}Kk^2 + a} \lambda_k^* \lambda_k$$

define $\tilde{\psi}_k = \psi_k - \frac{\lambda_k}{\frac{1}{2}Kk^2+a}$

$$\Rightarrow Z[\lambda] = \underbrace{\int D[\tilde{\psi}_k]\, e^{-\sum_k (\frac{1}{2}Kk^2+a)\tilde{\psi}_k^* \tilde{\psi}_k}}_{=Z[0]} e^{\sum_k \frac{1}{\frac{1}{2}Kk^2+a}|\lambda_k|^2} =$$

$$= Z[0]\, e^{\sum_k \frac{1}{\frac{1}{2}Kk^2+a}|\lambda_k|^2}$$

$$\Rightarrow \frac{\delta^2}{\delta\lambda_k \delta\lambda_k^*} Z[\lambda] = Z[0] \frac{\delta}{\delta\lambda_k}\left(\frac{\lambda_k}{\frac{1}{2}Kk^2+a} e^{\sum_k \frac{1}{\frac{1}{2}Kk^2+a}|\lambda_k|^2} \right)\Bigg|_{\lambda=0} =$$

$$= Z[0] \frac{1}{\frac{1}{2}Kk^2+a} \delta_{k,k'}$$

Hence

$$\langle \psi_k^* \psi_{k'} \rangle = \frac{\delta_{k,k'}}{\frac{1}{2}Kk^2+a}$$

and $\langle \psi^*(x_1)\psi(x_2)\rangle = \frac{1}{V}\sum_k \frac{e^{ik(x_1-x_2)}}{\frac{1}{2}Kk^2+a}$.

Good book: Negele + Orland: (Quantum theory of) many particle physics

Review: Path integrals

Today: Group theory (math)

Group: • set of elements $\underbrace{\{e, a, b, c, \dots\}}_{\text{number of elements = order of the group is finite}} = A$

• a way to combine them, an operation, multiplication

such that
1) if $a, b \in A$, then $ab \in A$
2) operation is transitive: $a(bc) = (ab)c$
3) identity e, such that $ae = ea = a \;\; \forall a \in A$
4) $\forall a \in A \;\; \exists$ inverse $a^{-1} \in A$ and $aa^{-1} = a^{-1}a = e$

Note: Usually $ab \neq ba$. If $ab = ba \;\; \forall a, b \in A$, then the group is Abelian.

Example: permutation group (aka symmetric group) S_3:

$☆, \triangle, \square \rightarrow \triangle, \square, ☆$ etc.

group elements are different permutations

notation: $[2\ 3\ 1](☆\ \square\ \triangle) = (\square\ \triangle\ ☆)$

group multiplication: $[3\ 2\ 1][2\ 3\ 1](☆, \square, \triangle) = (☆, \triangle, \square)$

but $[1\ 3\ 2](☆, \square, \triangle) = (☆, \triangle, \square)$

$\Rightarrow [3\ 2\ 1][2\ 3\ 1] = [1\ 3\ 2]$

order of $S_3 = 6 (= 3!)$

Subgroup: if $B \subset A$ and if $G = (A, \cdot)$ and $S = (B, \cdot)$ are groups, then S is a subgroup of G.

e.g. permutation: $e = [1\ 2\ 3]$, $a = [2\ 3\ 1]$, $b = [3\ 1\ 2]$,
$c = [2\ 1\ 3]$, $d = [1\ 3\ 2]$, $f = [3\ 2\ 1]$

Multiplication table:

second

first	e	a	b	c	d	f
e	e	a	b	c	d	f
a	a	b	e	d	f	c
b	b	e	a	f	c	d
c	c	f	d	e	b	a
d	d	c	f	a	e	b
f	f	d	c	b	a	e

$\Rightarrow$ (e, a, b) is a subgroup of S_3.
(e, c), (e, d), (e, f) are all subgroups
e is also a subgroup (but trivial)
Also the group is its own subgroup, but this is sometimes excluded.

Right coset: Sg = set of elements obtained by multiplying g by any element of S

S: subgroup of G; g: element of G

(1) either $Sg_1 = Sg_2$ or $Sg_1 \cap Sg_2 = \phi$

proof: Assume $g = s_1 g_1$ and $g = s_2 g_2$.

$$\Rightarrow g_2 = s_2^{-1} g = s_2^{-1}(s_1 g_1) = (s_2^{-1} s_1) g_1 = s_3 g_1$$

Hence $s_2 g_2 = (s_2 s_3) g_1 \Rightarrow Sg_2 = Sg_1$

(2) all elements of $S'g$ are different.

proof. Assume $s_1 g = s_2 g$ (ie the theorem is not true)

$$\Rightarrow s_1 g g^{-1} = s_2 g g^{-1} \Rightarrow s_1 = s_2$$

$\Rightarrow S'g$ has as many elements as S'. Let h' = order of S': $S'g$ has h' elements

(3) each element of G belongs to at least one coset $S'g$.

proof. $e \in S'$.

