Separation of variables

Spose have linear PDE

$\mathcal{L}_t y + \mathcal{K}_x y = 0$ diff op depending only on x

Write diff op depending only on t

$y(t,x) = T(t)\,X(x)$

Then

$\mathcal{L}_t T(t) X(x) + \mathcal{K}_x T(t) X(x) = 0$

$= X(x)\,\mathcal{L}_t T(t) + T(t)\,\mathcal{K}_x X(x)$

Divide by $T(t)X(x)$:

$$\underbrace{\frac{1}{T(t)} \mathcal{L}_t T(t)}_{\text{fn only of } t} + \underbrace{\frac{1}{X(x)} \mathcal{K}_x X(x)}_{\text{fn only of } x} = 0$$

So each term must be constant:

$$\frac{1}{T(t)} \mathcal{L}_t T(t) = \lambda = -\frac{1}{X(x)} \mathcal{K}_x X(x).$$

This is 2 eigenvalue eqs:

$\mathcal{L}_t T(t) = \lambda T(t)$

$\mathcal{K}_x X(x) = -\lambda X(x)$

Ex 1/, PS 6a

$Y_{\ell m}(\theta, \phi) = \Theta(\theta)\,\Phi(\phi)$

Example 3/
Separation of 3D Laplacian ∇^2 ~~&~~ Q: What is ∇^2 angular & radial parts.

$$\nabla^2 y = \left(\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{L^2}{r^2}\right) y = -k^2 y$$

$$y = R(r)\, Y(\hat{r})$$

$$\underbrace{\left(\frac{1}{R(r)}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{k^2}{r^2}\right)R}_{\text{indept of angular}} - \underbrace{\frac{1}{Y(\hat{r})} L^2 Y(\hat{r})}_{\text{indept of radial}} = -k^2$$

know

$$L^2 Y(\hat{r}) = \ell(\ell+1)\, Y(\hat{r})$$

$$\left(\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{k^2}{r^2}\right) R(r) = \ell(\ell+1)\, R(r)$$

ie $\left[r^2 \frac{\partial^2}{\partial r^2} + 2r\frac{\partial}{\partial r} + \frac{k^2}{r^2} - \ell(\ell+1)\right] R(r) = 0$

Write $R(r) = \frac{u(r)}{r^{\frac{1}{2}}}$.

Become Bessel eqn

$$\left[r^2 \frac{\partial^2}{\partial r^2} + r\frac{\partial}{\partial r} + k^2 - \frac{(\ell+\frac{1}{2})^2}{r^2}\right] u(r) = 0$$

Solutions are $u(r) = \left.\begin{matrix} J \\ Y \end{matrix}\right\}_{\ell+\frac{1}{2}}(kr)$

Example 2./

1D time-dependent wave eqn

$$\left(\frac{\partial^2}{\partial t^2} - c^2 \frac{\partial}{\partial x^2}\right) y = 0$$

c = wave speed

Write $y = T(t)\,X(x)$;

$$\frac{\partial^2}{\partial t^2} T(t)X(x) - c^2 \frac{\partial^2}{\partial x^2} T(t)X(x) = 0$$

Divide by $y = TX$;

$$\underbrace{\frac{1}{T(t)}\frac{\partial^2}{\partial t^2} T(t)}_{\text{indepr of } x} - c^2 \underbrace{\frac{1}{X(x)}\frac{\partial^2}{\partial x^2} X(x)}_{\text{indepr of } t} = 0$$

so both = constant, call it $-\omega^2$:

$$\frac{1}{T(t)}\frac{\partial^2}{\partial t^2} T(t) = -\omega^2 = \frac{c^2}{X(x)}\frac{\partial^2}{\partial x^2} X(x)$$

ie $\dfrac{\partial^2}{\partial t^2} T(t) = -\omega^2 T(t) \quad \Rightarrow T = e^{\pm i\omega t}$

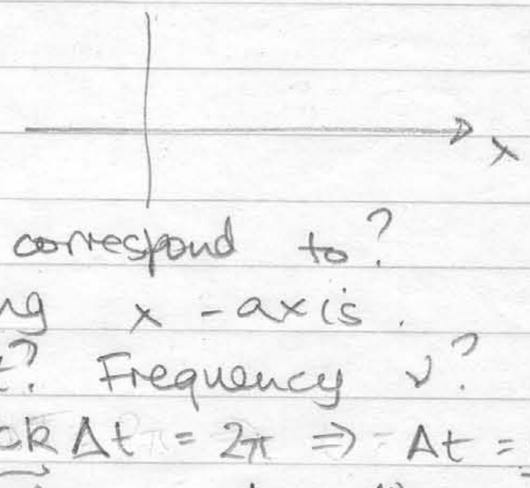
Q: solutions are?

$$\frac{\partial^2}{\partial x^2} X(x) = -\underbrace{\frac{\omega^2}{c^2}}_{\text{call this } k^2} X(x) \quad \Rightarrow X = e^{\pm ikx}$$

where $k \equiv \dfrac{\omega}{c}$

So solutions are

$$y = e^{\pm i\omega t \pm ikx} = e^{\pm ik(x \pm ct)}$$



Q: What do these solutions correspond to?

A: Waves moving at $\pm c$ along x-axis.

Q: Wavelength Δx? Period Δt? Frequency ν?

A: $k\Delta x = 2\pi \Rightarrow \Delta x = \dfrac{2\pi}{k}$, $\underbrace{ck}_{=\omega}\Delta t = 2\pi \Rightarrow \Delta t = \dfrac{2\pi}{\omega}$

$\nu = \dfrac{1}{\Delta t} = \dfrac{\omega}{2\pi}$.

Often, the fastest and most accurate way to compute common eigenfunctions numerically is with recurrence relations.

