Mathematical Methods, revision lectures

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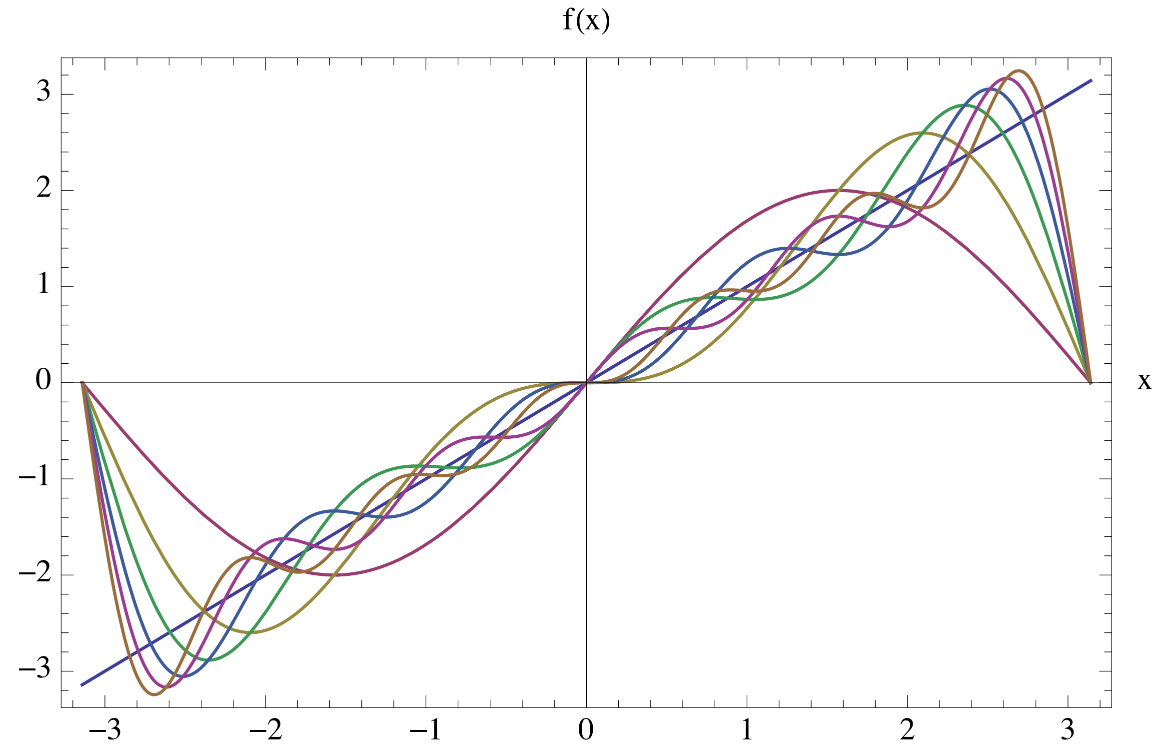


course website: http://www-thphys.physics.ox.ac.uk/people/AndreLukas/MathMeth/

lecture notes: http://www-thphys.physics.ox.ac.uk/people/AndreLukas/MathMeth/mmlecturenotes.pdf

Mathematica notebook: http://www-thphys.physics.ox.ac.uk/people/AndreLukas/MathMeth/mathmeth.nb

Overview

- Inner product vector spaces, Hilbert spaces
- Fourier analysis
- Orthogonal polynomials
- Ordinary linear differential equations
- Partial linear differential equations

Inner product vector spaces, Hilbert spaces

What is an inner product vector space?

A: A vector space with a scalar product.

Definition of a scalar product:

Definition 1.9. *A real scalar product on a vector space V over $F = \mathbb{R}$ and a hermitian scalar product on a vector space V over the field $F = \mathbb{C}$ is a map $\langle \cdot, \cdot \rangle : V \times V \to F$ which satisfies*

(S1) $\langle \mathbf{v}, \mathbf{w} \rangle = \langle \mathbf{w}, \mathbf{v} \rangle$, *for a real scalar product,* $F = \mathbb{R}$ ← symmetry

$\langle \mathbf{v}, \mathbf{w} \rangle = \langle \mathbf{w}, \mathbf{v} \rangle^*$, *for a hermitian scalar product,* $F = \mathbb{C}$ ← hermiticity

(S2) $\langle \mathbf{v}, \alpha\mathbf{u} + \beta\mathbf{w} \rangle = \alpha\langle \mathbf{v}, \mathbf{u} \rangle + \beta\langle \mathbf{v}, \mathbf{w} \rangle$ ← linearity

(S3) $\langle \mathbf{v}, \mathbf{v} \rangle > 0$ *if* $\mathbf{v} \neq \mathbf{0}$ ← positivity

for all vectors $\mathbf{v}, \mathbf{u}, \mathbf{w} \in V$ *and all scalars* $\alpha, \beta \in F$.

The norm associated to a scalar product

$$\| \mathbf{v} \| := \sqrt{\langle \mathbf{v}, \mathbf{v} \rangle}$$

satisfies the Cauchy-Schwarz and triangle inequalities

$$|\langle \mathbf{v}, \mathbf{w} \rangle| \leq \| \mathbf{v} \| \| \mathbf{w} \| \qquad\qquad \| \mathbf{v} + \mathbf{w} \| \leq \| \mathbf{v} \| + \| \mathbf{w} \|$$

Features of inner product vector spaces

- ortho-normal basis: vectors $\epsilon_i \in V$ with $\langle \epsilon_i, \epsilon_j \rangle = \delta_{ij}$.

Parseval's equation

coordinates relative to basis: $\mathbf{v} = \sum_{i=1}^{n} \alpha_i \, \boldsymbol{\epsilon}_i \quad \Longleftrightarrow \quad \alpha_i = \langle \boldsymbol{\epsilon}_i, \mathbf{v} \rangle$

scalar product in terms of coordinates: $\langle \mathbf{v}, \mathbf{w} \rangle = \sum_{i=1}^{n} \alpha_i^* \beta_i$, $\quad \| \, \mathbf{v} \, \|^2 = \sum_{i=1}^{n} |\alpha_i|^2$

matrix describing linear map $T : V \to V$: $\quad A_{ij} = \langle \boldsymbol{\epsilon}_i, T(\boldsymbol{\epsilon}_j) \rangle$

- hermitian conjugate $T^\dagger : V \to V$ of $T : V \to V$: $\langle \mathbf{v}, T\mathbf{w} \rangle = \langle T^\dagger \mathbf{v}, \mathbf{w} \rangle$ *for all* $\mathbf{v}, \mathbf{w} \in V$.

$$A_{ij} = \langle \boldsymbol{\epsilon}_i, T(\boldsymbol{\epsilon}_j) \rangle \, , \qquad (A^\dagger)_{ij} = \langle \boldsymbol{\epsilon}_i, T^\dagger(\boldsymbol{\epsilon}_j) \rangle \, .$$

- hermitian maps: $\langle \mathbf{v}, T(\mathbf{w}) \rangle = \langle T(\mathbf{v}), \mathbf{w} \rangle$ *for all* $\mathbf{v}, \mathbf{w} \in V$. or $T^\dagger = T$ (observables in QM)

$A_{ij} = \langle \boldsymbol{\epsilon}_i, T(\boldsymbol{\epsilon}_j) \rangle$ is a hermitian matrix

Theorem 1.24. *Let V be an inner product vector space. If $T : V \to V$ is self-adjoint then*

(i) All eigenvalues of T are real.
(ii) Eigenvectors for different eigenvalues are orthogonal.

- unitary linear maps: linear map $U : V \to V$ with $\langle U(\mathbf{v}), U(\mathbf{w}) \rangle = \langle \mathbf{v}, \mathbf{w} \rangle$ *for all* $\mathbf{v}, \mathbf{w} \in V$.

$$\Leftrightarrow \qquad U^\dagger U = \mathrm{id}$$

$U_{ij} = \langle \boldsymbol{\epsilon}_i | U | \boldsymbol{\epsilon}_j \rangle$ is a unitary matrix (time evolution in QM: $U = e^{-iHt}$)

Dirac notation

The map $\imath : V \to V^*$ defined by $\imath(\mathbf{v})(\mathbf{w}) := \langle \mathbf{v}, \mathbf{w} \rangle$ is bijective, so vectors and dual vectors can be identified. Dirac notation makes this manifest:

$$\imath(\mathbf{v}) \to \langle \mathbf{v}| \qquad \mathbf{w} \to |\mathbf{w}\rangle \qquad \imath(\mathbf{v})(\mathbf{w}) = \langle \mathbf{v}, \mathbf{w} \rangle = \langle \mathbf{v}|\mathbf{w}\rangle$$

bra ket bra-c-ket

matrix elements: $T_{ij} = \langle \epsilon_i | T | \epsilon_j \rangle = \langle \epsilon_i, T(\epsilon_j) \rangle$

operators in terms of ortho-normal basis: $T = \sum_{k,l=1}^{n} T_{kl} |\epsilon_k\rangle\langle\epsilon_l|$

identity in terms of ortho-normal basis: $\mathrm{id} = \sum_{i=1}^{n} |\epsilon_i\rangle\langle\epsilon_i|$

components of a vector: $|\mathbf{v}\rangle = \sum_{i=1}^{n} |\epsilon_i\rangle\langle\epsilon_i|\mathbf{v}\rangle$

scalar product: $\langle \mathbf{v}|\mathbf{w}\rangle = \sum_{i=1}^{n} \langle \mathbf{v}|\epsilon_i\rangle\langle\epsilon_i|\mathbf{w}\rangle \, , \qquad \| \, |\mathbf{v}\rangle \, \|^2 = \langle \mathbf{v}|\mathbf{v}\rangle = \sum_{i=1}^{n} \langle \mathbf{v}|\epsilon_i\rangle\langle\epsilon_i|\mathbf{v}\rangle$

In Hilbert space with ortho-normal basis finite-dimensional expressions generalise to infinite dimensions.

Examples of inner product vector spaces

- $\mathbb{R}^n$ or $\mathbb{C}^n$ with standard scalar product $\langle \mathbf{v}, \mathbf{w} \rangle := \sum_{i=1}^{n} v_i^* w_i$
- function vector spaces, e.g. $\mathcal{C}[a,b]$ with $\langle f, g \rangle := \int_a^b dx\, f(x)^* g(x)$. Interesting operators:

- multiplication with function, $M_p(f)(x) := p(x) f(x)$: $M_p^\dagger = M_{p^*}$ since

$$\langle f, M_p(g) \rangle = \int_a^b dx\, f(x)^* (p(x) g(x)) = \int_a^b (p(x)^* f(x))^* g(x) = \langle M_{p^*}(f), g \rangle$$

- multiplication with phase $e^{iu(x)}$ is unitary since

$$M_p \circ M_q = M_{pq}\,, \qquad M_1 = \mathrm{id} \qquad\qquad M_{e^{iu}}^\dagger \circ M_{e^{iu}} = M_{e^{-iu}} \circ M_{e^{iu}} = M_1 = \mathrm{id}$$

- translation operator $T_a(f)(x) := f(x-a)$. Its adjoint is $T_a^\dagger = T_{-a}$ since

$$\langle f, T_a(g) \rangle = \int_{-\infty}^{\infty} dx\, f(x)^* g(x-a) \overbrace{=}^{y=x-a} \int_{-\infty}^{\infty} dy\, f(y+a)^* g(y) = \langle T_{-a}(f), g \rangle$$

- the translation operator is unitary, since $T_a^\dagger \circ T_a = T_{-a} \circ T_a = \mathrm{id}$

- the differential operator $D = d/dx$ has adjoint $\left(\frac{d}{dx}\right)^\dagger = -\frac{d}{dx}$, $\left(\pm i \frac{d}{dx}\right)^\dagger = \pm i \frac{d}{dx}$ since

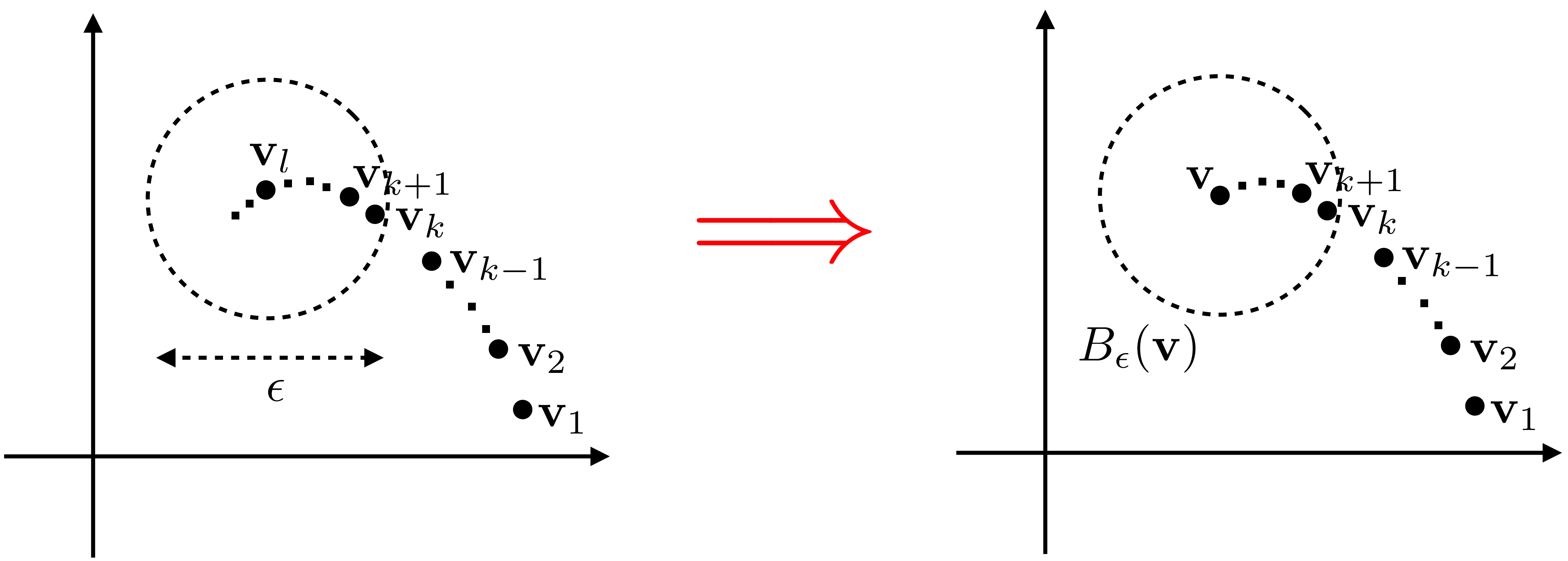
$$\langle f, D(g) \rangle = \int_{-\infty}^{\infty} dx\, f(x)^* g'(x) = \underbrace{[f(x)^* g(x)]_{-\infty}^{\infty}}_{=0} - \int_{-\infty}^{\infty} dx\, f'(x)^* g(x) = \langle -D(f), g \rangle$$

(assuming functions vanish at boundaries)

What is a Hilbert space?