(1) $\wedge$ (3) $\Rightarrow$ each element of G belongs to exactly one disjoint coset. Number of disjoint cosets $= n \Rightarrow n \cdot h' = h$ = the order of $G \Rightarrow h/h' \in \mathbb{N}$

• <u>Order of an element</u>: if $a^n = e$ and $a^m \neq e$, $m < n$, the order of a is n.

• <u>equivalence</u>: 2 elements a, b of G are equivalent if there $\exists$ an element $g \in G$ such that $g^{-1} a g = b$.
cf. change of basis

• <u>Class</u>: set of equivalent elements

example: S_3: (i) e forms a class: $g^{-1} e g = e \ \forall g$.

(ii) $c^{-1} = c$ (from the table). Hence $c^{-1} a c = c d = b$: $\{a, b\}$ form a class.

(iii) $a^{-1} = b$, $a^{-1} c a = b f = d$. $b^{-1} c b = a d = f$
$\Rightarrow \{c, d, f\}$ form a class.

• elements in a class have the same order.

$$b^n = (g^{-1} a g)^n = g^{-1} a^n g = g^{-1} e g = e$$

- invariant subsets: if S' is a subgroup of G', and if $g^{-1}Sg = S \ \forall g$ the S' is an invariant subgroup and contains only complete classes.

Representation:

The set of $n \times n$ matrices $\{M_j\}$ is a representation of the group G if

$$g_i \cdot g_j = g_k \Rightarrow M_i M_j = M_k$$

(note that $\Leftarrow$ is not true in general)

$\Rightarrow$ each group has a trivial representation $M_j = I \ \forall j$.

- if $g_i \neq g_j \Rightarrow M_i \neq M_j$, the groups G and M are isomorphic ($\sim$ perfectly equivalent).

- if several $g \in G$ are representated by the same matrix, the groups G and M are homomorphic (M preserves some of the structure of G).

- Two representations $D(g)$ and $D'(g)$ are equivalent if there $\exists$ a non-singular matrix S such that $D'(g) = S^{-1} D(g) S$

- if there $\exists$ a matrix S such that all matrices $D(g)$ become block-diagonal:

$$S'^{-1} D S' = \begin{pmatrix} D^{(1)}(g) & 0 \\ 0 & D^{(2)}(g) \end{pmatrix}$$

$D(g) = n \times n$
$D^{(1)}(g) = n_1 \times n_1$
$D^{(2)}(g) = n_2 \times n_2$
$n = n_1 + n_2$

then the representation $D(g)$ is reducible,

$$D(g) = D^{(1)}(g) \oplus D^{(2)}(g).$$

If no such transformation $\exists$, $D(g)$ is irreducible.

Theorems 1., 2., 3. in the book

4. If h is the order of G, and if G has the equivalent irreducible representation $D^{(j)}$ with dimensionalities n_j, then

$$\sum_g \underbrace{\left[D^{(j)}_{\alpha\beta}(g)\right]^* \; D^{(i)}_{\gamma\delta}(g)}_{\text{matrix elements}} = \frac{h}{n_i}\,\delta_{ij}\,\delta_{\alpha\gamma}\,\delta_{\beta\delta}$$

regard $D^{(i)}_{\alpha\beta}$ as an $\sum_i \underbrace{n_i^2}_{n_i \times n_i}$ - dimensional vector, then

$D^{(i)}_{\alpha\beta}$ form an orthogonal basis with as many vectors as there are elements in G $(=h)$.