E.g. - spherical harmonics $Y_{\ell m} \propto P_\ell^m(\theta) e^{im\phi}$
- Bessel functions
- (bound, at least) hydrogenic wavefunctions = (Laguerre)
- simple harm osc wavefunctions = Hermite

Sometimes, as with spher harmonics, there are several recurrence relations to choose from.
But not all are good for num computation...

This is especially true when you need a full set of eigfns, not just one, as is typically the case.

Q: When folks work numerically with $Y_{\ell m}$ they typically work up to ℓ_{max}
ie $\ell = 0$ to ℓ_{max}
$m = -\ell$ to ℓ.
Why full set of m,
NOT $m = -m_{max}$ to m_{max}?

A: ~~So~~ treatment is indept of arbitrary axis.

Q: How do $Y_{\ell m}$ transform under rotations?

A: $Y_{\ell m} \to \sum_{m'} R_{\ell m m'} Y_{\ell m'}$
so ℓ is preserved.

Q: Why is ℓ preserved? A: Because $L^2 = \ell(\ell+1)$ is preserved.

Stability of recurrence relation

Consider recurrence

$$a X_{n+1} = b X_n + c X_{n-1}$$

Could also apply this in reverse dirn

$$c X_{n-1} = -b X_n + a X_{n+1}$$

Q: Expect how many indept solns? A: 2.

Rewrite as

$$X_{n+1} + \mu X_n = \lambda (X_n + \mu X_{n-1})$$

Requires

$$\frac{b}{a} = \lambda - \mu \quad , \quad \frac{c}{a} = \lambda\mu$$

Eliminate μ; $\lambda \frac{b}{a} + \frac{c}{a} = \lambda(\lambda - \mu) + \lambda\mu = \lambda^2$

ie $a\lambda^2 - b\lambda - c = 0$ ← characteristic eq

ie $\lambda_\pm = +\frac{b}{2a} \pm \sqrt{\frac{b^2}{4a^2} + \frac{c}{a}}$

and $\overset{\lambda_\pm - \frac{b}{a}}{\overset{\parallel}{\mu_\pm}} = -\frac{b}{2a} \pm \sqrt{\frac{b^2}{4a^2} + \frac{c}{a}} = -\lambda_\mp$

ie

$$\boxed{X_{n+1} - \lambda_\mp X_n = \lambda_\pm (X_n - \lambda_\mp X_{n-1})}$$

For constant a,b,c, soln after n steps is

$$X_{n+1} - \lambda_\mp X_n = \lambda_\pm^n (X_1 - \lambda_\mp X_0).$$

2 solutions.

Q: Which soln grows faster (in abs value)?

A: One with larger $|\lambda_\pm|$

If roots $\lambda_\pm$ are complex conj ⇒ neutral stab.

Ex 1./ Bessel functions $J_\nu(x)$

$$J_{\nu+1}(x) = \frac{2\nu}{x} J_\nu(x) - J_{\nu-1}(x)$$

equivalently $J_{\nu-1}(x) = \frac{2\nu}{x} J_\nu(x) - J_{\nu+1}(x)$

$$a = 1, \quad b = \frac{2\nu}{x}, \quad c = -1$$

$$\lambda_\pm = \frac{\nu}{x} \pm \sqrt{\frac{\nu^2}{x^2} - 1}$$

Case $|\nu| < |x|$

$\lambda_\pm$ are complex conjugate.

$$\lambda_\pm = \exp\left(\pm i \cos^{-1} \frac{\nu}{x}\right)$$

Stability is neutral.

Case $|\nu| > |x|$

$$\lambda_\pm = \exp\left(\pm \cosh^{-1} \frac{\nu}{x}\right)$$

has growing and decaying solutions.

Which way is recurrence stable?

Take series soln:

$$J_\nu(x) = \sum_{k=0}^{\infty} \frac{(-)^k (x/2)^{\nu+2k}}{k! \underbrace{(\nu+k)!}_{= \Gamma(\nu+k+1)}}$$

$$= \frac{(x/2)^\nu}{\nu!} + \dots$$

This gets tiny for small x, large ν.

You want to recurse in direction where $J_\nu(x)$ is increasing,

ie downard, from large to small ν.

Mathematica jl.nb

PS 7

Ex 7/ $P_\ell^m(x)$ recurrence in ℓ:

$$\underbrace{(\ell-m+1)}_{a} P^m_{\ell+1} = \underbrace{(2\ell+1)x}_{b} P^m_\ell - \underbrace{(\ell+m)}_{c} P^m_{\ell-1}$$

so

$$\lambda_\pm = \overbrace{\frac{(2\ell+1)x}{2(\ell-m+1)}}^{\frac{b}{2a}} \pm \sqrt{\overbrace{\frac{(2\ell+1)^2x^2}{4(\ell-m+1)^2}}^{\frac{b^2}{4a^2}} - \overbrace{\frac{(\ell+m)}{2(\ell-m+1)}}^{+\frac{c}{a}}}$$

$$\cancel{= \frac{1}{2(\ell-m+1)}\left[(2\ell+1)x + \sqrt{(2\ell+1)^2x^2 - 4(\ell-m+1)(\ell+m)}\right]}$$

$$\xrightarrow{\ell \gg m} \quad x \pm \sqrt{\underbrace{x^2-1}_{-ve}}$$

$x = \cos\theta$ runs from $+1$ to -1.

Stability is neutral for $\ell \to \infty$.