Maths answer: An inner product vector space which is complete.
Physics answer: The arena for quantum mechanics.

Complete means that every Cauchy sequence converges.



$(\mathbf{v}_k)$ Cauchy sequence

$(\mathbf{v}_k)$ converges to $\mathbf{v}$

Hilbert space has an ortho-normal basis iff it is separable
-> previous formulae generalise . . .

Hilbert space which appear in practice are separable . . .

Examples of Hilbert spaces

- $\mathbb{R}^n$ and $\mathbb{C}^n$ with standard scalar product
  (the latter for finite-dimensional quantum systems)

- general construction: measure set (X, Σ, μ) -> $L^2(X)$

- $(\mathbb{N}, \Sigma_c, \mu_c)$ with counting measure μ_c -> ℓ^2 sequences $(x_i)_{i=1}^{\infty}$, $\left(\sum_{i=1}^{\infty} |x_i|^2\right)^{1/2}$ finite

  scalar product: $\langle (x_i), (y_i) \rangle = \sum_{i=1}^{\infty} \bar{x}_i y_i$

  (quantum mechanics in ``matrix mechanics" formulation)

- Lebesgue measure space $(U, \Sigma_L(U), \mu_L)$, $U \subset \mathbb{R}^n$ -> $L^2(U)$ = measurable functions $f : U \to \mathbb{R}$ with $\left(\int_U dx\, |f(x)|^2\right)^{1/2}$ finite.

  scalar product: $\langle f, g \rangle = \int_U dx\, f(x)^* g(x)$

  (quantum mechanics in ``wave function" formulation)

- Generalisation to include weight function $w : [a,b] \to \mathbb{R}^{>0}$ -> $L^2_w([a,b])$ = measurable function $f : [a,b] \to \mathbb{R}$ with $\left(\int_{[a,b]} dx\, w(x) |f(x)|^2\right)^{1/2}$ finite.

  scalar product: $\langle f, g \rangle := \int_{[a,b]} dx\, w(x) f(x)^* g(x)$

Fourier analysis

(a) Fourier series

Maths idea: find an ortho-normal basis for $L^2([a,b])$ based on sine and cosine

Physics idea: discrete frequency decomposition: coordinates=frequency strength

The Fourier series comes in four flavours:

- Cosine Fourier series on $L^2_{\mathbb{R}}([0,a])$:

basis: $\tilde{c}_0 = \frac{1}{\sqrt{a}}\,, \qquad \tilde{c}_k := \sqrt{\frac{2}{a}}\cos\left(\frac{k\pi x}{a}\right)\,, \quad k = 1,2,\dots\,.$

series: $f(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty} a_k \cos\left(\frac{k\pi x}{a}\right) \quad \text{where} \quad a_k = \frac{2}{a}\int_0^a dx\, \cos\left(\frac{k\pi x}{a}\right) f(x)$

Parseval's eqn.: $\frac{2}{a}\int_0^a dx\, |f(x)|^2 = \frac{|a_0|^2}{2} + \sum_{k=1}^{\infty} |a_k|^2$

- Sine Fourier series on $L^2_{\mathbb{R}}([0,a])$:

basis: $\tilde{s}_k = \sqrt{\frac{2}{a}}\sin\left(\frac{k\pi x}{a}\right)\,, \quad k = 1,2,\dots$

series: $f(x) = \sum_{k=1}^{\infty} b_k \sin\left(\frac{k\pi x}{a}\right) \quad \text{where} \quad b_k = \frac{2}{a}\int_0^a dx\, \sin\left(\frac{k\pi x}{a}\right) f(x)$

Parseval's eqn.: $\frac{2}{a}\int_0^a dx\, |f(x)|^2 = \sum_{k=1}^{\infty} |b_k|^2$

- Real standard Fourier series on $L^2_{\mathbb{R}}([-a,a])$:

basis: $c_0 := \frac{1}{\sqrt{2a}}\ , \quad c_k := \frac{1}{\sqrt{a}}\cos\left(\frac{k\pi x}{a}\right)\ , \quad s_k := \frac{1}{\sqrt{a}}\sin\left(\frac{k\pi x}{a}\right)\ , \quad k = 1, 2, \ldots\ ,$

series: $$f(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty}\left(a_k \cos\left(\frac{k\pi x}{a}\right) + b_k \sin\left(\frac{k\pi x}{a}\right)\right)$$

$$a_0 = \frac{1}{a}\int_{-a}^{a} dx\, f(x)\ , \quad a_k = \frac{1}{a}\int_{-a}^{a} dx\, \cos\left(\frac{k\pi x}{a}\right) f(x)\ , \quad b_k = \frac{1}{a}\int_{-a}^{a} dx\, \sin\left(\frac{k\pi x}{a}\right) f(x)$$

Parseval's eqn.: $$\frac{1}{a}\int_{-a}^{a} dx\, |f(x)|^2 = \frac{|a_0|^2}{2} + \sum_{k=1}^{\infty}(|a_k|^2 + |b_k|^2)$$

- Complex standard Fourier series on $L^2_{\mathbb{C}}([-a,a])$:

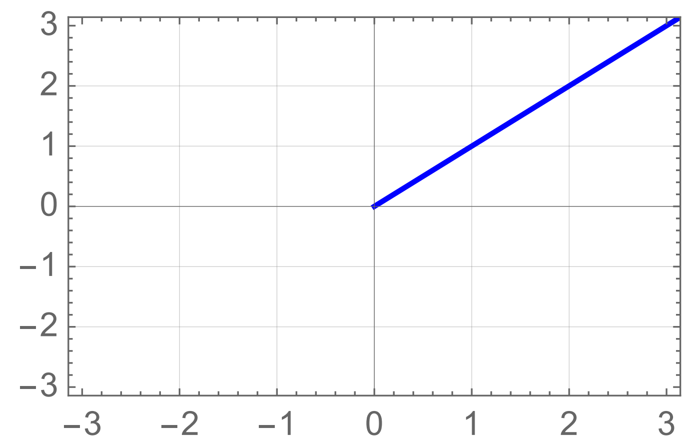
basis: $e_k := \frac{1}{\sqrt{2a}}\exp\left(\frac{ik\pi x}{a}\right)\ , \quad k \in \mathbb{Z}$

series: $$f(x) = \sum_{k\in\mathbb{Z}} a_k \exp\left(\frac{ik\pi x}{a}\right) \quad \text{where} \quad a_k = \frac{1}{2a}\int_{-a}^{a} dx\, \exp\left(\frac{-ik\pi x}{a}\right) f(x)$$

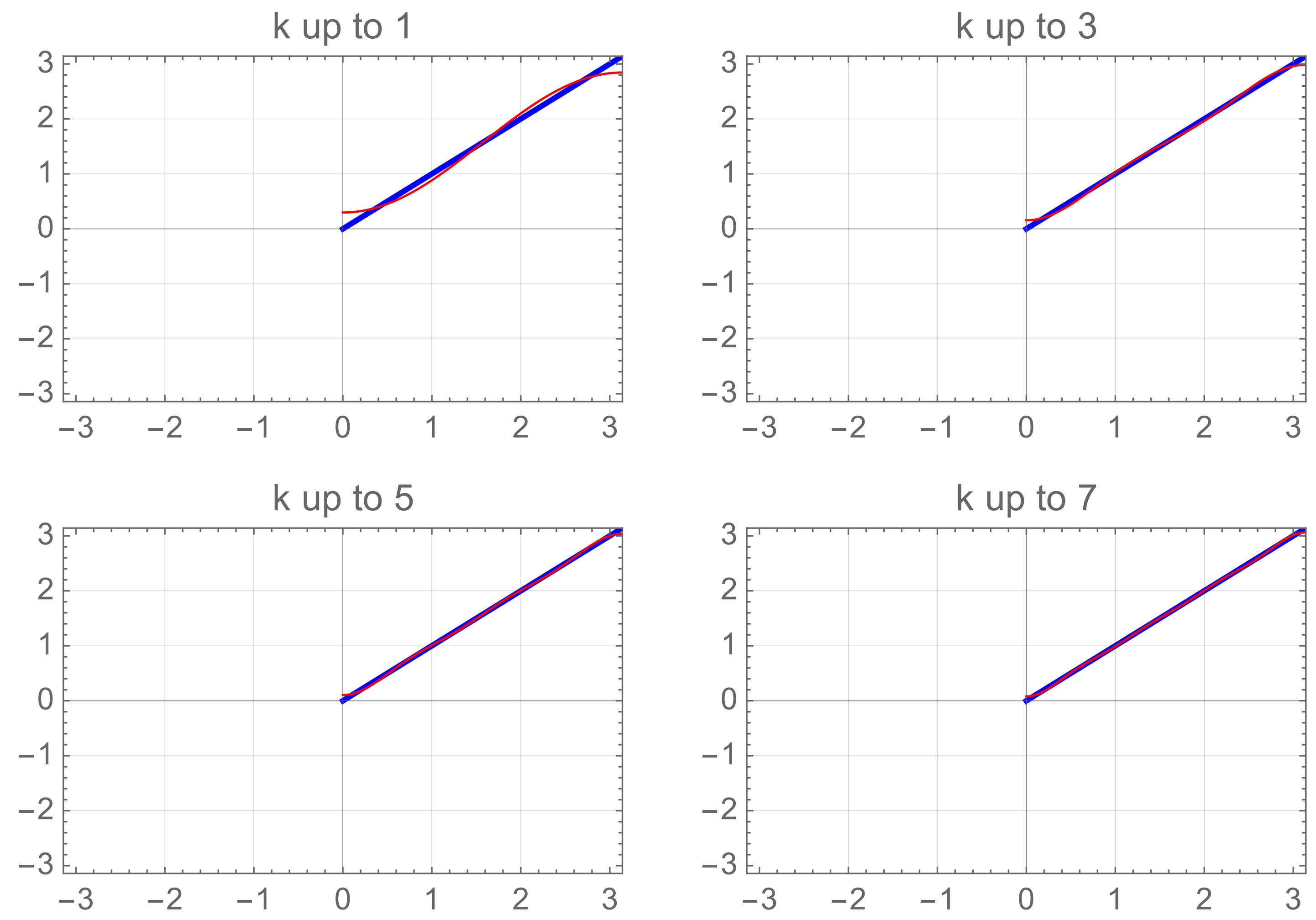
Parseval's eqn.: $$\frac{1}{2a}\int_{-a}^{a} dx\, |f(x)|^2 = \sum_{k\in\mathbb{Z}} |a_k|^2$$

Fourier series example

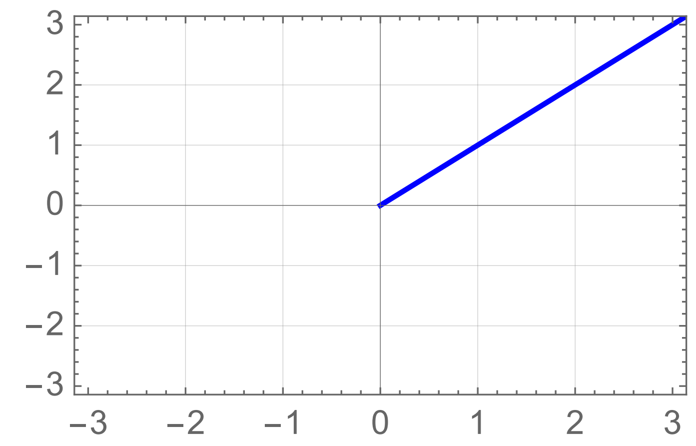
- **Cosine series:** $f(x) = x\ , \quad x \in [0, \pi]$



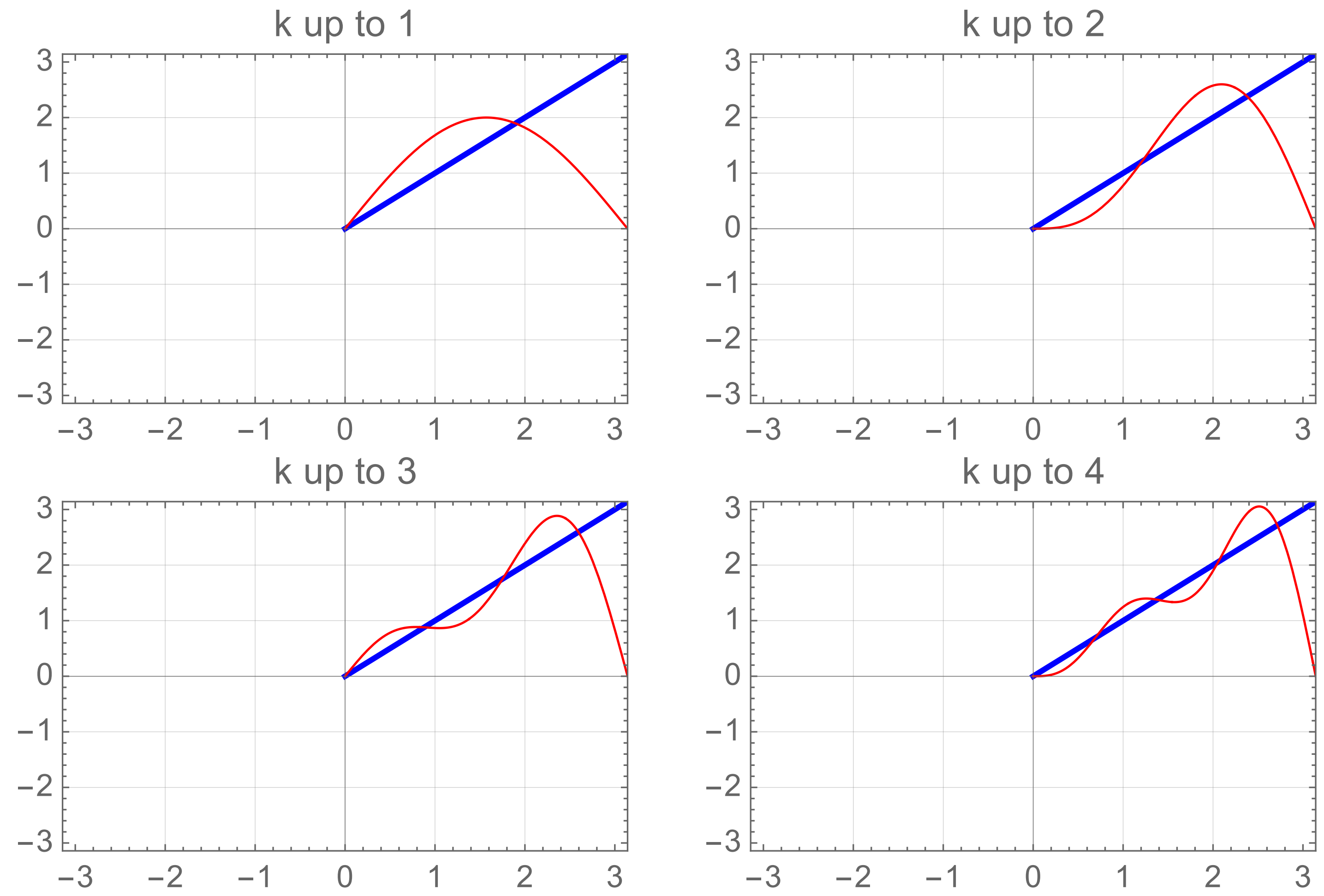
$$f(x) = \frac{\pi}{2} - \frac{4}{\pi} \sum_{k=1,3,5,\ldots} \frac{\cos(kx)}{k^2}$$