$\Rightarrow$ $h \le \sum_i n_i^2$: equality holds: $\sum_i n_i^2 = h$ (more advanced techniques required)

$\Rightarrow$ limits the number of irred. reps.

example: S_3 : $h=6$ $\Rightarrow$ $6 = \sum_i n_i^2$

either 1) $6 = 1+1+\ldots+1$ (6 1-dim representations)

or 2) $6 = 2^2+1+1$ (2 1-dim reps, 1 2-D reps)

Character: $\chi^{(i)}(g) = \operatorname{Tr} D^{(i)}(g) = \sum_\alpha D^{(i)}_{\alpha\alpha}(g)$

If g_1 and g_2 belongs to the same class, then

$$\chi^{(i)}(g_1) = \chi^{(i)}(g_2)$$

proof: $g_1 = g^{-1} g_2 g \Rightarrow \chi^{(i)}(g_1) = \operatorname{Tr} D^{(i)}(g_1) =$

$= \operatorname{Tr} D^{(i)}(g^{-1} g_2 g) =$

$= \operatorname{Tr}\left[D^{(i)}(g^{-1}) D^{(i)}(g_2) D^{(i)}(g)\right] =$

$= \operatorname{Tr}\left[D^{(i)}(g_2) D^{(i)}(g) D^{(i)}(g^{-1})\right] =$

$= \operatorname{Tr}\left[D^{(i)}(g_2) D^{(i)}(g g^{-1})\right] =$

$= \operatorname{Tr} D^{(i)}(g_2) =$

$\chi^{(i)}(g_2)$

if their are s classes C_k $(k=1,\dots,s)$ with p_k elements in class C_k, then

$$\sum_{k=1}^{s} p_k \chi^{(i)}(C_k)^* \chi^{(j)}(C_k) = h\delta_{ij}$$

$\Rightarrow$ $\sqrt{\frac{p_k}{h}}\,\chi^{(i)}(C_k)$ are orthonormal vectors in an s-dim space.

number of vectors = number of irred. reps.

$\Rightarrow$ no. of irred. reps $\leq$ no. of classes (equality holds)

For a reducable representation

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

each irred. reps $D^{(i)}(g)$ can appear c_i times

$\Rightarrow$ $D(g) = c_1 D^{(1)}(g) \oplus c_2 D^{(2)}(g) \oplus \dots$

$\Rightarrow$ $\chi(C_k) = c_1 \chi^{(1)}(C_k) + c_2 \chi^{(2)}(C_k) + \dots$

Multiply both sides with $p_k \chi^{(j)}(C_k)^*$

$\Rightarrow$ $p_k \chi^{(j)}(C_k)^* \chi(C_k) =$

$$= p_k c_1 \chi^{(1)}(C_k)^* \chi^{(1)}(C_k) + \dots$$

Sum over k:

$$\Rightarrow \sum_{k=1}^{s} p_k \chi^{(j)}(C_k)^* \chi(C_k) = h c_j$$

$$\Rightarrow c_j = \frac{1}{h}\sum_{k=1}^{s} p_k \chi^{(j)}(C_k)^* \chi(C_k) = \frac{1}{h}\sum_{g} \chi^{(j)}(g)^* \chi(g)$$

Review: finite groups, representations

Today: applications in physics

Hamiltonian H with a symmetry group G, i.e

$$\underbrace{[H,g]}_{\text{commutator}} = 0 \quad \text{for } \underbrace{g}_{\text{some operation}} \in G$$

$$(Hg - gH)|\psi\rangle = 0$$

$\Rightarrow$ if $\psi(\vec{r})$ is an eigenfunction of H with energy E, so is $g\psi(\vec{r})$.

$\Rightarrow$ if $\psi(\vec{r})$ is non-degenerate, then $g\psi(\vec{r}) = e^{i\alpha}\psi(\vec{r})$.

If $\psi(\vec{r})$ is degenerate, meaning that if there are states $\{\psi_j(\vec{r})\}_{j=1}^{N}$ all with energy E, then

$$g\psi_i(\vec{r}) = \sum_{j=1}^{N} \psi_j(\vec{r}) \underbrace{D_{ji}(g)}_{\text{coefficient (matrix)}}$$

$D_{ij}(g)$ form a representation of G:

$$g_2 g_1 \psi_i = g_2 \sum_k \psi_k(\vec{r}) D_{ki}(g_1) =$$

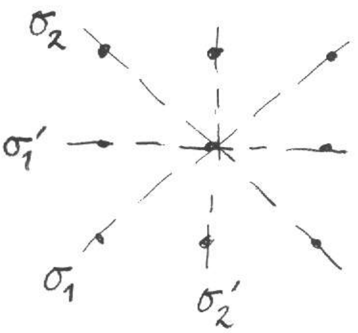
$$= \sum_j \psi_j(\vec{r}) \underbrace{\sum_k D_{jk}(g_2) D_{ki}(g_1)}_{} =$$

$$= \sum_j \psi_j(\vec{r}) D_{ji}(g_2 g_1)$$

$\Rightarrow$ all (non-accidental) degeneracies correspond to representations of the symmetry group; dimension of rep. = number of degenerate states.