Most dangerous case is $|x|$ near 1

Roots are real for

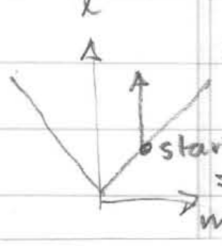
$$x^2 > \frac{4(\ell+m)(\ell-m+1)}{(2\ell+1)^2} = \frac{(2\ell+1)^2-(2m+1)^2}{(2\ell+1)^2}$$

$$= 1 - \left(\frac{2m+1}{2\ell+1}\right)^2$$

Series expansion near $|x| = 1$:

$$P_\ell^m(x) \approx (-)^m \frac{(\ell+m)!}{(\ell-m)!}\left(\frac{1-x^2}{4}\right)^{m/2}$$

$$\frac{P^m_{\ell+1}(x)}{P^m_\ell(x)} \approx \frac{\ell+m+1}{\ell-m+1} > 1 \quad \text{ie } P_\ell^m \text{ increases with } \ell.$$



$\Rightarrow$ Recurr is stable in dirn of increasing ℓ.

Ex 3 / $P_\ell^m(x)$ recurrence in m

$$P_\ell^{m+1} = \underbrace{\frac{2mx}{\sqrt{1-x^2}}}_{b} P_\ell^m - \underbrace{(\ell-m)(\ell+m-1)}_{c} P_\ell^{m-1}$$

$a=1$

$$\lambda_\pm = \overset{\frac{b}{2a}}{\frac{-mx}{\sqrt{1-x^2}}} \pm \sqrt{\overset{\frac{b^2}{4a^2}}{\frac{m^2x^2}{1-x^2}} \overset{+\ \frac{c}{a}}{-} \underbrace{(\ell-m)(\ell+m-1)}_{=\ell^2-m^2-\ell+m}}$$

Arg of $\sqrt{\ }$ is ≥ 0 when

$$x^2 \geq \frac{(\ell-m)(\ell+m-1)}{\ell^2-\ell+m} = \frac{\ell^2-\ell-m^2+m}{\ell^2-\ell+m}$$

ie $$x^2 \geq 1 - \frac{m^2}{\ell^2-\ell+m}$$

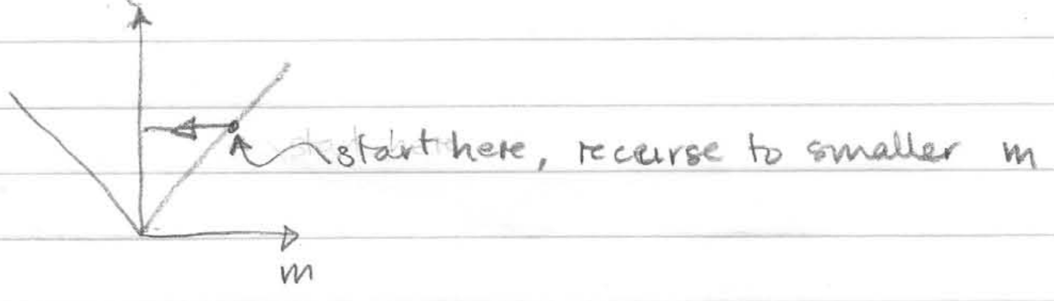
So roots are real when x is near 1.

Again $P_\ell^m(x) \simeq (-)^m \frac{(\ell+m)!}{(\ell-m)!}\left(\frac{1-x^2}{4}\right)^{m/2}$ near $|x| \simeq 1$

so $$\frac{P_\ell^{m+1}(x)}{P_\ell^m(x)} \simeq -(\ell+m)(\ell+m+1)\left(\frac{1-x^2}{4}\right)^{\frac{1}{2}}$$

in abs value decreases as m increases.

So recurrence is stable in dirn of decreasing m.



Fourier Series. RHB Ch. 12

Let $\mathcal{L} = \dfrac{d^2}{dx^2}$, Q: lin diff op? A: yes

Eigenvalue eq

$$\mathcal{L} y = -k^2 y$$

has eigensolutions

$$y \propto e^{\pm ikx}$$

with eigenvalue $-k^2$.

Take interval of x to be $[-\pi, \pi]$

ie take inner product to be

$$a \cdot b \equiv a^\dagger b = \langle a | b \rangle = \int_{-\pi}^{\pi} a^*(x)\, b(x)\, dx$$

could also take interval to be $[0, 2\pi]$ ...

Q: Where might such b.c.s arise physically? A: fns defined on a circle, x = az angle 

Q: Is $\mathcal{L}$ self-adjoint?

A: $\mathcal{L}^\dagger$ = swap coeffs, make odd derivs $-$ve

$\Rightarrow \mathcal{L}^\dagger = \mathcal{L}$ ✓.

Q: what are possible k for periodic eigfns?
A: $k = 0, \pm 1, \ldots$ ie k integral

Repeat integration by parts.

$$y_a^\dagger \mathcal{L} y_b$$

$$= \int_{-\pi}^{\pi} y_a^* \frac{d^2}{dx^2} y_b \, dx$$

$$= \left[y_a^* \frac{dy_b}{dx} \right]_{-\pi}^{\pi} - \int_{-\pi}^{\pi} \frac{dy_a^*}{dx} \frac{dy_b}{dx} \, dx$$

$$= \left[y_a^* \frac{dy_b}{dx} \right]_{-\pi}^{\pi} - \left[\frac{dy_a^*}{dx} y_b \right]_{\pi}^{\pi} + \int_{-\pi}^{\pi} \frac{d^2 y_a^*}{dx^2} y_b \, dx$$

$$= \left[y_a^* \frac{dy_b}{dx} - \frac{dy_a^*}{dx} y_b \right]_{-\pi}^{\pi} + y_a^\dagger \mathcal{L}^\dagger y_b$$

$= y_a^\dagger \mathcal{L}^\dagger y_b$ provided surface term vanishes.

True provided that y_a, y_b periodic over $[-\pi, \pi]$, ie provided that k integral.