- **Sine series:** $f(x) = x \;, \quad x \in [0, \pi]$



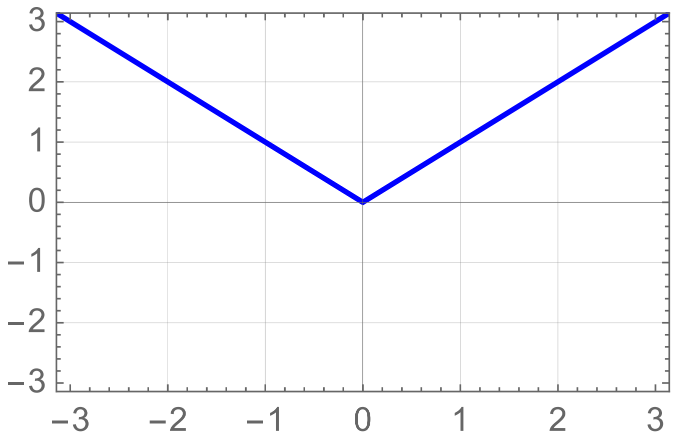
$$f(x) = 2 \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k} \sin(kx)$$



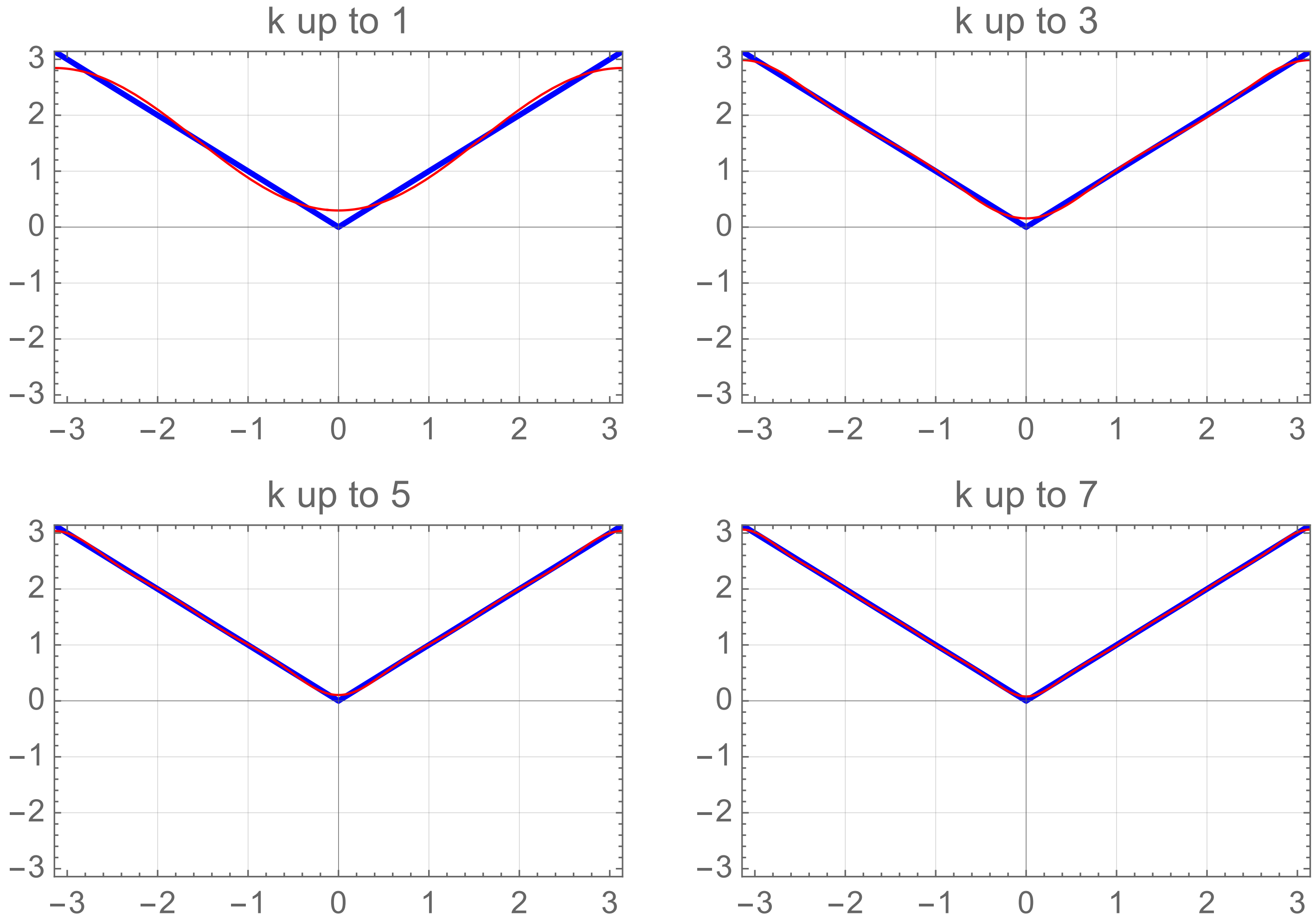
- Real standard Fourier series:

$$f(x) = |x| \, , \quad x \in [-\pi, \pi]$$

(even extension)



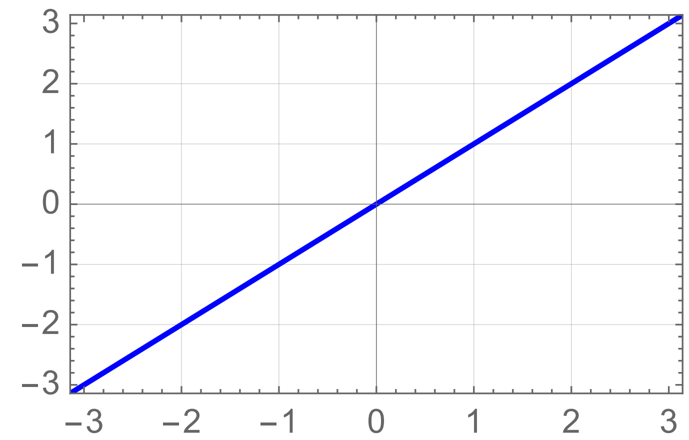
$$f(x) = \frac{\pi}{2} - \frac{4}{\pi} \sum_{k=1,3,5,\ldots} \frac{\cos(kx)}{k^2}$$

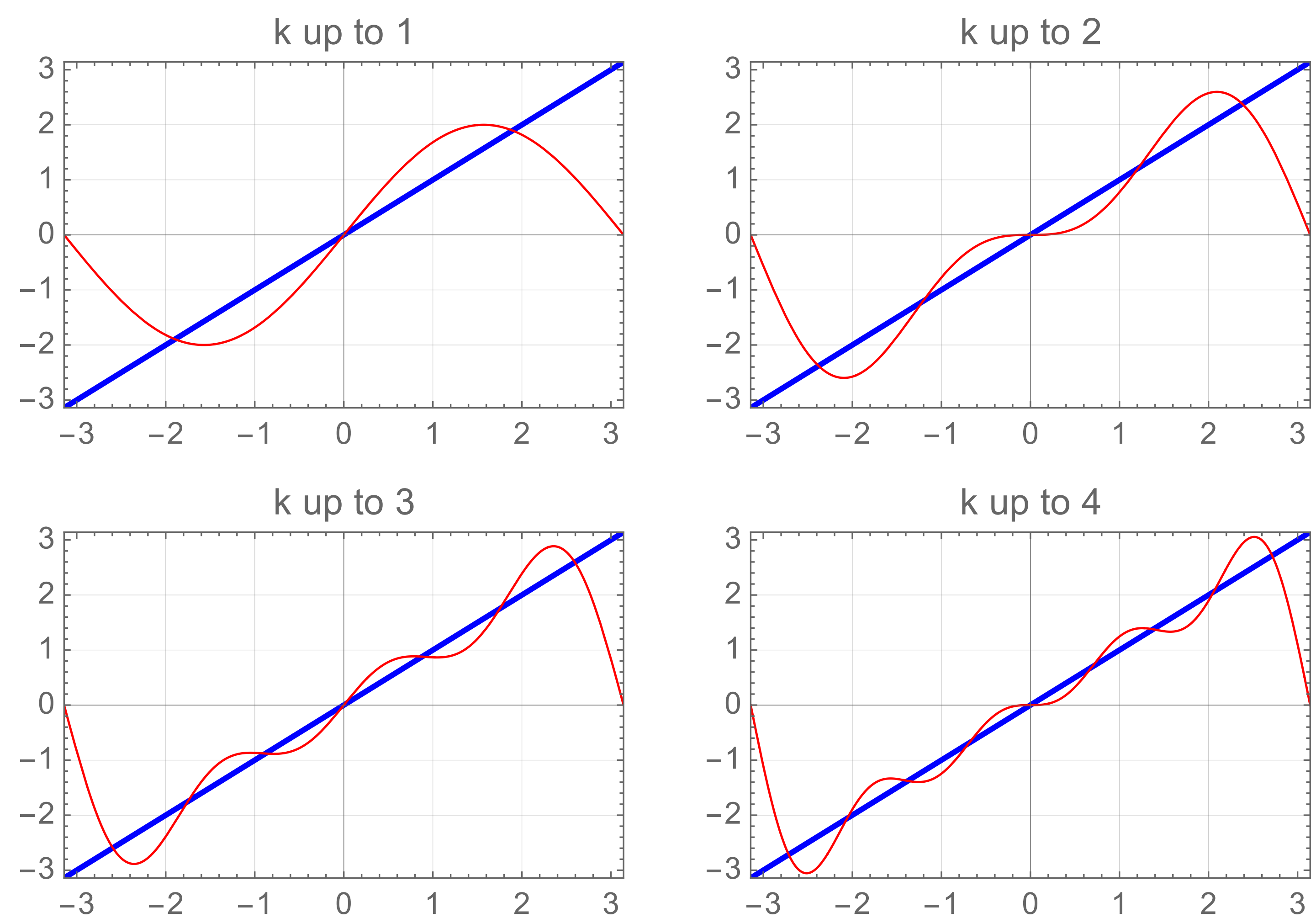


• Real standard Fourier series

$$f(x) = x \ , \qquad x \in [-\pi, \pi]$$

(odd extension)





$$f(x) = 2\sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k} \sin(kx)$$

complex Fourier series

$$\frac{1}{2i}(e^{ikx} - e^{-ikx})$$

Parseval: $\displaystyle \frac{2\pi^2}{3} = \frac{1}{\pi}\int_{-\pi}^{\pi} dx\, x^2 = \sum_{k=1}^{\infty} |b_k|^2 = 4\sum_{k=1}^{\infty} \frac{1}{k^2}$

(b) Fourier transform

Maths idea: Fourier transform is a unitary map $\mathcal{T} : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$

Physics idea: frequency analysis, in QM: relation between wave fct. in position and momentum space

- Definition of Fourier transform

$$\boxed{\begin{aligned} \hat{f}(\mathbf{k}) = \mathcal{F}(f)(\mathbf{k}) &:= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} d^n x \; \exp(-i\mathbf{x}\cdot\mathbf{k}) f(\mathbf{x}) \\ \tilde{\mathcal{F}}(\hat{f})(\mathbf{x}) &:= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} dk^n \; \hat{f}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} \qquad \text{(inverse FT)} \end{aligned}} \Longrightarrow \quad \tilde{\mathcal{F}} \circ \mathcal{F}(f) = \mathcal{F} \circ \tilde{\mathcal{F}}(f) = f$$

- Interpretation

$$f(x) = \frac{1}{\sqrt{2\pi}} \exp(ik_0 x) \quad \Rightarrow \quad \hat{f}(k) = \frac{1}{2\pi} \int_{\mathbb{R}} dx \exp(i(k_0 - k)x) = \delta(k - k_0)$$

plain wave with wave number k_0 -> FT has sharp peak at k_0

$$f(x) = \frac{1}{\sqrt{2\pi}} \sum_i \exp(ik_i x) \quad \Rightarrow \quad \hat{f}(k) = \sum_i \delta(k - k_i)$$

superposition with wave numbers k_i -> FT has sharp peaks at k_i

$$f_a(\mathbf{x}) = e^{-\frac{|\mathbf{x}|^2}{2a^2}} \quad \Rightarrow \quad \widehat{f}_a(\mathbf{k}) = a^n e^{-a^2|\mathbf{k}|^2/2}$$