$\Rightarrow$ Symmetries can be used to determine degeneracies in the spectrum of a Hamiltonian.

Bandstructure of a 2D solid with a square lattice:



symmetry operations $\{E, C_4, C_4^{-1}, C_2, \sigma_1, \sigma_2, \sigma_1', \sigma_2'$

E = identity

C_4 = rotation by $\frac{2\pi}{4}$

C_4^{-1} = rotation in opposite direction

C_2 = similar

σ_1 = reflection

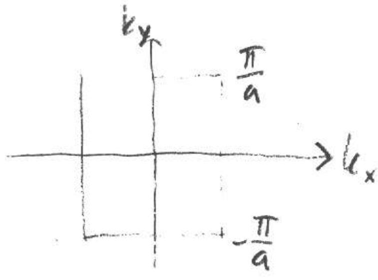
$\sigma_2, \sigma_1', \sigma_2'$ = similar

This group is called C_{4v}, containing 8 operations.

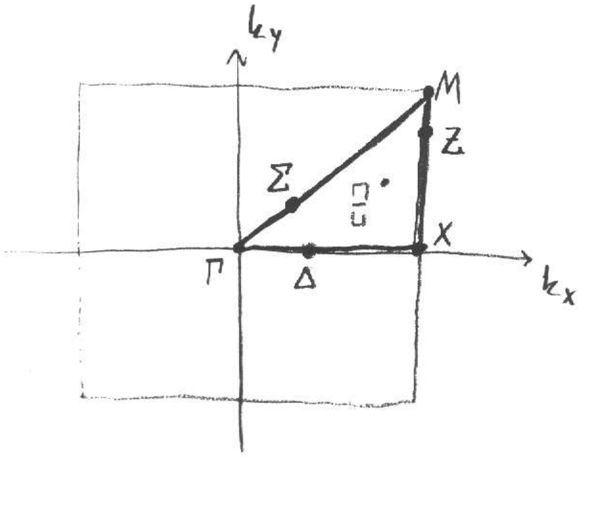
Condensed matter physics: Bloch's theorem:

all points in $\vec{k}$-space that differ from a reciprocal lattice vector $\vec{G} = \frac{2\pi}{a}(n\hat{i} + m\hat{j})$ are equivalent

$\Rightarrow$ need only to consider some k-values (lowest Brillouin-zone)



Symmetry operations can be used to relate parts of the lowest BZ onto each other.



symmetry operations at $\Gamma, \Delta, X, Z, M, \Sigma$, ⊟:

operations that map these points to points that are equivalent to them

$\Gamma: C_{4v}$, $X: \{E, C_2, \sigma_1', \sigma_2'\}$

$\Delta: \{E, \sigma_1'\}$, $Z: \{E, \sigma_2'\}$, $\Sigma: \{E, \sigma_1\}$

⊟$: \{E\}$, $M: C_{4v}$

Figure out the degeneracies $\Rightarrow$ need representations

eg Γ-point:

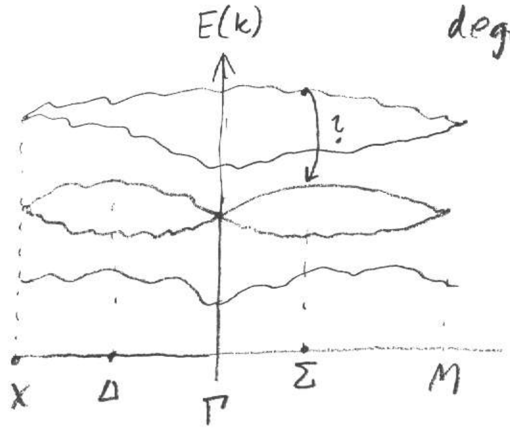
Classes: $\{E\}, \{C_4, C_4^{-1}\}, \{C_2\}, \{\sigma_1, \sigma_2\}, \{\sigma_1', \sigma_2'\}$

5 classes $\Rightarrow$ 5 irreducible reps.

8 elements in C_{4v} $\Rightarrow$ $8 = \sum_{i=1}^{5} n_i^2$

$\Rightarrow$ four 1-dim reps, and one 2-dim rep.

$\Rightarrow$ energy bands at Γ-point at most double degenerate.



$\leftarrow$ Energy diagram

note: course on symmetry analysis $\exists$!