Q: Is $\mathcal{L}$ Hermitian?
A: Yes, with respect to functions that are periodic over $[-\pi, \pi]$.
Q: Is $\mathcal{L} \equiv \frac{d^2}{dx^2}$ Hermitian with respect to other sets of functions?
A: Yes, could choose any other interval, and functions periodic over it.

Check theorems:
Thm 1. Eigvals are real?
$k = 0, \pm 1, \pm 2, \ldots$
So eigvals $-k^2$ are real. ✓
Thm 2. Eigfns are orthogonal?
Take eigfns $y_a = e^{ik_a x}$, $y_b = e^{ik_b x}$

$$\int_{-\pi}^{\pi} y_a^* y_b \, dx$$

$$= \int_{-\pi}^{\pi} e^{-ik_a x} e^{ik_b x} \, dx$$

$$= \int_{-\pi}^{\pi} e^{i(k_b - k_a)x} \, dx$$

$$= \left[\frac{e^{i(k_b - k_a)x}}{i(k_b - k_a)} \right]_{-\pi}^{\pi} \quad \text{for } k_b \neq k_a$$

$$= 0 \quad ✓$$

Inner product of eigfn $y_a = e^{ik_a x}$ with itself?

$$\int_{-\pi}^{\pi} y_a^* y_a \, dx = \int_{-\pi}^{\pi} e^{-ik_a x} e^{ik_a x} \, dx$$

$$= \int_{-\pi}^{\pi} dx = 2\pi.$$

So normalized eigfns are

$$\boxed{y_k = \frac{1}{\sqrt{2\pi}} e^{ikx}}$$

for k integral constitute an orthonormal set.

Fourier transform u_k of a function $u(x)$

Suppose $u(x)$, periodic over $[-\pi, \pi]$, can be written

$$\boxed{u(x) = \sum_{k=-\infty}^{\infty} u_k \, y_k(x)} \quad , \quad y_k(x) = \frac{e^{ikx}}{\sqrt{2\pi}}$$

What are the u_k?

Invoke orthogonality of eigfns:

$$\int y_k \cdot u \equiv y_k^\dagger u \equiv \langle y_k | u \rangle$$ various alt notations

$$= \int_{-\pi}^{\pi} y_k^*(x) \, u(x) \, dx$$

$$= \int_{-\pi}^{\pi} y_k^*(x) \sum_{k'=-\infty}^{\infty} u_{k'} \, y_{k'}(x) \, dx$$

a mathematician would be much more careful about swapping order of $\int \Sigma$

$$= \sum_{k'=-\infty}^{\infty} u_{k'} \underbrace{\int_{-\pi}^{\pi} y_k^*(x) \, y_{k'}(x) \, dx}_{= \delta_{kk'}}$$

$$= u_k \, .$$

That is

$$\boxed{u_k = \int_{-\pi}^{\pi} u(x) \frac{e^{-ikx}}{\sqrt{2\pi}} \, dx} \, .$$

u_k, $k = 0, \pm 1, \pm 2, \ldots$

is the Fourier transform of $u(x)$.

Thm 3 Eigfns form complete set ?

Is it true that any periodic function $u(x)$ can be expressed as

$$u(x) = \sum_{k=-\infty}^{\infty} u_k \frac{e^{ikx}}{\sqrt{2\pi}} \quad ?$$

Yes and no.

That is, there are conditions.

A rather general set of conditions is:

If $u(x)$ is square integrable, ie if

$$u^\dagger u \equiv \int_{-\pi}^{\pi} u^*(x)\, u(x)\, dx = \int_{-\pi}^{\pi} |u(x)|^2 dx$$

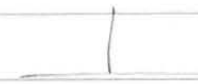
is finite,

then $\exists\ u_k$ s.t

$$\int_{-\pi}^{\pi} \left| u(x) - \sum_{k=-\infty}^{\infty} u_k \frac{e^{ikx}}{\sqrt{2\pi}} \right|^2 dx = 0$$

Comments

1. In non-relativistic quantum mechanics, physical wavefunctions are square-integrable, and 2 wavefns ψ and ϕ are the same iff
$$\int |\psi - \phi|^2 d^3x = 0$$
So there's some physics here, not just mathematics.

(2) What about a function like the Dirac delta-function $\delta(x-x_0)$? 

[Actually, to make it periodic require $\sum_{k=-\infty}^{\infty} \delta(x - x_0 + 2\pi k)$ ]

$\delta(x-x_0)$ is not square-integrable:

$$\int_{-\pi}^{\pi} |\delta(x-x_0)|^2 \, dx$$

$$= \int_{-\pi}^{\pi} \delta(x-x_0)\,\delta(x-x_0)\, dx$$

because $\int f(x)\,\delta(x-x_0)\,dx = f(x_0)$ for any $f(x)$

$$= \delta(x_0 - x_0)$$

$$= \infty$$

Fourier transform of $\delta(x-x_0)$ is

$$\int_{-\pi}^{\pi} \delta(x-x_0) \frac{e^{-ikx}}{\sqrt{2\pi}}\, dx = \frac{e^{-ikx_0}}{\sqrt{2\pi}}$$

whose coeff all have abs value $\frac{1}{\sqrt{2\pi}}$.

Functions like $\delta(x-x_0)$ should be considered as limits of a sequence of square-integrable functions.

Legitimate to use $\delta(x-x_0)$ as long as you remember it's really the limit of a sequence.

Inner product in Fourier space

Think of $u(x)$ as a vector in Hilbert space
  u_x in real space
  u_k is Fourier space.

You demand that the inner product

$$u \cdot v$$

of two vectors u & v
be the same in any space,
regardless of the basis of eigenfuncs.