Gaussian with width a -> Gaussian with width 1/a

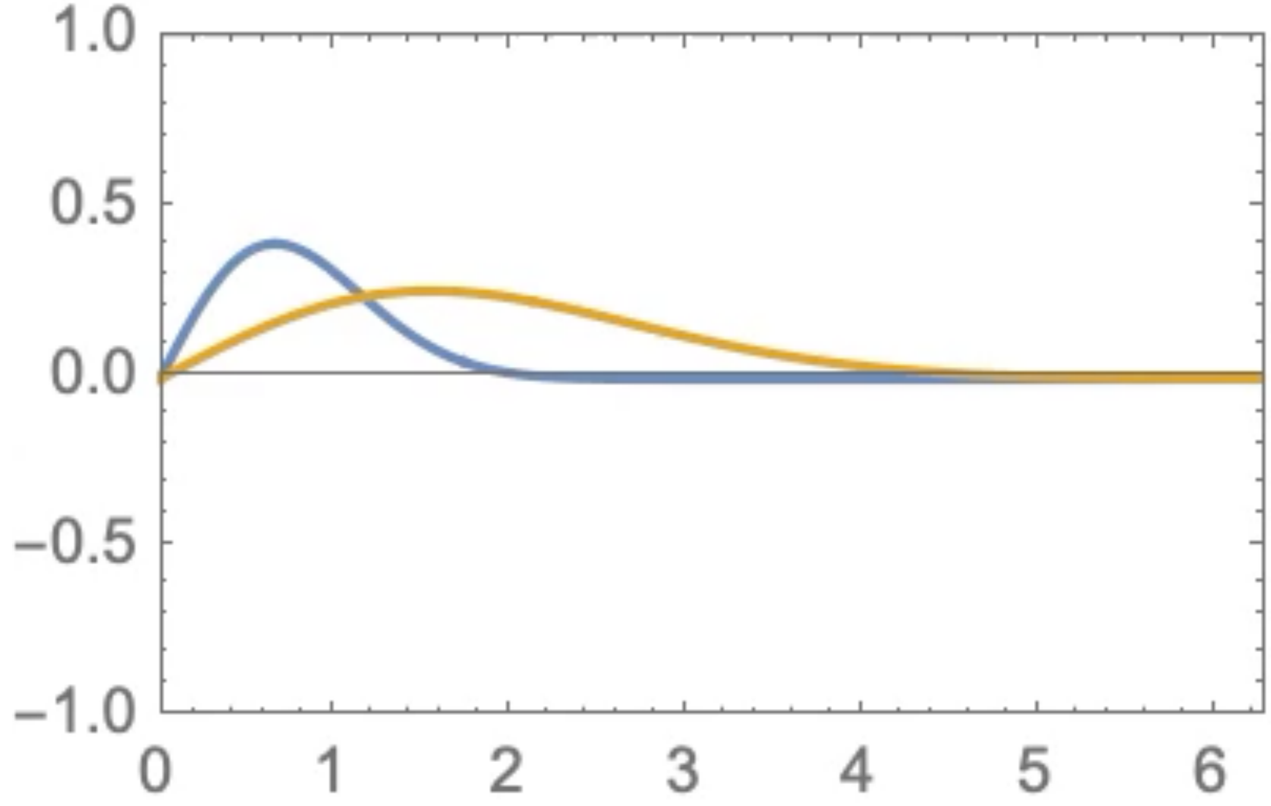
$$\Delta x \sim a\,, \quad \Delta k \sim 1/a \quad \Rightarrow \quad \Delta x\, \Delta k \sim 1$$

uncertainty relation

$$f(x) = e^{-x^2} \sin(k_0 x)$$ (blue)

$$|\mathcal{F}(f)(x)|$$ (yellow)

$k_0 \in [1, 5]$



- How does FT intertwine with other linear operators?

translation	modulation	dilatation	multiplication
$T_{\mathbf{a}}(f)(\mathbf{x}) := f(\mathbf{x}-\mathbf{a})$,	$E_{\mathbf{b}}(f)(\mathbf{x}) := \exp(i\mathbf{b}\cdot\mathbf{x})f(\mathbf{x})$,	$\mathcal{D}_\lambda(f)(\mathbf{x}) := f(\lambda\mathbf{x})$,	$M_g(f)(\mathbf{x}) := g(\mathbf{x})f(\mathbf{x})$

$\mathcal{F}\circ T_{\mathbf{a}} = E_{-\mathbf{a}}\circ\mathcal{F}$ $\qquad$ $\mathcal{F}\circ E_{\mathbf{b}} = T_{\mathbf{b}}\circ\mathcal{F}$ $\qquad$ ``exchanges translation and modulation"

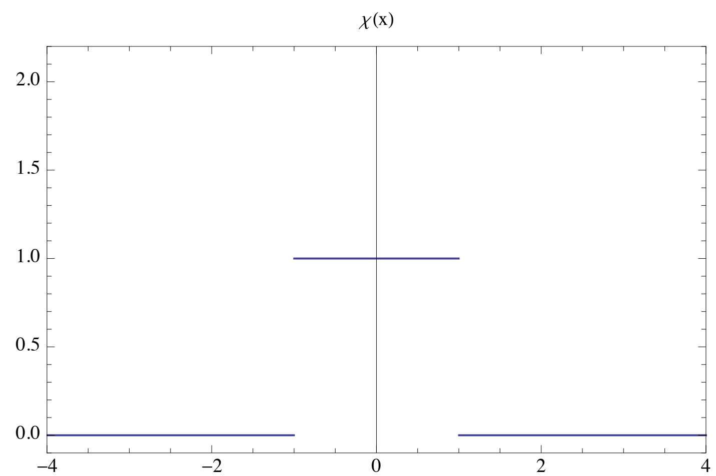
$\mathcal{F}\circ\mathcal{D}_\lambda = \frac{1}{|\lambda|^n}\mathcal{D}_{1/\lambda}\circ\mathcal{F}$ $\qquad$ ``dilation with λ to dilation with $1/\lambda$"

$\mathcal{F}\circ D_{x_j} = M_{ik_j}\circ\mathcal{F}$ $\qquad$ $\mathcal{F}\circ M_{x_j} = iD_{k_j}\circ\mathcal{F}$. $\qquad$ ``exchanges differentiation and multiplication"

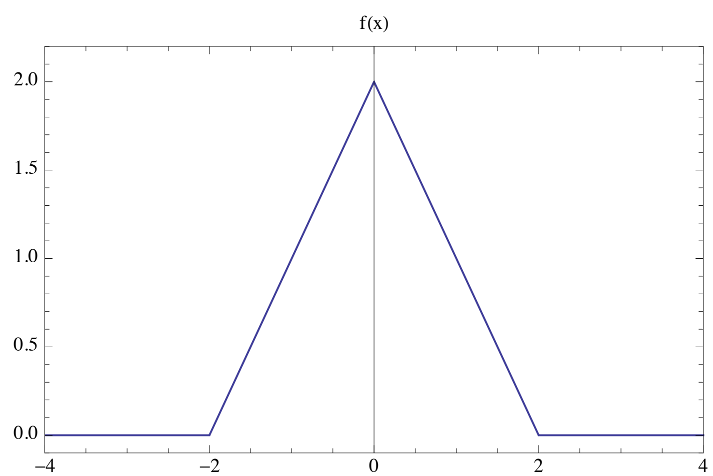
- Convolution

$$(f\star g)(\mathbf{x}) := \int_{\mathbb{R}^n} dy^n\, f(\mathbf{y})g(\mathbf{x}-\mathbf{y}) \qquad \Rightarrow \qquad \widehat{f\star g} = (2\pi)^{n/2}\hat{f}\,\hat{g}$$

Example:



$\xrightarrow{\chi\star\chi}$



$$\hat{\chi}(k) = \frac{1}{\sqrt{2\pi}}\int_{-1}^{1} dx\, e^{-ikx} = \sqrt{\frac{2}{\pi}}\frac{\sin k}{k} \qquad \hat{f}(k) = \widehat{\chi\star\chi}(k) = \sqrt{2\pi}\,\hat{\chi}^2(k) = 2\sqrt{\frac{2}{\pi}}\frac{\sin^2 k}{k^2}$$

Orthogonal polynomials

Setting: $L^2_w([a,b])$ with scalar product $\langle f, g\rangle = \int_a^b dx\, w(x) f(x) g(x)$

Q: Can we find an ortho-normal basis of polynomials on this space?

$$(P_n)_{n=0}^{\infty} \qquad P_n \text{ is of degree } n \qquad \langle P_n, P_m\rangle = h_n\, \delta_{nm}$$

If we can find such a basis then every $f \in L^2_w([a,b])$ can be expanded as

$$f(x) = \sum_{n=0}^{\infty} a_n \hat{P}_n(x)\ , \qquad a_n = \int_a^b dx\, w(x) \hat{P}_n(x) f(x) \qquad \hat{P}_n := \frac{1}{\| P_n \|} P_n = \frac{1}{\sqrt{h_n}} P_n$$

We can indeed find such polynomial bases and thinking about the different types of intervals and different weight functions leads to a classification.

(An elementary method to obtain the orthogonal polynomials is to apply the Gram-Schmidt procedure to the monomials $(1, x, x^2, x^3, \cdots)$.)

Types of orthogonal polynomials

$[a,b]$	$\alpha,\ \beta$	X	$w(x)$	name	symbol
$[-1,1]$	$\alpha>-1,\ \beta>-1$	x^2-1	$(1-x)^\alpha(x+1)^\beta$	Jacobi	$P_n^{(\alpha,\beta)}$
$[-1,1]$	$\alpha=\beta>-1$	x^2-1	$(1-x)^\alpha(x+1)^\alpha$	Gegenbauer	$P_n^{(\alpha,\alpha)}$
$[-1,1]$	$\alpha=\beta=\pm\frac{1}{2}$	x^2-1	$(1-x)^{\pm 1/2}(x+1)^{\pm 1/2}$	Chebyshev	$T_n^{(\pm)}$
$[-1,1]$	$\alpha=\beta=0$	x^2-1	1	Legendre	P_n
$[0,\infty]$	$\alpha>-1$	x	$e^{-x}x^\alpha$	Laguerre	$L_n^{(\alpha)}$
$[0,\infty]$	$\alpha=0$	x	e^{-x}	Laguerre	L_n
$[-\infty,\infty]$		1	e^{-x^2}	Hermite	H_n

Rodriguez formula:

$$P_n(x)=\frac{1}{K_n w(x)}\frac{d^n}{dx^n}\left(w(x)X^n\right)\ ,\qquad X=\begin{cases}(b-x)(a-x) & \mathit{for}\quad |a|,|b|<\infty\\ x-a & \mathit{for}\quad |a|<\infty\,,\ b=\infty\\ 1 & \mathit{for}\quad -a=b=\infty\end{cases}$$

$$w(x)=\begin{cases}(b-x)^\alpha(x-a)^\beta & \mathit{for}\quad |a|,|b|<\infty\\ e^{-x}(x-a)^\alpha & \mathit{for}\quad |a|<\infty\,,\ b=\infty\\ e^{-x^2} & \mathit{for}\quad -a=b=\infty\end{cases}$$

All these different types of orthogonal polynomials have common features:

Recursion formula: $P_{n+1}(x) = (A_n x + B_n)P_n(x) - C_n P_{n-1}(x)$

Differential equation: $Xy'' + K_1 P_1 y' - n\left(k_1 K_1 + \frac{n-1}{2}X''\right)y = 0$

Generating function: $G(x,z) = \sum_{n=0}^{\infty} P_n(x) z^n$

Where do they appear in physics?

- Legendre: problem with an angle θ so that $\cos(\theta) \in [-1,1]$,
  problems with spherical coordinates (r,θ,ϕ),
  Laplacian on sphere, spherical harmonics,
  E&M: multipole expansion, QM: angular part of H wave function.

- Laguerre: typically function of a radial coordinate $r \in [0,\infty]$,
  QM: radial part of H wave function.

- Hermite: depend on coordinate $x \in [-\infty,\infty]$,
  QM: essentially wave function of quantum harmonic oscillator.

(a) Legendre polynomials

- Orthogonal polynomials P_n on $L^2([-1,1])$
- Rodriguez formula: $P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n$
- First few: $P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = \frac{1}{2}(3x^2-1), \quad P_3(x) = \frac{1}{2}(5x^3-3x), \quad P_4(x) = \frac{1}{8}(35x^4-30x^2+3)$.
- Expansion: $f(x) = \sum_{n=0}^{\infty} a_n P_n(x)$, $\qquad a_n = \frac{2n+1}{2}\int_{-1}^{1} dx\, P_n(x) f(x)$
- Recursion formula: $(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x)$
- Differential equation: $(1-x^2)y'' - 2xy' + n(n+1)y = 0$
- Generating function: $G(x,z) = \frac{1}{\sqrt{1-2xz+z^2}} = \sum_{n=0}^{\infty} P_n(x) z^n$

Application: Multipole expansion of Coulomb term

$$V(\mathbf{r},\mathbf{r}') = \frac{1}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{r}\frac{1}{\sqrt{1-2\left(\frac{r'}{r}\right)\cos\theta + \left(\frac{r'}{r}\right)^2}} = \frac{1}{r}G(x,z) = \frac{1}{r}\sum_{n=0}^{\infty} P_n(\cos\theta)\left(\frac{r'}{r}\right)^n$$

(a) Hermite polynomials

- Orthogonal polynomials H_n on $L^2_w(\mathbb{R})$, where $w(x) = e^{-x^2}$
- Rodriguez formula: $H_n(x) = (-1)^n e^{x^2} \dfrac{d^n}{dx^n} e^{-x^2}$
- First few: $H_0(x) = 1\ ,\quad H_1(x) = 2x\ ,\quad H_2(x) = 4x^2 - 2\ ,\quad H_3(x) = 8x^3 - 12x$
- Recursion relation: $H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$
- Differential equation: $y'' - 2xy' + 2ny = 0$
- Generating function: $G(x,z) = \exp\left(2xz - z^2\right) = \displaystyle\sum_{n=0}^{\infty} H_n(x) \frac{z^n}{n!}$

Application: Quantum harmonic oscillator

$$H\Psi = E\Psi \qquad\qquad H = -\frac{\hbar^2}{2m}\frac{d^2}{d\xi^2} + \frac{1}{2}m\omega^2\xi^2$$

define $x = \sqrt{\frac{m\omega}{\hbar}}\xi\ ,\ \ \epsilon = \frac{E}{\hbar\omega}$

$$\mathcal{H}\psi = \epsilon\psi \qquad\qquad \mathcal{H} = \frac{1}{2}\left(-\frac{d^2}{dx^2} + x^2\right)$$

(i) wave function treatment

if = 2n -> Hermite diff. eq.

$$\psi(x) = y(x)e^{-x^2/2} \xrightarrow{\text{into Schroedinger eq.}} y'' - 2xy' + (2\epsilon - 1)y = 0$$

$$\psi_n(x) = H_n(x)e^{-x^2/2}/A_n \qquad \epsilon_n = n + \frac{1}{2} \qquad E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