In real space:

$$u \cdot v \equiv u^\dagger v$$

$$= \int_{-\pi}^{\pi} u^*(x)\, v(x)\, dx$$

$$= \int_{-\pi}^{\pi} \left(\sum_{k'=-\infty}^{\infty} u_{k'} \frac{e^{ik'x}}{\sqrt{2\pi}} \right)^* \left(\sum_{k=-\infty}^{\infty} v_k \frac{e^{ikx}}{\sqrt{2\pi}} \right) dx$$

$$= \sum_{k'} \sum_{k} u_{k'}^* v_k \underbrace{\int_{-\pi}^{\pi} \frac{e^{-ik'x}}{\sqrt{2\pi}} \frac{e^{ikx}}{\sqrt{2\pi}}\, dx}_{= \delta_{k'k}}$$

$$= \sum_{k=-\infty}^{\infty} u_k^* v_k$$

Thus the inner product is, in Fourier space

$$\boxed{u^\dagger v = \sum_{k=-\infty}^{\infty} u_k^* v_k} \qquad \left(\; u_k^* \; \right) \begin{pmatrix} v_k \end{pmatrix}$$

The fact that

$$u \cdot v \equiv u^\dagger v = \int_{-\pi}^{\pi} u^*(x)\, v(x)\, dx = \sum_{k=-\infty}^{\infty} u_k^* v_k$$

is called Parseval's theorem.

Can abbreviate
$u \cdot v = u_x^* v_x = u_k^* v_k$
with implicit integration/summation over x, k, just like finite-dimensional vectors.

It is extremely useful ~~that~~ that the inner product (of a Hilbert space) is the same regardless of basis (real, Fourier, ...), because it allows you to flip between bases without explicit calculation.
~~For ex,~~ if $\mathcal{L}$ is some diff op, then

$$\langle u | \mathcal{L} | v \rangle = \int_{-\pi}^{\pi} u^*(x)\, \mathcal{L}_x v(x)\, dx$$

$$= \sum_k u_k^* \mathcal{L}_k v_k$$

is the same in real and Fourier space.
Just as regard function $u(x)$ as vector u_x
so also regard $y_k(x) = \frac{e^{ikx}}{\sqrt{2\pi}}$ as a matrix y_{xk}
that transforms from Fourier to real space:

$$u(x) = \sum_k y_k(x)\, u_k$$

$$u_x = y_{xk} u_k$$

And the inverse of matrix y_{xk} is?

$$u_k = \int_{-\pi}^{\pi} \frac{e^{-ikx}}{\sqrt{2\pi}} u(x)\, dx$$

$$u_k = y^*_{xk} u_x = y^\dagger_{kx} u_x$$

Inverse of y_{xk} is $y^\dagger_{kx}$, its Hermitian conj. Nice!

Convolution theorem

Convolution in real space $\equiv$ multiplication in Fourier space

— Fourier — $\equiv$ — real —

Fourier transform of product $a(x)b(x)$ is

$$\int_{-\pi}^{\pi} a(x)\,b(x)\,\frac{e^{-ikx}}{\sqrt{2\pi}}\,dx$$

$$= \int_{-\pi}^{\pi}\left(\sum_{m=-\infty}^{\infty} a_m \frac{e^{imx}}{\sqrt{2\pi}}\right)\left(\sum_{n=-\infty}^{\infty} b_n \frac{e^{inx}}{\sqrt{2\pi}}\right)\frac{e^{-ikx}}{\sqrt{2\pi}}\,dx$$

$$= \sum_m \sum_n a_m b_n \underbrace{\int_{-\pi}^{\pi} \frac{e^{i(m+n-k)x}}{(2\pi)^{3/2}}\,dx}_{=\frac{1}{\sqrt{2\pi}}\delta_{m,k-n}}$$

$$= \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} a_{k-n}\, b_n$$

Convolution of $a(x)$ and $b(x)$ in real space is

$$\int_{-\pi}^{\pi} a(x-x')\,b(x')\,dx'$$

FT of this is

$$\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} a(x-x')\,b(x')\,dx'\,\frac{e^{-ikx}}{\sqrt{2\pi}}\,dx$$

$$= \int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\left(\sum_{m=-\infty}^{\infty} a_m \frac{e^{im(x-x')}}{\sqrt{2\pi}}\right)\left(\sum_{n=-\infty}^{\infty} b_n \frac{e^{inx'}}{\sqrt{2\pi}}\right)\frac{e^{-ikx}}{\sqrt{2\pi}}\,dx'\,dx$$

$$= \frac{1}{(2\pi)^{3/2}} \sum_m \sum_n a_m b_n \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \underbrace{e^{i(n-m)x'}\,dx'}_{=2\pi\delta_{nm}}\ \underbrace{e^{i(m-k)x}\,dx}_{2\pi\delta_{mk}}$$

$$= \sqrt{2\pi}\; a_k\, b_k$$

CUT — see next page

Convolution of a_k and b_k in Fourier space is

$$\sum_{n=-\infty}^{\infty} a_{k-n} b_n$$

FT of this is

$$\sum_k \sum_n a_{k-n} b_n \frac{e^{+ikx}}{\sqrt{2\pi}}$$

$$= \sum_k \sum_n \left(\int_{-\pi}^{\pi} a(x') \frac{e^{-i(k-n)x'}}{\sqrt{2\pi}} dx \right) \left(\int_{\pi}^{\pi} b(x'') \frac{e^{-inx''}}{\sqrt{2\pi}} dx'' \right) \frac{e^{ikx}}{\sqrt{2\pi}}$$

$$= \frac{1}{(2\pi)^{3/2}} \int_{-\pi}^{\pi} \frac{a(x') b(x'')}{dx'' \, dx'} \underbrace{\sum_k e^{ik(x-x')}}_{= 2\pi \, \delta_D(x-x')} \underbrace{\sum_n e^{in(x'-x'')}}_{= 2\pi \, \delta_D(x'-x'')}$$

$$= \sqrt{2\pi} \; a(x) \, b(x)$$

Continuous Fourier Transform

With Fourier series, considered functions $u(x)$ periodic over $[-\pi, \pi]$.
But what if $u(x)$ is not periodic?
Consider making the periodic interval wider & wider – maybe as wide as the whole Universe!

$$\text{Write } x = \underset{\text{some real constant}}{a} r, \quad \text{so } r = x/a$$

If x is periodic over $[-\pi, \pi]$,
then r is periodic over $\left[\frac{-\pi}{a}, \frac{\pi}{a}\right]$

Interested in limit of small a, $a \to 0$.
Eigfns are

$$y_k(x) = \frac{e^{ikx}}{\sqrt{2\pi}} \qquad k = 0, \pm 1, \pm 2, \ldots$$

$$= \frac{e^{ikar}}{\sqrt{2\pi}}$$

$$= \frac{e^{ipr}}{\sqrt{2\pi}} \qquad p = ka = 0, \pm a, \pm 2a, \ldots$$

$$\equiv Z_p(r)$$

$$Z_p \equiv e^{ipr}/\sqrt{2\pi}$$

$$\frac{d^2 Z_p}{dr^2} = -\underbrace{p^2}_{\text{eigenvalues}} Z_p$$

Q: Is it just a trick to derive continuous FT from Fourier series in limit of ∞-ly wide periodic interval?
A: It's not a trick. It is fundamental that cts Fourier modes are limit of countable sequence of modes.

Orthogonality.

As usual, for eigfns $y_k(x) = e^{ikx}/\sqrt{2\pi}$

$$\int_{x=-\pi}^{\pi} y_{k'}^*(x)\, y_k(x)\, \underbrace{dx}_{=a\,r} = \delta_{kk'}$$

$$= \int_{r=-\pi/a}^{\pi/a} z_{p'}^*(r)\, z_p(r)\, a\, dr$$

$\begin{cases} 1 \text{ if } k=k' \text{ ie if } p=p' \\ 0 \text{ if } k \neq k' \text{ ie if } p \neq p' \end{cases}$

So

$$\int_{-\pi/a}^{\pi/a} z_{p''}^*(r)\, z_p(r)\, dr = \frac{\delta_{kk'}}{a} = \frac{\delta_{pp'}}{a}$$

Take limit $a \to 0$.

Apparently

$$\int_{-\infty}^{\infty} z_{p''}^*(r)\, z_p(r)\, dr = \delta_D(p'-p) = \begin{cases} \infty & \text{if } p=p' \\ 0 & \text{if } p \neq p' \end{cases}$$

How to interpret weird function $\delta_D(p'-p)$?

$$\int \underbrace{\delta_D(p'-p)}_{= \frac{\delta_{p'p}}{a} = \frac{\delta_{k'k}}{a}} \underbrace{dp}_{=a\,dk}$$

any interval of p containing p'

arises as limit of finite sum

$$\sum_k \frac{\delta_{k'k}}{a}\, a = 1$$

any sum over integers k including k'

So regard

$$\int \delta_D(p'-p)\, dp = 1$$

Evidently δ_D is the Dirac delta-function.

To summarize: In the continuous limit $a \to 0$,

$$z_p(r) = \frac{e^{ipr}}{\sqrt{2\pi}}$$

are eigenfunctions of

$$\frac{d^2 z}{dr^2} = -p^2 z$$

with eigenvalues $-p^2$ with $p \in (-\infty, \infty)$.

Orthonormality condition is

$$\int_{-\infty}^{\infty} z_{p'}^*(r)\, z_p(r)\, dr = \int_{-\infty}^{\infty} \frac{e^{-ip'r}}{\sqrt{2\pi}} \frac{e^{ipr}}{\sqrt{2\pi}}\, dr = \delta_D(p'-p)$$

Continuous Fourier Transform

Suppose — tilde signifies Fourier space

$$v(r) = \int_{-\infty}^{\infty} \tilde{v}(p) \frac{e^{ipr}}{\sqrt{2\pi}}\, dp$$

Consider

$$\int_{-\infty}^{\infty} v(r) \frac{e^{-ipr}}{\sqrt{2\pi}}\, dr$$

$$= \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} \tilde{v}(p') \frac{e^{ip'r}}{\sqrt{2\pi}}\, dp' \right) \frac{e^{-ipr}}{\sqrt{2\pi}}\, dr$$

change order of integration

$$= \int_{-\infty}^{\infty} \tilde{v}(p') \underbrace{\left(\int_{-\infty}^{\infty} \frac{e^{ip'r}}{\sqrt{2\pi}} \frac{e^{-ipr}}{\sqrt{2\pi}}\, dr \right)}_{= \delta_D(p'-p)} dp'$$

$$= \tilde{v}(p)$$

ie

$$\tilde{v}(p) = \int_{-\infty}^{\infty} v(r) \frac{e^{-ipr}}{\sqrt{2\pi}}\, dr$$

Summarize:

$$\boxed{\begin{aligned} v(r) &= \int_{-\infty}^{\infty} \tilde{v}(p) \frac{e^{ipr}}{\sqrt{2\pi}} dp \\ \tilde{v}(p) &= \int_{-\infty}^{\infty} v(r) \frac{e^{-ipr}}{\sqrt{2\pi}} dr \end{aligned}}$$

constitute FT pair.