(ii) operator treatment

define $a = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right)$, $a^\dagger = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right)$ and $N = a^\dagger a$

$$\Rightarrow \qquad \mathcal{H} = N + \tfrac{1}{2} \qquad [a, a^\dagger] = 1 \qquad [N, a^\dagger] = a^\dagger \qquad [N, a] = -a$$

define ground state $|0\rangle$ by $a|0\rangle = 0$, and state $|n\rangle$ by $|n\rangle = \frac{1}{\sqrt{n}}a^\dagger|n-1\rangle$

$$\Rightarrow \qquad N|n\rangle = n|n\rangle \qquad \mathcal{H}|n\rangle = \left(n + \frac{1}{2}\right)|n\rangle$$

(iii) relation between (i) and (ii)

$$\psi_n(x) = \langle x|n\rangle$$

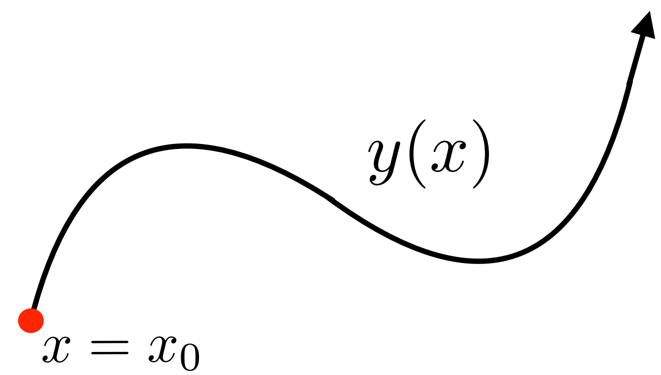
Ordinary linear differential equations

The problem

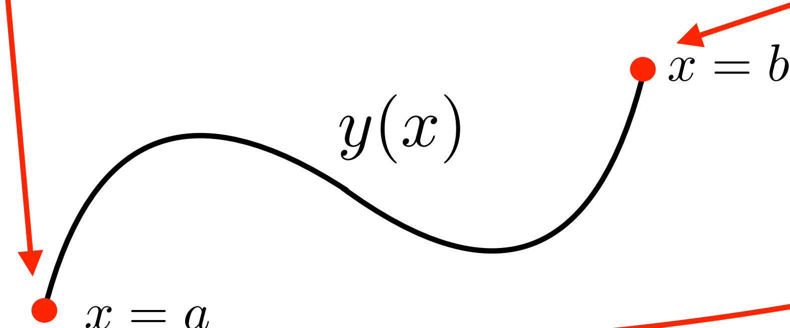
Solve ordinary, second order homogeneous or inhomogeneous diff. eqs.:

$$\left.\begin{array}{rcl} \alpha_2(x)y'' + \alpha_1(x)y' + \alpha_0(x)y & = & f(x) \\ \alpha_2(x)y'' + \alpha_1(x)y' + \alpha_0(x)y & = & 0 \end{array}\right\} \quad \text{or} \quad \left.\begin{array}{rcl} Ty & = & f \\ Ty & = & 0 \end{array}\right\} \qquad T = \alpha_2 D^2 + \alpha_1 D + \alpha_0$$

Initial conditions: $\boxed{\begin{array}{l} y(x_0) = y_0 \\ y'(x_0) = y'_0 \end{array}}$



boundary conditions: $\overset{\text{Dirichlet}}{\boxed{d_a y(a)}} + \overset{\text{von Neumann}}{\boxed{n_a y'(a)}} = c_a\,, \qquad \overset{\text{Dirichlet}}{\boxed{d_b y(b)}} + \overset{\text{von Neumann}}{\boxed{n_b y'(b)}} = c_b$



focus

Solutions and how to find them

- structure of solution space

$$V_I = y_0 + V_H$$

2d space of inhom. solutions

particular inhom. solution

2d vector space of hom. solutions

Two solutions $y_1, y_2 \in V_H$ form a basis of V_H iff the Wronski determinant

$$W := \det \begin{pmatrix} y_1 & y_2 \\ y_1' & y_2' \end{pmatrix} (x) = (y_1 y_2' - y_2 y_1')(x)$$

is non-zero.

Example: $y'' + y = 0 \quad \rightarrow \quad y_1(x) = \sin(x)\ , \quad y_2(x) = \cos(x)$

$$W = -\sin^2(x) - \cos^2(x) = -1 \quad \Rightarrow \quad (y_1, y_2) \text{ basis of } V_H$$

- How to get an inhom. solution y from a basis (y_1, y_2) of V_H :

$$y(x) = \int_{x_0}^{x} dt\, G(x,t) f(t) \qquad G(x,t) = \frac{y_1(t)y_2(x) - y_1(x)y_2(t)}{\alpha_2(t)W(t)}$$

Green function

Example: $Ty = f \;, \qquad T = \frac{d^2}{dx^2} + 1$

$$\Rightarrow \; V_H = \mathrm{Span}(y_1 = \sin \;\; y_2 = \cos) \;, \quad W = -1 \;, \quad \alpha_2 = 1$$

$$\Rightarrow \; G(x,t) = \sin(x - t)$$

$$y_0(x) = \int_{x_0}^{x} dt\, G(x,t) f(t) = \int_{x_0}^{x} dt\, \sin(x-t) f(t)$$

$$V_I = y_0 + V_H$$

- How to find a solution to the hom. eqs. (if you already have one)

Suppose y is a solution, $Ty = 0$. Then, another solution $\tilde{y}$ can be obtained by

$$\tilde{y}(x) = y(x)u(x) \ , \qquad u'(x) = \frac{1}{y(x)^2} \exp\left(- \int_{x_0}^{x} dt \, \frac{\alpha_1(t)}{\alpha_2(t)} \right)$$

Example: The other solution to the (n=1) Legendre diff. eqn.

$$(1-x^2)y'' - 2xy' + 2y = 0 \quad \text{solved by} \quad y(x) = P_1(x) = x$$

$$\alpha_1(x) = -2x \qquad \alpha_2(x) = 1 - x^2$$

$$\Rightarrow \quad u'(x) = \frac{1}{x^2} \exp\left(\int^{x} dt \, \frac{2t}{1-t^2} \right) = \frac{1}{x^2(1-x^2)}$$

$$\Rightarrow \quad u(x) = -\frac{1}{x} + \frac{1}{2} \ln \frac{1+x}{1-x}$$

$$\Rightarrow \quad \tilde{y}(x) = x u(x) = \frac{x}{2} \ln \frac{1+x}{1-x} - 1$$

- How to find a solution to the hom. eqs. in the first place

Power series Ansatz: $y(x) = \sum_{k=0}^{\infty} a_k x^k$

Insert and determine recursion formula for coefficients a_k

Works well if $\alpha_2,\ \alpha_1,\ \alpha_0$ are polynomial . . .

Example: Legendre differential equation

$$(1-x^2)y'' - 2xy' + n(n+1)y = 0$$

$$\Rightarrow \quad \sum_{k=0}^{\infty} \left[(k+2)(k+1)a_{k+2} - (k(k+1) - n(n+1))a_k\right] x^k = 0$$

$$\Rightarrow \quad a_{k+2} = \frac{k(k+1) - n(n+1)}{(k+1)(k+2)} a_k \ , \qquad k = 0, 1, \ldots$$

- How to satisfy the boundary conditions

  - Find all hom. solutions, V_H
  - Find all solutions in V_H which satisfy the right boundary conditions
  - Construct inhom. solution which satisfies the right boundary conditions ← ???

- How to find a solution to inhom. eqs. which satisfies boundary conditions

E.g. Dirichlet: $\alpha_2(x)y'' + \alpha_1(x)y' + \alpha_0(x)y = f(x)\ , \qquad y(a) = 0\ , \qquad y(b) = 0$

$$y(x) = \int_a^b dt\, G(x,t) f(t) \qquad G(x,t) = \frac{y_1(t)y_2(x)\theta(x-t) + y_1(x)y_2(t)\theta(t-x)}{\alpha_2(t)W(t)}$$

(where $y_1(a) = y_2(b) = 0$)

Example: $Ty = f\ , \qquad T = \frac{d^2}{dx^2} + 1 \qquad y(0) \ = \ y(\pi/2) \ = \ 0$

$$y_1 = \sin,\ y_2 = \cos,\ W = -1,\ \alpha_2 = 1$$

$$\Rightarrow \quad G(x,t) = -\sin(t)\cos(x)\,\theta(x-t) - \sin(x)\cos(t)\,\theta(t-x)$$

$$\Rightarrow \quad y(x) = \int_0^{\pi/2} dt\, G(x,t) f(t)$$

Sturm Liouville operators

Every $T = \alpha_2(x)\frac{d^2}{dx^2} + \alpha_1(x)\frac{d}{dx} + \alpha_0(x)$ can be re-written in SL form

$$T_{\rm SL} = \frac{1}{w(x)}\left[\frac{d}{dx}\left(p(x)\frac{d}{dx}\right) + q(x)\right]$$

where $p(x) = \exp\left(\int_{x_0}^{x} dt\, \frac{\alpha_1(t)}{\alpha_2(t)}\right)$, $\quad w(x) = \frac{p(x)}{\alpha_2(x)}$, $\quad q(x) = \alpha_0(x)w(x)$

Why is this interesting?

A: $T_{\rm SL}$ is a hermitian operator for the scalar product $\langle f, g\rangle = \int_a^b dx\, w(x)f(x)g(x)$
(if boundary terms can be made to vanish)

Consider Sturm-Liouville eigenvalue problem: $T_{\rm SL}y = \lambda y$

-> eigenfunctions are orthogonal w.r.t. above scalar product

Example: Hermite differential equation in SL form

$$T = \frac{d^2}{dx^2} - 2x\frac{d}{dx} \qquad \Rightarrow \qquad \alpha_2 = 1\,, \quad \alpha_1 = -2x\,, \quad \alpha_0 = 0$$

$$p = \exp\left(\int^x dx\,\frac{\alpha_1}{\alpha_2}\right) = \exp\left(-2\int^x dx\,x\right) = e^{-x^2} \qquad\qquad w = \frac{p}{\alpha_2} = e^{-x^2}$$

$$\Rightarrow \qquad T_{\mathrm{SL}} = \frac{1}{w}\frac{d}{dx}\left(p\frac{d}{dx}\right) = e^{x^2}\left(\frac{d}{dx}e^{-x^2}\frac{d}{dx}\right)$$

Orthogonal functions can be understood in terms of SL eigenvalue problem:

name	DEQ	p	q	w	$\mathcal{L}_{\mathrm{SL}}[a,b]$	bound. cond.	λ	y
sine Fourier	$y'' = \lambda y$	1	0	1	$\mathcal{L}_b([0,a])$	$y(0) = y(\pi) = 0$	$-\frac{\pi^2 k^2}{a^2}$	$\sin\left(\frac{k\pi x}{a}\right)$
cosine Fourier	$y'' = \lambda y$	1	0	1	$\mathcal{L}_b([0,a])$	$y'(0) = y'(\pi) = 0$	$-\frac{\pi^2 k^2}{a^2}$	$\cos\left(\frac{k\pi x}{a}\right)$
Fourier	$y'' = \lambda y$	1	0	1	$\mathcal{L}_p([-a,a])$	periodic	$-\frac{\pi^2 k^2}{a^2}$ $-\frac{\pi^2 k^2}{a^2}$	$\sin\left(\frac{k\pi x}{a}\right)$ $\cos\left(\frac{k\pi x}{a}\right)$
Legendre	$(1-x^2)y'' - 2xy' = \lambda y$	$1-x^2$	0	1	$\mathcal{L}([-1,1])$		$-n(n+1)$	P_n
Laguerre	$xy'' + (1-x)y' = \lambda y$	xe^{-x}	0	e^{-x}	$\mathcal{L}([0,\infty])$		$-n$	L_n
Hermite	$y'' - 2xy' = \lambda y$	e^{-x^2}	0	e^{-x^2}	$\mathcal{L}([-\infty,\infty])$		$-2n$	H_n
Bessel	$y'' + \frac{1}{x}y' - \frac{\nu^2}{x^2}y = \lambda y$	x	$-\frac{\nu^2}{x^2}$	x	$\mathcal{L}_b([0,a])$	$y(0) = y(a) = 0$	$-\frac{z^2_{\nu k}}{a^2}$	$\hat{J}_{\nu k}$

Partial linear differential equations

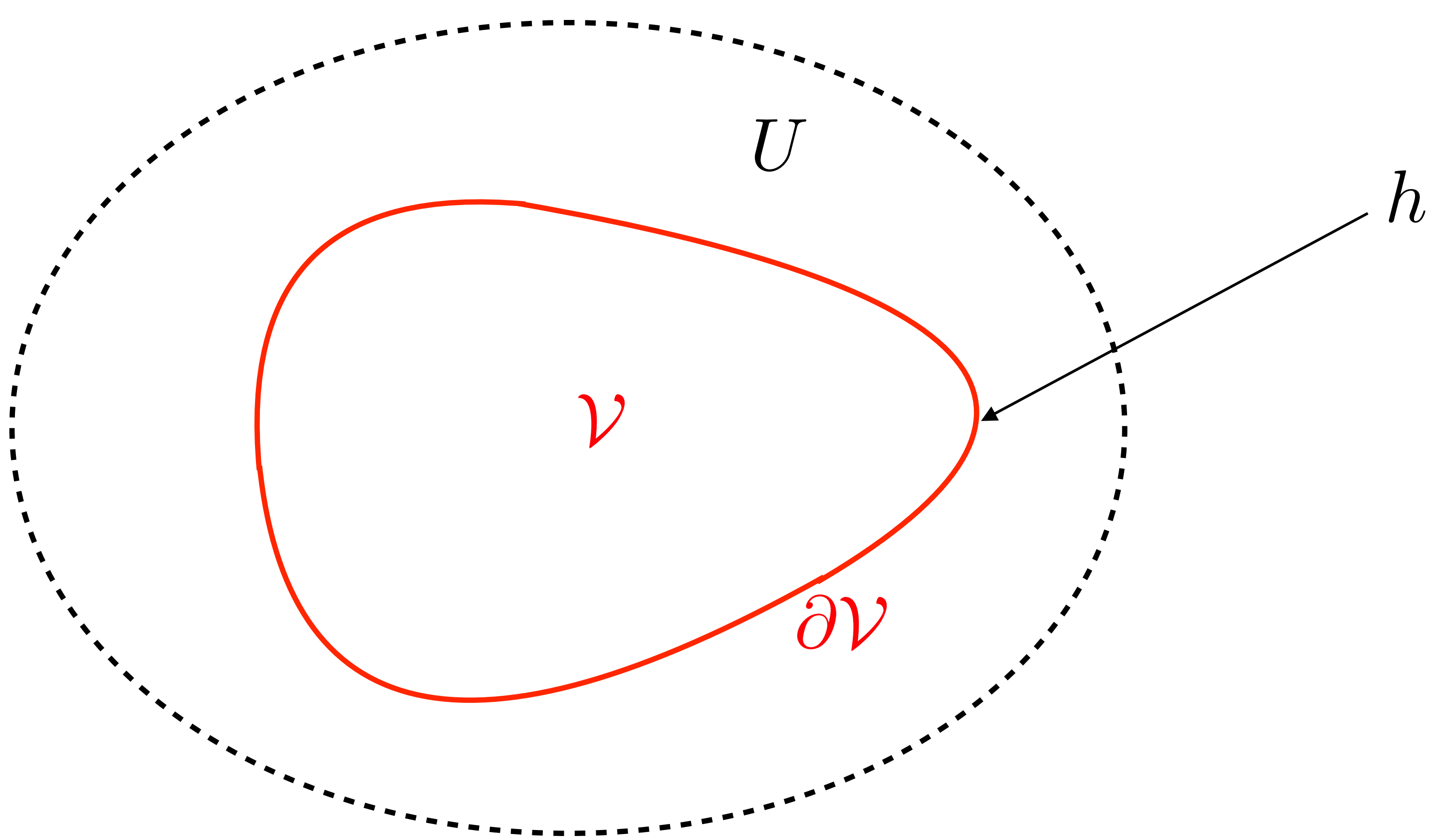
Laplace equation

- typical problem

On some region $\mathcal{V} \subset U \subset \mathbb{R}^n$ solve

$$\Delta\phi = 0 \quad \text{or} \quad \Delta\phi = \rho \qquad \text{(where } \Delta = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2} \text{)}$$

with boundary condition $\phi|_{\partial\mathcal{V}} = h$ (Dirichlet) or $\mathbf{n}\cdot\nabla\phi|_{\partial\mathcal{V}} = h$ (von Neumann)



- Laplacian in different coordinates

  - 2d Cartesian: $\Delta_2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ ⟵ rectangular boundary conditions

  - 2d complex: $\Delta_2 = 4\frac{\partial^2}{\partial z \partial \bar{z}}$ ⟵ "2d slices", use holomorphic fcts.

  - 2d polar: $\Delta_{2,\mathrm{pol}} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}$ ⟵ circle boundaries

  - 3d Cartesian: $\Delta_3 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ ⟵ rectangular boundary conditions

  - 3d cylindrical: $\Delta_3 = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2} + \frac{\partial^2}{\partial z^2} = \Delta_{2,\mathrm{pol}} + \frac{\partial^2}{\partial z^2}$ ⟵ cylindrical boundaries

  - on sphere: $\Delta_{S^2} = \frac{1}{\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \varphi^2}$

  - 3d spherical: $\Delta_{3,\mathrm{sph}} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \varphi^2}\right]$

$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\Delta_{S^2}$$ ⟵ spherical boundaries

$= -L^2$ -> quantum mechanics

- Green function of Laplacian (= Coulomb potential)

$$G(\mathbf{x}-\mathbf{a}) = G_{\mathbf{a}}(\mathbf{x}) = \begin{cases} -\frac{1}{(n-2)v_n}\frac{1}{|\mathbf{x}-\mathbf{a}|^{n-2}} & \text{for} \quad n>2 \\ \frac{1}{2\pi}\ln|\mathbf{x}-\mathbf{a}| & \text{for} \quad n=2 \end{cases} \qquad \Rightarrow \qquad \Delta G(\mathbf{x}-\mathbf{a}) = \delta(\mathbf{x}-\mathbf{a})$$

Then, we can write down the solutions to $\Delta\phi = \rho$ as

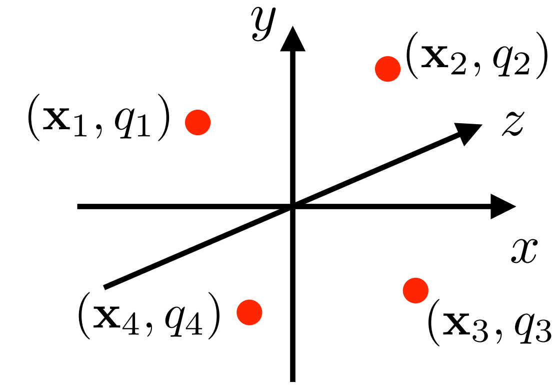
$$\boxed{\phi(\mathbf{x}) = \phi_H(\mathbf{x}) + \int_{\mathbb{R}^n} dy^n\, G(\mathbf{x}-\mathbf{y})\rho(\mathbf{y}) \quad \text{where} \quad \Delta\phi_H = 0}$$

can be chosen to satisfy
boundary conditions

check: $$\Delta_{\mathbf{x}}\phi(\mathbf{x}) = \underbrace{\Delta_{\mathbf{x}}\phi_H(\mathbf{x})}_{=0} + \int_{\mathbb{R}^n} d^n y\, \underbrace{\Delta_{\mathbf{x}} G(\mathbf{x}-\mathbf{y})}_{=\delta(\mathbf{x}-\mathbf{y})}\rho(\mathbf{y}) = \rho(\mathbf{x})$$

And now for explicit solution methods . . .

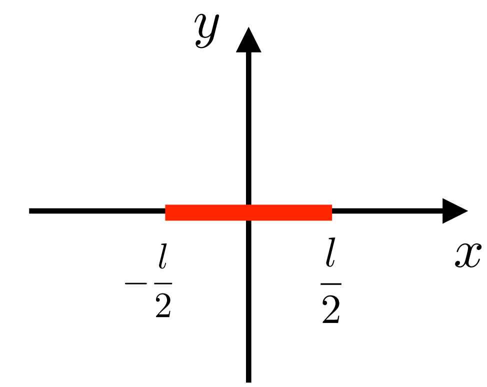
Example: Point sources in three dimensions



$$G(\mathbf{x}) = -\frac{1}{4\pi|\mathbf{x}|} \qquad \rho(\mathbf{x}) = \sum_i q_i \delta(\mathbf{x} - \mathbf{x}_i)$$

$$\Rightarrow \quad \phi(\mathbf{x}) = \int_{\mathbb{R}^3} d^3y\, G(\mathbf{x}-\mathbf{y})\rho(\mathbf{y}) = -\sum_i q_i \int_{\mathbb{R}^3} d^3y \frac{\delta(\mathbf{y}-\mathbf{x}_i)}{4\pi|\mathbf{x}-\mathbf{y}|} = -\sum_i \frac{q_i}{4\pi|\mathbf{x}-\mathbf{x}_i|}$$

Example: Rod in two dimensions



$$G(\mathbf{x}) = \frac{1}{2\pi}\ln(|\mathbf{x}|) \qquad \rho(\mathbf{x}) = \begin{cases} q\delta(y) & \text{for } -l/2 \le x \le l/2 \\ 0 & \text{otherwise} \end{cases}$$

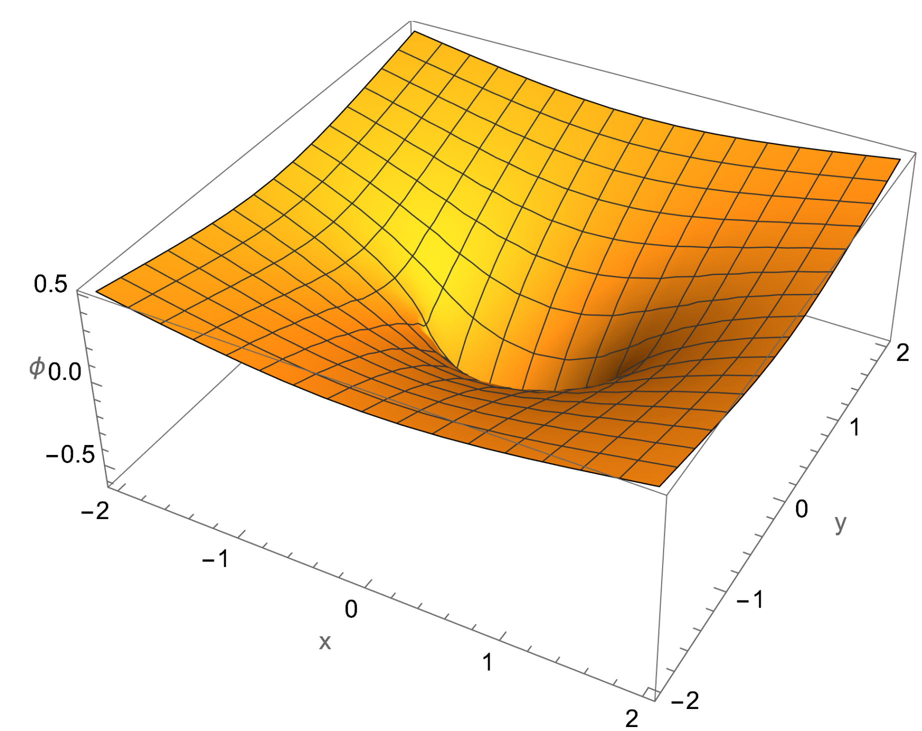
$$\mathbf{x} = (x, y)\,, \quad \mathbf{y} = (x', y')$$

$$\Rightarrow \quad \phi(\mathbf{x}) = \int_{\mathbb{R}^2} d^2y\, G(\mathbf{x}-\mathbf{y})\rho(\mathbf{y})$$

$$= \frac{q}{4\pi}\int_{-l/2}^{l/2} dx' \int_{\mathbb{R}} dy'\, \delta(y')\ln((x-x')^2 + (y-y')^2)$$

$$= \frac{q}{4\pi}\int_{-l/2}^{l/2} dx' \; \ln(y^2 + (x-x')^2)$$

$$= \text{ a bit horrible} \ldots$$



• Quick and dirty - separation of variables

e.g. 2d Cartesian coordinates: $\Delta\phi = 0$, $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$

separation Ansatz: $\phi(x,y) = X(x)Y(y)$

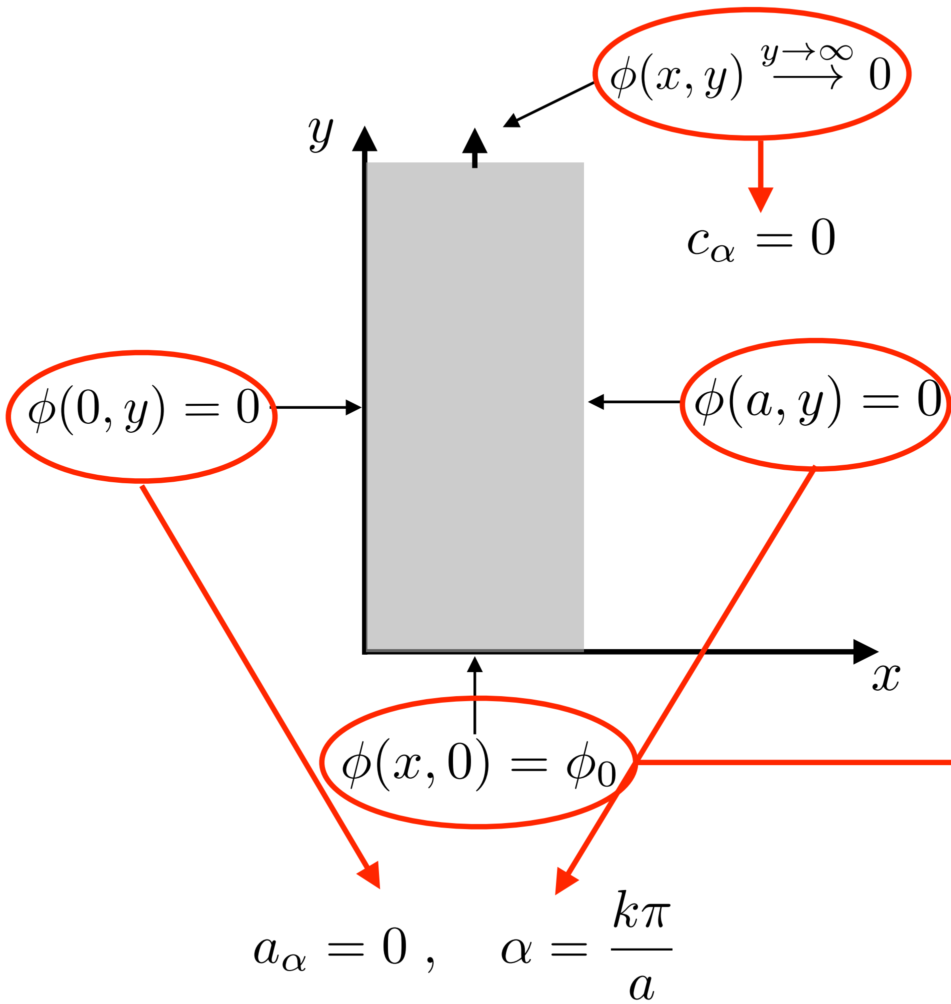
$$\Rightarrow \underbrace{\frac{X''}{X}(x)}_{=-\alpha^2} + \underbrace{\frac{Y''}{Y}(y)}_{=\alpha^2} = 0 \quad \rightarrow \quad X'' = -\alpha^2 X \;, \qquad Y'' = \alpha^2 Y$$

$$\Rightarrow \; X(x) = a_\alpha \cos(\alpha x) + b_\alpha \sin(\alpha x) \;, \qquad Y(y) = c_\alpha e^{\alpha y} + d_\alpha e^{-\alpha y}$$

$$\boxed{\phi(x,y) = \sum_\alpha (a_\alpha \cos(\alpha x) + b_\alpha \sin(\alpha x))(c_\alpha e^{\alpha y} + d_\alpha e^{-\alpha y})}$$