How does this compare to Fourier series FT?

$$u(x) = \sum_{k=-\infty}^{\infty} u_k \frac{e^{ikx}}{\sqrt{2\pi}}$$

$$u_k = \int_{-\pi}^{\pi} u(x) \frac{e^{-ikx}}{\sqrt{2\pi}} \underbrace{dx}_{= a\,dr}$$

Transformation is

$$x = ar \quad \Rightarrow \quad dx = a \int dr$$

$$p = k/a$$

so if

$$v(r) = u(x) = u(ar)$$

then

$$\tilde{v}(p) = a u_k$$

$$\int \tilde{v}(p)\, dp = a u_k \frac{dk}{a} = u_k \underbrace{dk}_{\int dk \to \sum_k}$$

convolution theorem for continuous FT

Convolution of $a(x)$ and $b(x)$ in real space is

$$\int_{-\infty}^{\infty} a(x-x')\, b(x')\, dx' \quad \text{continuous limit of} \quad \int_{-\pi}^{\pi} a(x-x')\, b(x')\, dx'$$

FT of this is

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} a(x-x')\, b(x')\, dx' \,\frac{e^{-ikx}}{\sqrt{2\pi}}\, dx$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} \tilde{a}(p) \frac{e^{ip(x-x')}}{\sqrt{2\pi}}\, dp \right)\left(\int_{-\infty}^{\infty} \tilde{b}(q) \frac{e^{iqx'}}{\sqrt{2\pi}}\, dq \right) \frac{e^{-ikx}}{\sqrt{2\pi}}\, dx'\, dx$$

$$= \frac{1}{(2\pi)^{3/2}} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \tilde{a}(p)\, \tilde{b}(q)\, dp\, dq\, \underbrace{\int_{-\infty}^{\infty} e^{i(q-p)x'}\, dx'}_{=2\pi\,\delta_D(q-p)}\ \underbrace{\int_{-\infty}^{\infty} e^{i(p-k)x}\, dx}_{=2\pi\,\delta_D(p-k)}$$

$$= \sqrt{2\pi}\; \tilde{a}(k)\, \tilde{b}(k)$$

Likewise conv of $\tilde{a}(k)$ and $\tilde{b}(k)$ in Fourier space is

$$\int_{-\infty}^{\infty} \tilde{a}(k-k')\, \tilde{b}(k')\, dk' \quad \text{continuous limit of} \quad \sum_{k'=-\infty}^{\infty} \tilde{a}_{k-k'}\, \tilde{b}_{k'}$$

FT of this is

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \tilde{a}(k-k')\, \tilde{b}(k')\, dk' \,\frac{e^{ikx}}{\sqrt{2\pi}}\, dk$$

= as above!

$$= \sqrt{2\pi}\; a(x)\, b(x)$$

Comments

1. Notation $\tilde{v}(p)$ for FT of $v(r)$ is common, but by no means universal. My own preference is to drop the tilde, recognizing that v is the same vector in Hilbert space with components

$$v_r = v(r) \text{ in real space}$$
$$v_p = v(p) \; (\doteq \tilde{v}(p)) \text{ in Fourier space).}$$

2. The choice of sign in e^{ipr} is not universal.
Choice here agrees with standard convention in quantum mechanics that momentum operator is

$$\hat{p} = -i\frac{d}{dr} \qquad \left(\text{or } \hat{\mathbf{p}} = -i\frac{\partial}{\partial \mathbf{r}} \text{ in 3D}\right)$$

hat for operator

3. Disposition of (2π) factors is not universal.
Different disciplines follow different conventions.
Alternative 1:
$$v(r) = \int_{-\infty}^{\infty} \tilde{v}(p)\, e^{2\pi i p r}\, dp, \quad \tilde{v}(p) = \int_{-\infty}^{\infty} v(r)\, e^{-2\pi i p r}\, dr$$
Alternative 2:
$$v(r) = \int_{-\infty}^{\infty} \tilde{v}(p)\, e^{ipr}\, \frac{dp}{2\pi}, \quad \tilde{v}(p) = \int_{-\infty}^{\infty} v(r)\, e^{-ipr}\, dr.$$
This last one is the cosmological convention.
FOLLOW WHAT'S CONVENTIONAL IN YOUR DISCIPLINE!

Differentiation

Consider

$$\frac{dv(r)}{dr} \overset{\text{expand } v}{\underset{\text{in Fourier modes}}{=}} \frac{d}{dr}\int_{-\infty}^{\infty} v(p)\,\frac{e^{ipr}}{\sqrt{2\pi}}\,dp$$

$$= \int_{-\infty}^{\infty} v(p)\, ip\, \frac{e^{ipr}}{\sqrt{2\pi}}\,dp$$

= Fourier transform of $ip\,v(p)$

$\Rightarrow$ $\boxed{\text{Differentiation in real space} \equiv \text{multiplication by } ip \text{ in Fourier space}}$

Action of momentum operator —

$$\hat{p} \equiv -i\frac{d}{dr}$$

$\equiv$ multiply by p in Fourier space

Q: True also for Fourier series?
A: Yes. Q: Discrete FT?
A: Y & N.

Q: Does this seem to confuse an operator with an eigenvalue?

A: In Fourier space, the momentum operator $\hat{p}$ is a diagonal matrix with diagonal values equal to its eigenvalues p.

Instead of regarding Fourier modes as eigenmodes of $\frac{d^2 v}{dr^2} = -p^2 v$

can equally well regard them as eigenmodes of $-i\frac{d}{dr}v = p\,v$.

Linear differential equations whose coefficients are constants routinely occur in perturbation theory (small amplitude waves) on uniform (translation invariant) background. The universal professional approach to such equations is to Fourier transform them, causing the differential equations to become algebraic.