Fix range of α and constants from boundary conditions

Example: Potential on an infinite strip



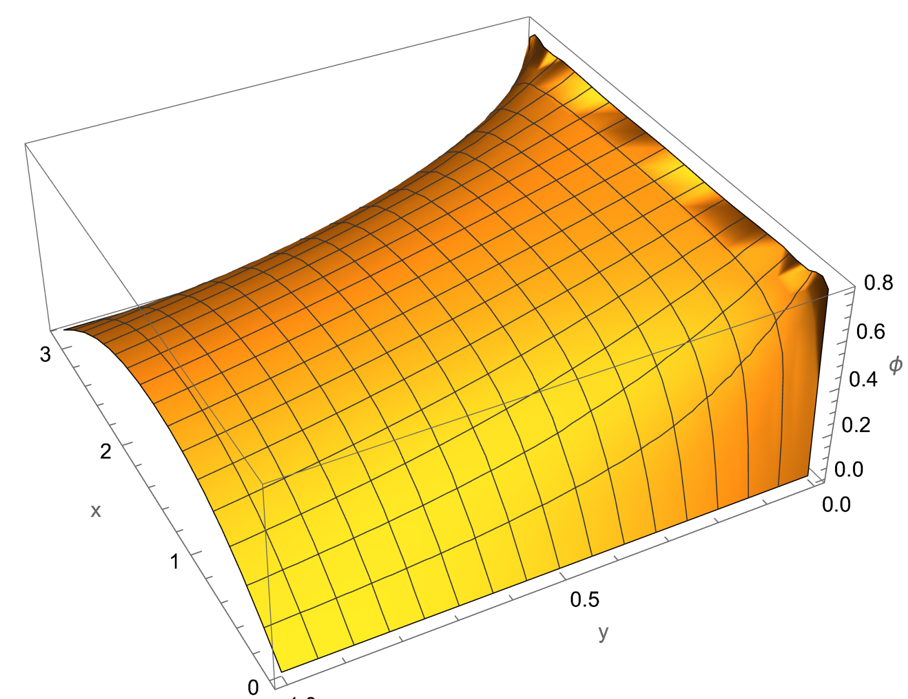
(1) $$\phi(x,y) = \sum_\alpha (a_\alpha \cos(\alpha x) + b_\alpha \sin(\alpha x))(c_\alpha e^{\alpha y} + d_\alpha e^{-\alpha y})$$

(2) $$\phi(x,y) = \sum_{k=1,2,\ldots} b_k\, e^{-k\pi y/a} \sin\left(\frac{k\pi x}{a}\right)$$

(3) $$\phi_0 = \phi(x,0) = \sum_{k=1,2,\ldots} b_k \sin\left(\frac{k\pi x}{a}\right)$$

(4) $$b_k = \frac{2}{a}\int_0^a dx\, \sin\left(\frac{k\pi x}{a}\right)\phi_0 = \begin{cases} \frac{\phi_0}{k\pi} & \text{for } k \text{ odd} \\ 0 & \text{for } k \text{ even} \end{cases}$$

(5) $$\phi(x,y) = \frac{\phi_0}{\pi} \sum_{k=0,1,\ldots} \frac{1}{2k+1} \sin\left(\frac{(2k+1)\pi x}{a}\right) e^{-(2k+1)\pi y/a}$$



- More systematic - expanding in an orthonormal function system

e.g. 2d polar coordinates: $\Delta\phi = 0$ $\quad\quad \Delta = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}$

Fouries series in φ: $\phi(r,\varphi) = \frac{A_0(r)}{2} + \sum_{k=1}^{\infty}(A_k(r)\cos(k\varphi) + B_k(r)\sin(k\varphi))$

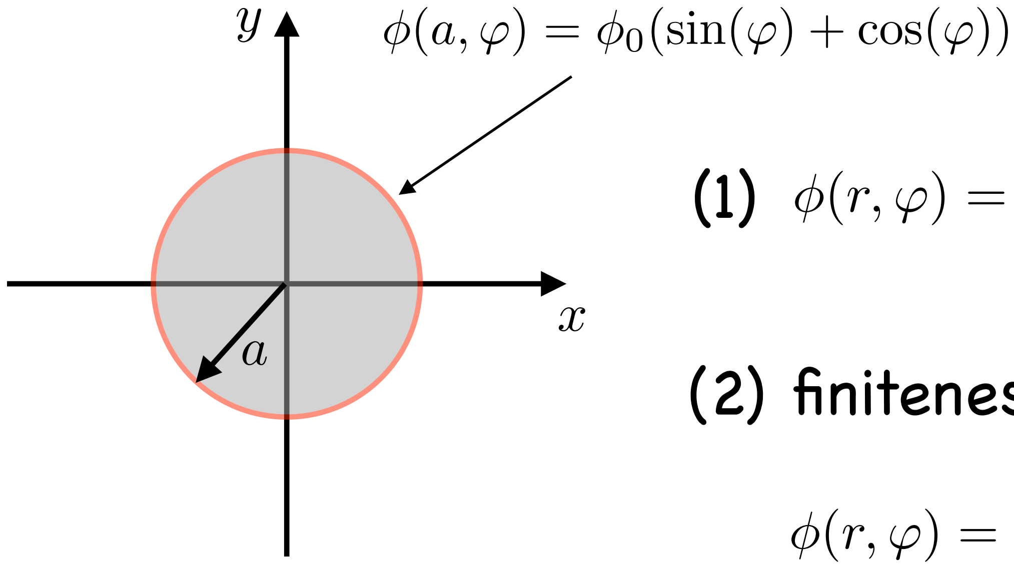
$$\Rightarrow \quad \frac{1}{r}(rA_0')' + \sum_{k=1}^{\infty}\left(\frac{1}{r}(rA_k')' - \frac{k^2}{r^2}A_k\right)\cos(k\varphi) + \sum_{k=1}^{\infty}\left(\frac{1}{r}(rB_k')' - \frac{k^2}{r^2}B_k\right)\sin(k\varphi) = 0$$

$$\Rightarrow \quad A_0(r) = a_0 + \tilde{a}_0\ln r\ , \qquad A_k(r) = a_k r^k + \tilde{a}_k r^{-k}\ , \qquad B_k(r) = b_k r^k + \tilde{b}_k r^{-k}$$

$$\boxed{\phi(r,\varphi) = \frac{a_0}{2} + \frac{\tilde{a}_0}{2}\ln r + \sum_{k=1}^{\infty}(a_k r^k + \tilde{a}_k r^{-k})\cos(k\varphi) + \sum_{k=1}^{\infty}(b_k r^k + \tilde{b}_k r^{-k})\sin(k\varphi)}$$

Fix constants from boundary conditions

Example: Potential on a disk



(1) $\phi(r,\varphi) = \frac{a_0}{2} + \frac{\tilde{a}_0}{2}\ln r + \sum_{k=1}^{\infty}(a_k r^k + \tilde{a}_k r^{-k})\cos(k\varphi) + \sum_{k=1}^{\infty}(b_k r^k + \tilde{b}_k r^{-k})\sin(k\varphi)$

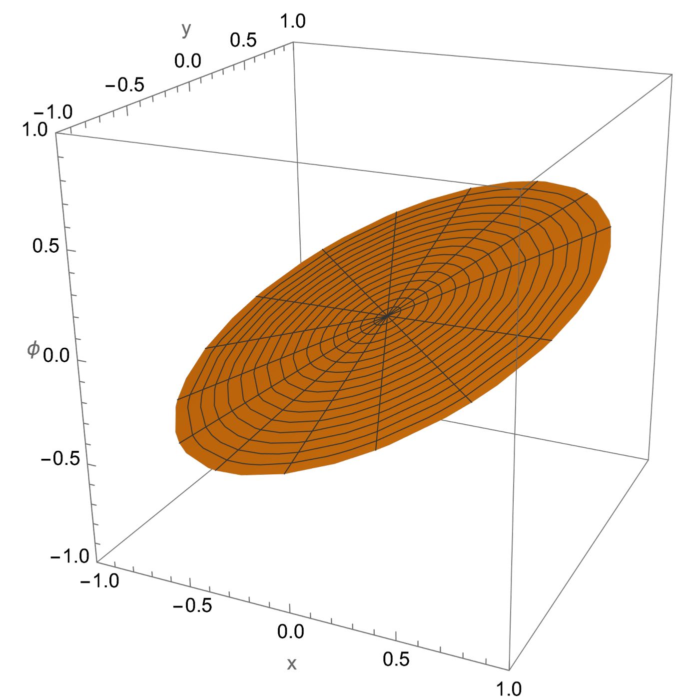
(2) finiteness of potential on disk: $\tilde{a}_k = \tilde{b}_k = 0$

$$\phi(r,\varphi) = \frac{a_0}{2} + \sum_{k=1}^{\infty} r^k (a_k\cos(k\varphi) + b_k\sin(k\varphi))$$

(3) $\phi(a,\varphi) = \frac{a_0}{2} + \sum_{k=1}^{\infty} a^k (a_k\cos(k\varphi) + b_k\sin(k\varphi)) \stackrel{!}{=} \phi_0(\sin(\varphi) + \cos(\varphi))$

$$\Rightarrow \qquad a_1 = \frac{\phi_0}{a}\,, \quad b_1 = \frac{\phi_0}{a}\,, \quad \text{all others } 0$$

(4) $\phi(r\varphi) = \frac{\phi_0 r}{a}(\sin(\varphi) + \cos(\varphi)) = \frac{\phi_0}{a}(x+y)$



• Laplacian on the two-sphere

eigenvalue problem: $\Delta_{S^2}\, f = \lambda f$

eigenfcts. are spherical harmonics:

$$Y_l^m(\theta,\varphi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)e^{im\varphi}\ , \qquad l=0,1,\dots\ , \quad m=-l,\dots,l\ .$$

$$Y_l^0(\theta,\varphi) = \sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta) \longrightarrow \varphi \text{ independent problems}$$

$$\Rightarrow \qquad \Delta_{S^2}\, Y_l^m = -l(l+1)Y_l^m$$

The spherical harmonics form on ortho-normal basis on $L^2(S^2)$ w.r.t. scalar product

$$\langle f,g\rangle_{S^2} = \int_{S^2} f(x)^* g(x)\, dS\ , \qquad dS = \sin\theta d\theta\, d\varphi$$

- Laplacian in 3d spherical coordinates

want to solve $\Delta\phi = 0$ $\Delta_{3,\text{sph}} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\Delta_{S^2}$

expand in spherical harmonics: $\phi(r,\theta,\varphi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} R_{lm}(r)Y_{lm}(\theta,\varphi)$

$$\Rightarrow \quad \frac{d}{dr}\left(r^2 R'_{lm}\right) = l(l+1)R_{lm} \quad \Rightarrow \quad R_{lm}(r) = A_{lm}r^l + B_{lm}r^{-l-1}$$

$$\boxed{\begin{aligned} &\phi(r,\theta,\varphi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}(A_{lm}r^l + B_{lm}r^{-l-1})Y_{lm}(\theta,\varphi) \\ &\phi(r,\theta) = \sum_{l=0}^{\infty}(A_l r^l + B_l r^{-l-1})P_l(\cos\theta) \longrightarrow \varphi \text{ independent problems} \end{aligned}}$$

Fix constants from boundary conditions

Example: Sphere with constant potential

$$\phi(a,\theta,\varphi) = \phi_0 \ , \quad \phi(r,\theta,\varphi) \stackrel{r\to\infty}{\longrightarrow} 0$$

$$\phi(r,\theta,\varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (A_{lm} r^l + B_{lm} r^{-l-1}) Y_{lm}(\theta,\varphi)$$

inside:

(1) finiteness implies $B_{lm} = 0$

(2) $\phi(a,\theta,\varphi) = \sum_{l,m} A_{lm} a^l Y_{lm}(\theta,\varphi) \stackrel{!}{=} \phi_0$

$\Rightarrow \quad A_{lm} = 0 \text{ for } l > 0$

(3) $\phi(r,\theta,\varphi) = \phi_0 \text{ for } r \leq a$

outside:

(1) vanishing at infinity: $A_{lm} = 0$

(2) $\phi(a,\theta,\varphi) = \sum_{l,m} B_{lm} a^{-l-1} Y_{lm}(\theta,\varphi) \stackrel{!}{=} \phi_0$

$\Rightarrow \quad B_{lm} = 0 \text{ for } l > 0$

(3) $\phi(a,\theta,\varphi) = \dfrac{a\,\phi_0}{r} \text{ for } r \geq a$

Helmholz equation

$$(\Delta + k^2)\psi = 0\,, \qquad (\Delta + k^2)\psi = f$$

homogeneous eq.: eigenvalue problem for Laplacian

inhomogeneous eq.: Green function $G = AG_+ + BG_-$, $A + B = 1$ where

$$G_\pm(r) = \frac{e^{\pm ikr}}{r}$$

$$\boxed{\begin{aligned} &(\Delta + k^2)G(\mathbf{x}) = -4\pi\delta(\mathbf{x}) \\ &\qquad\qquad \psi(\mathbf{x}) = \psi_{\mathrm{hom}}(\mathbf{x}) - \frac{1}{4\pi}\int_{\mathbb{R}^3} d^3y\, G(\mathbf{x}-\mathbf{y})f(\mathbf{y}) \end{aligned}}$$

Example: Infinite spherical well

Problem: solve eigenvalue problem $-\Delta\psi = E\psi$ with boundary cond. $\psi|_{|\mathbf{x}|=a} = 0$

(1) recall: $\Delta_{3,\text{sph}} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2}\Delta_{S^2}$ $\qquad \Delta_{S^2} Y_{lm} = -l(l+1)Y_{lm}$

(2) expand: $\psi(r,\theta,\varphi) = \sum_{l.m} R_{l,m}(r) Y_{lm}(\theta,\varphi)$

Bessel diff. eq. for $\nu = l + \frac{1}{2}$

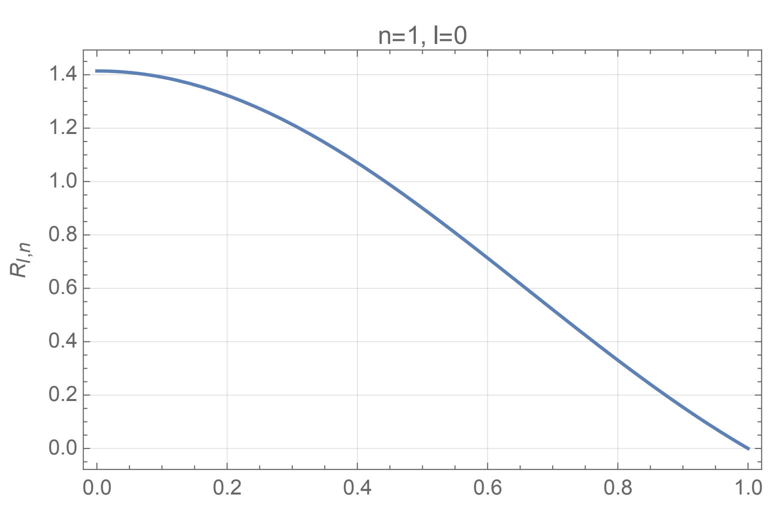
(3) insert and find eq. for radial part $R_{l,m}$: $\rho^2 \tilde{y}'' + \rho\tilde{y}' + (\rho^2 - (l+1/2)^2)\tilde{y} = 0$