Ex/ Homog simple harmonic oscillator

$$\left(\frac{d^2}{dx^2} + 2a\frac{d}{dx} + \omega^2\right) y(x) = 0$$

FT by inspection $\frac{d}{dx} \to ik$ (revert to common notation k for wavenumber)

$$(-k^2 + 2iak + \omega^2)\, y(k) = 0$$

More pedantically, expand

$$y(x) = \int_{-\infty}^{\infty} y(k) \frac{e^{ikx}}{\sqrt{2\pi}}\, dk$$

$$0 = \left(\frac{d}{dx^2} + 2a\frac{d}{dx} + \omega^2\right) \int_{-\infty}^{\infty} y(k) \frac{e^{ikx}}{\sqrt{2\pi}}\, dk$$

$$= \int_{-\infty}^{\infty} (-k^2 + 2iak + \omega^2)\, y(k) \frac{e^{ikx}}{\sqrt{2\pi}}\, dk$$

$$= \text{FT of } (-k^2 + 2iak + \omega^2)\, y(k).$$

Damped SHO

$$\left(\frac{d^2}{dt^2} + 2a\frac{d}{dt} + k^2\right) y(t) = 0$$

FT by inspection $\frac{d}{dt} \to \overset{\text{physics convention}}{-} i\omega$

$$(-\omega^2 - 2ai\omega + k^2)\, y_\omega = 0$$

Non-trivial ($y_\omega \neq 0$) solns satisfy

$$\omega = -ia \pm \sqrt{-a^2 + k^2}$$

Take damping coeff a to be small, $k^2 > a^2$.

Uhoh. Isn't ω supposed to be real in Fourier expansion $y(t) = \int_{-\infty}^{\infty} y_\omega \frac{e^{-i\omega t}}{\sqrt{2\pi}}\, d\omega$?

In real space, solutions are

$$y(t) = e^{-at \pm iqt} \qquad q \equiv \sqrt{k^2 - a^2}$$

FT is

$$\int_{-\infty}^{\infty} e^{-at \pm iqt} \frac{e^{i\omega t}}{\sqrt{2\pi}}\, dt = \frac{1}{2\pi}\left[e^{(-a \pm iq + i\omega)t} \right]_{-\infty}^{\infty}$$

diverges at $t \to -\infty$; FT does not exist!

Diagnosis?

Duh, damped oscillator diverges as $t \to -\infty$.

Must introduce source at finite t to get finite result. For example GF

$$\left(\frac{d^2}{dt^2} + 2a\frac{d}{dt} + k^2\right) G(t, t_0) = \delta(t - t_0)$$

physically: unit whack at $t = t_0$
math: unit mx

FT GF by inspection:

$$\underbrace{(-\omega^2 - 2ai\omega + k^2)}_{= (a - i\omega)^2 + q^2} G_{\omega,\omega_0} = \underbrace{\delta_D(\omega + \omega_0)}_{\text{unit matrix in Fourier space}}$$

Check FT of $\delta_D(t-t_0)$: $\leftarrow \langle t_0 | 1 | t \rangle$

$$\iint \delta_D(t-t_0) \frac{e^{i\omega t}}{\sqrt{2\pi}} \frac{e^{+i\omega_0 t_0}}{\sqrt{2\pi}} \, dt \, dt_0 \quad \leftarrow \langle \omega_0 | 1 | \omega \rangle$$

$$= \int \frac{e^{i(\omega+\omega_0)t}}{2\pi} \, dt$$

$$= \delta_D(\omega - \omega_0)$$

Hence

$$\boxed{G_{\omega,\omega_0} = \frac{\delta_D(\omega-\omega_0)}{(a-i\omega)^2 + q^2}}$$

<u>WKB</u>

SHO with 'slowly' varying frequency^2 $k(x)$

$$f'' + k(x)^2 f = 0$$

eg. Schrod eqn $\dfrac{d^2\psi}{dx^2} + \dfrac{2m}{\hbar^2}\left[E - V(x)\right]\psi = 0$

If $k(x)$ were constant, solution would be

$$f = A\cos\left[k(x)\, x\right] + B\sin\left[k(x)\, x\right]$$

or equivalently

$$f = A e^{ik(x)x} + B e^{-ik(x)x}$$

So write
$$f = e^{i\phi(x)}$$
$$f' = i\phi' e^{i\phi}$$
$$f'' = (i\phi'' - \phi'^2)e^{i\phi}$$

whence diff eq becomes

$$i\phi'' - \phi'^2 + k^2 = 0$$

If ϕ'' is small ('slowly varying'), then

$$\phi'^2 = k^2 + i\phi'' \approx k^2$$

ie $\phi \approx \pm\int k\, dx$

In this approx, $\phi'' = \pm\dfrac{d}{dx}k$

Plug back in to get next approx

$$\phi'^2 \approx k^2 \underbrace{\pm i\frac{dk}{dx}}_{\text{small}}$$

ie $\phi' \approx \pm\left[k^2 \pm i\dfrac{dk}{dx}\right]^{\frac{1}{2}} \approx \pm k\left(1 \pm \dfrac{i}{2k^2}\dfrac{dk}{dx}\right)$

WKB 2

17.12

$$= \pm k + \frac{i}{2k}\frac{dk}{dx}$$

$$= \pm k + \frac{i}{2}\frac{d\ln k}{dx}$$

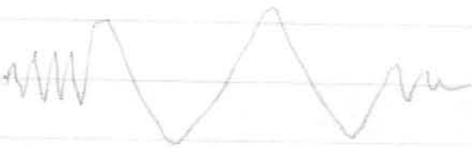
integration const

$$\text{so} \quad \phi \approx \pm \int k \, dx + \frac{i}{2}\ln k + \text{const}$$

whence

const

$$\boxed{f \equiv e^{i\phi} \approx \underbrace{\frac{A}{k^{1/2}}}_{\text{amplitude}} \underbrace{e^{\pm i \int k \, dx}}_{\text{phase}}}$$



$$\text{Amplitude} \underset{\sim}{\propto} \frac{1}{\text{frequency}^{1/2}}$$

For negative $k^2(x)$

$$f \approx \frac{A}{|k|^{1/2}} e^{\pm \int |k| \, dx}$$