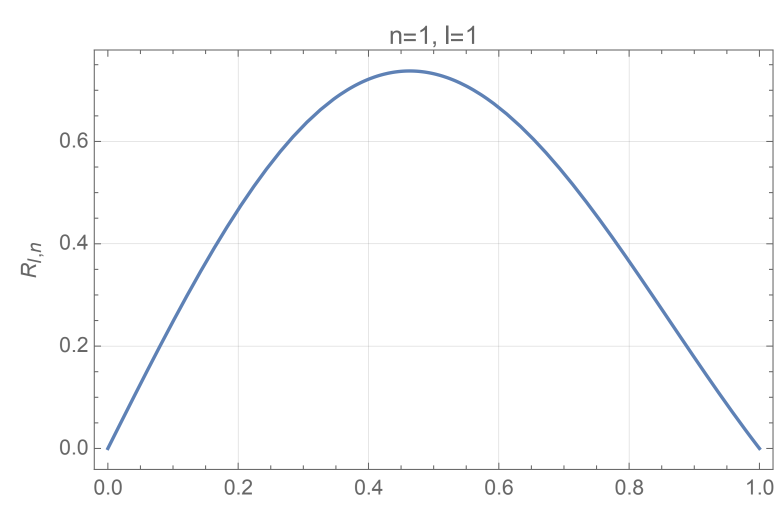
$\tilde{y} = \sqrt{\rho} y \qquad \rho = \sqrt{E} r$

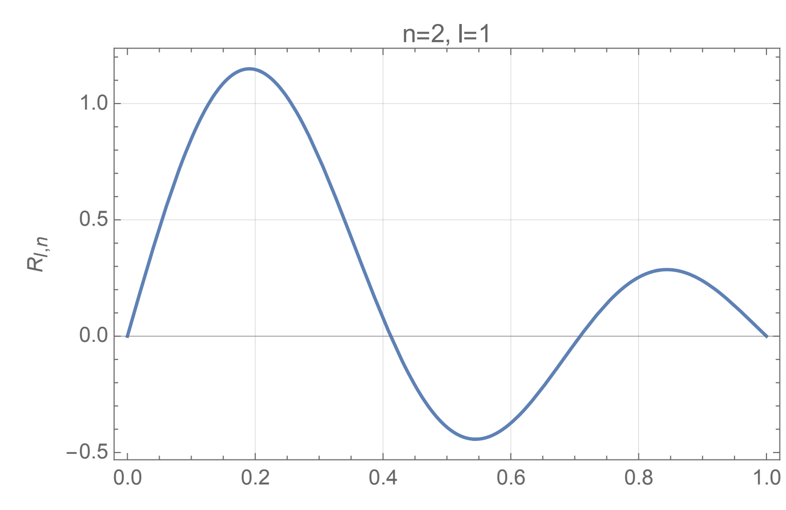
(4) radial part: $R_{l,m}(r) \sim \frac{1}{\sqrt{r}} J_{l+1/2}(\sqrt{E} r)$

(5) $R_{l,m}(a) = 0 \quad \Rightarrow \quad E = \frac{z_{l,n}^2}{a^2}$ $\longleftarrow$ zeros of Bessel function $J_{l+1/2}$

(6) $\psi_{n,l,m}(r,\theta,\varphi) \sim \frac{1}{\sqrt{r}} J_{l+1/2}\left(\frac{z_{l,n} r}{a}\right) Y_{lm}(\theta,\varphi)$







Time evolution

Many problems in physics are of the form

(i) $H\psi = \frac{1}{c}\dot{\psi}$ (ii) $H\psi = \ddot{\psi}$

e.g. Schroedinger eq. e.g. wave equations in E&M

where $\psi = \psi(t, \mathbf{x})$ and H is a second order diff. operator in $\mathbf{x}$.

If $(\phi_i)_{i=1}^{\infty}$ is an ortho-normal basis of eigenfunctions of H,

$$H\phi_i = \lambda_i \phi_i$$

we can expand $\psi(t, \mathbf{x}) = \sum_i A_i(t)\phi_i(\mathbf{x})$. The full solution is then

(i) $\psi(t, \mathbf{x}) = \sum_i a_i \phi_i(\mathbf{x}) e^{c\lambda_i t}$ (ii) $\psi(t, \mathbf{x}) = \sum_i \left(a_i \sin\left(\sqrt{|\lambda_i|}\, t\right) + b_i \cos\left(\sqrt{|\lambda_i|}\, t\right)\right) \phi_i(\mathbf{x})$

$\lambda_i < 0$

Fix constants from initial conditions on $\psi(0, \mathbf{x})$ and $\dot{\psi}(0, \mathbf{x})$

Example: Evolution of a spin system

Hilbert space: $\mathcal{H} = \{c|\uparrow\rangle + d|\downarrow\rangle \,|\, c,d \in \mathbb{C}\}$ $\qquad \langle\uparrow|\uparrow\rangle = \langle\downarrow|\downarrow\rangle = 1 \qquad \langle\uparrow|\downarrow\rangle = 0$

Hamiltonian: $H_{ij} = \langle i|\hat{H}|j\rangle = a\delta_{ij} + \sum_i b_\alpha(\sigma_\alpha)_{ij}$, e.g. $H = \begin{pmatrix} a & b_1 \\ b_1 & a \end{pmatrix}$

$$\Rightarrow \quad \hat{H}|E_\pm\rangle = E_\pm|E_\pm\rangle$$

$$|E_\pm\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \pm |\downarrow\rangle)$$

eigenvalues $E_\pm = a \pm b_1$

eigenvectors $\mathbf{v}_\pm = (1, \pm 1)^T/\sqrt{2}$

time evolution: $|\psi(t)\rangle = \beta_+ e^{-iE_+t}|E_+\rangle + \beta_- e^{-iE_-t}|E_-\rangle$

initial condition: $|\psi(0)\rangle = |\uparrow\rangle = \frac{1}{\sqrt{2}}(|E_+\rangle + |E_-\rangle) \quad \Rightarrow \quad |\psi(t)\rangle = \frac{e^{-iat}}{\sqrt{2}}\left(e^{-ib_1t}|E_+\rangle + e^{ib_1t}|E_-\rangle\right)$

probability of finding spin down:

$$p_\downarrow = |\langle\downarrow|\psi(t)\rangle|^2 = \frac{1}{4}\left|(\langle E_+| - \langle E_-|)(e^{-ib_1t}|E_+\rangle + e^{ib_1t}|E_-\rangle)\right|^2 = \sin^2(b_1t)$$

$$p_\uparrow = |\langle\uparrow|\psi(t)\rangle|^2 = \cos^2(b_1t)$$

Wave equation

$$\left(\Delta_n - \frac{\partial^2}{\partial t^2}\right)\psi = 0\,, \qquad \left(\Delta_n - \frac{\partial^2}{\partial t^2}\right)\psi = f$$

- Solving the homogeneous equation by (spatial) Fourier transform

$$\psi(t,\mathbf{x}) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} d^n k\, \tilde{\psi}(t,\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{x}}$$

$$\Rightarrow \quad \ddot{\tilde{\psi}} = -|\mathbf{k}|^2 \tilde{\psi} \qquad \Rightarrow \qquad \tilde{\psi}(t,\mathbf{k}) = \psi_+(\mathbf{k}) e^{i|\mathbf{k}|t} + \psi_-(\mathbf{k}) e^{-i|\mathbf{k}|t}$$

$$\boxed{\psi(t,\mathbf{x}) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} d^n k\, (\psi_+(\mathbf{k}) e^{i|\mathbf{k}|t} + \psi_-(\mathbf{k}) e^{-i|\mathbf{k}|t}) e^{-i\mathbf{k}\cdot\mathbf{x}}}$$

initial conditions $\psi(0,\mathbf{x}) = \psi_0(\mathbf{x})$ and $\dot{\psi}(0,\mathbf{x}) = \dot{\psi}_0(\mathbf{x}) \;\Rightarrow\; \psi_\pm = \frac{1}{2}\tilde{\mathcal{F}}\left(\psi_0 \mp \frac{i}{|\mathbf{k}|}\dot{\psi}_0\right)$

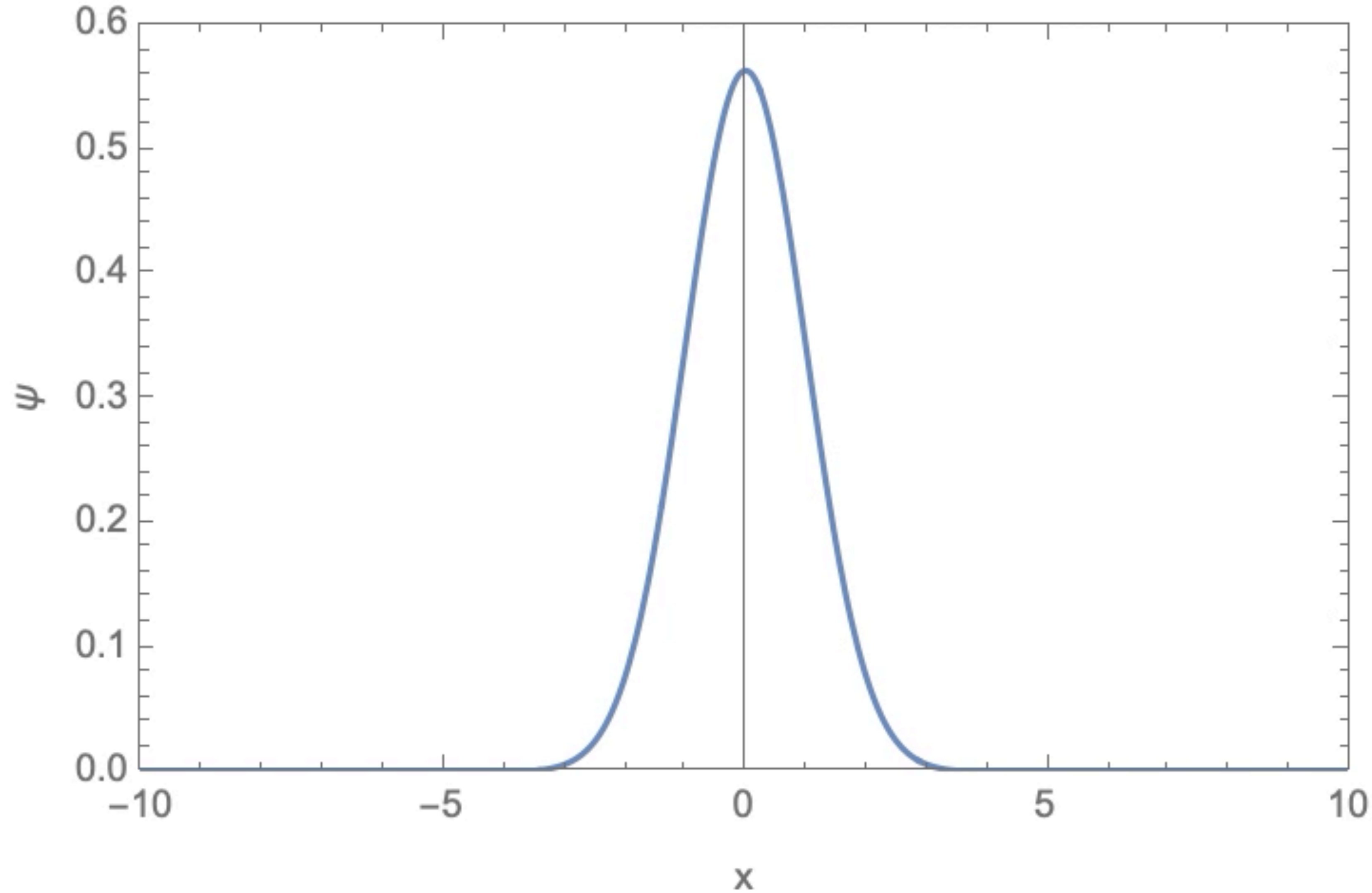
Example: Evolution of a 1d wave

Initial condition: $\psi_0(x) := \psi(0,x) = \dfrac{e^{-x^2/2}}{\sqrt{\pi}}$, $\dot{\psi}(0,x) = 0$

$$\Rightarrow \quad \psi_\pm(k) = \frac{1}{2}\tilde{\mathcal{F}}(\psi_0)(k) = \frac{e^{-k^2/2}}{\sqrt{2\pi}}$$

recall: $\psi(t,\mathbf{x}) = \dfrac{1}{(2\pi)^{n/2}} \displaystyle\int_{\mathbb{R}^n} d^n k \, (\psi_+(\mathbf{k}) e^{i|\mathbf{k}|t} + \psi_-(\mathbf{k}) e^{-i|\mathbf{k}|t}) e^{-i\mathbf{k}\cdot\mathbf{x}}$

$$= \frac{1}{2\pi} \int_{\mathbb{R}} dk \, e^{-k^2/2} \left(e^{i(|k|t - kx)} + e^{i(-|k|t - kx)} \right) = \frac{e^{-\frac{1}{2}(t+x)^2} \left(e^{2tx} + 1 \right)}{2\sqrt{\pi}}$$



0.6
0.5
0.4
0.3
0.2
0.1
0.0
ψ
−10
−5
0
5
10
x

- Solving the inhomogeneous equation with Green function

$$G_{\pm}(t,\mathbf{x}) = \frac{\delta(t \mp |\mathbf{x}|)}{|\mathbf{x}|} \qquad \left(\Delta_3 - \frac{\partial^2}{\partial t^2}\right) G(t,\mathbf{x}) = -4\pi\delta(t)\delta(\mathbf{x})$$

$$\boxed{\begin{aligned} \psi(t,\mathbf{x}) &= \psi_{\mathrm{hom}}(t,\mathbf{x}) - \frac{1}{4\pi}\int_{\mathbb{R}^4} dt'\, d^3x'\, G_{+}(t-t',\mathbf{x}-\mathbf{x}')f(t',\mathbf{x}') \\ &= \psi_{\mathrm{hom}}(t,\mathbf{x}) - \frac{1}{4\pi}\int_{\mathbb{R}^4} dt'\, d^3x'\, \frac{\delta(t-t'-|\mathbf{x}-\mathbf{x}'|)}{|\mathbf{x}-\mathbf{x}'|} f(t',\mathbf{x}') \\ &= \psi_{\mathrm{hom}}(t,\mathbf{x}) - \frac{1}{4\pi}\int_{\mathbb{R}^3} d^3x'\, \left(\frac{f(t',\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}\right)_{t'=t-|\mathbf{x}-\mathbf{x}'|} \end{aligned}}$$

Good luck!