2. The Free Schrödinger Equation

Notes:
- From now on we use natural units, i.e., $\hbar = m = 1$.
- For $\psi: \mathbb{R}\times\mathbb{R}^d \to \mathbb{C}$, partial derivatives are defined in the usual way:
  $\partial_x \psi(t,x) := \partial_x \mathrm{Re}\,\psi(t,x) + i\partial_x \mathrm{Im}\,\psi(t,x)$

Free one-particle SE: $V=0$, i.e., $i\partial_t \psi(t,x) = -\frac{1}{2}\Delta_x \psi(t,x)$, $\psi: \mathbb{R}_t \times \mathbb{R}^d_x \to \mathbb{C}$

Recall: solutions to the stationary SE $-\frac{1}{2}\Delta_x \phi(x) = E\,\phi(x)$
give us solutions $\psi(t,x) = e^{-iEt}\phi(x)$

Formally, the "eigenfunctions" of $-\frac{1}{2}\Delta_x$ are $\boxed{\text{plane waves}}$

$$\boxed{\phi_k(x) = e^{ik\cdot x}} = e^{i\sum_{j=1}^{d} k_j x_j}, \text{ for any } k\in\mathbb{R}^d \quad \left(\text{since } -\tfrac{1}{2}\Delta_x \phi_k(x) = \tfrac{1}{2}k^2 \phi_k(x)\right)$$

$\Rightarrow$ this gives solutions $\psi_k(t,x) = e^{-i\frac{k^2}{2}t}e^{ikx}$ of the free SE

But $|\psi_k(t,x)|^2 = 1$, so on $\mathbb{R}^d$ $\int_{\mathbb{R}^d} |\psi_k(t,x)|^2 dx = \infty$, but we want $\int_{\mathbb{R}^d}|\psi|^2 = 1$.

By linearity, we find that formally $\psi(t,x) = \int f(k)\psi_k(t,x)dx = \int f(k) e^{-i\frac{k^2}{2}t}e^{ikx}dx$
is also a solution, and $f: \mathbb{R}^d \to \mathbb{C}$ is determined by the initial condition:
$\psi(0,x) = \int f(k)e^{ikx}dx$

Conclusion: we need to study the Fourier transform on $\mathbb{R}^d$.

2.1 Fourier Transform on Schwartz Space

We often use the following function spaces:

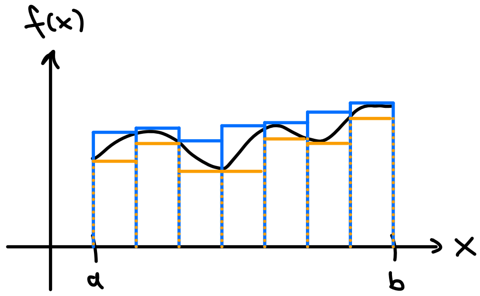
$$\boxed{L^p(\mathbb{R}^d) := \left\{ f:\mathbb{R}^d \to \mathbb{C} : \underbrace{\|f\|_p}_{p\text{-norm}} = \left(\int |f|^p\right)^{\frac{1}{p}} < \infty \right\}}, \quad 1 \le p < \infty$$

Note: All integrals in this class refer to the Lebesgue integral.

Quick introduction to the Lebesgue integral: (here just for $d=1$)

Recall: $f:[a,b]\to\mathbb{R}$ bounded is Riemann integrable if upper and lower Riemann integral coincide

$$\text{upper: } \inf_{\substack{\text{partitions}\\ \text{of } [a,b]}} \sum_{i=1}^m \underbrace{M_i}_{=\sup_{x\in[x_{i-1},x_i]} f(x)} \Delta x_i \qquad \text{lower: } \sup_{\substack{\text{partitions}\\ \text{of } [a,b]}} \sum_{i=1}^m \underbrace{m_i}_{=\inf_{x\in[x_{i-1},x_i]} f(x)} \Delta x_i$$



Examples: • continuous functions are Riemann integrable

• $\mathbb{1}_{\mathbb{Q}}|_{[0,1]}$ is not Riemann integrable

↳ note: for $S\subset\mathbb{R}^d$, we define the indicator function $\mathbb{1}_S(x) := \begin{cases} 1 & \text{for } x\in S \\ 0 & \text{for } x\notin S \end{cases}$

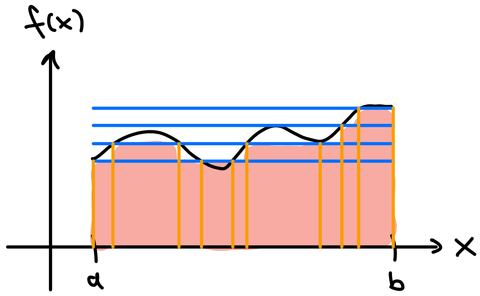
Note: • Improper Riemann integrals might exist if $a=-\infty$ or $b=\infty$ or f is not bounded.

• If $(f_n)_n \xrightarrow{n\to\infty} f$ uniformly, then $\lim_{n\to\infty} \int_a^b f_n(x)\,dx = \int_a^b \underbrace{\lim_{n\to\infty} f_n(x)}_{f(x)}\,dx$.

But this might fail for improper integrals (e.g., $\lim_{n\to\infty} \int_{-\infty}^{\infty} n^{-1}\, \mathbb{1}_{[0,n]}(x)\,dx = 1 \neq 0$).

The Lebesgue integral addresses the difficulties with exchanging limits and integration.

Idea of the construction: partition y-axis instead of x-axis



Steps in constructing the Lebesgue integral:

a collection of subsets of Ω — $\mu: \Sigma \to \mathbb{R}_+$ satisfying reasonable axioms — e.g., $\Omega = \mathbb{R}$

- define "size" of a subset $S \subset \mathbb{R}$; this leads to measure spaces (Ω, Σ, μ); e.g., $\mu([a,b]) = b-a$.

- approximate f by "simple functions" $\sum_k a_k \mathbb{1}_{S_k}$
  ↳ then $\int \sum_k a_k \mathbb{1}_{S_k} \, d\mu = \sum_k a_k \mu(S_k)$

- then $\int f \, d\mu := \sup\{\int s \, d\mu : 0 \le s \le f, s \text{ simple}\}$ for $f \ge 0$

- in general: $\int f \, d\mu := \int f^+ d\mu - \int f^- d\mu$ if one of the integrals is finite
  (positive part of f; negative part of f)

Note: · $f: [a,b] \to \mathbb{R}$ (bounded) Riemann integrable $\Rightarrow$ f Lebesgue integrable

· $\int \mathbb{1}_{\mathbb{Q}}|_{[0,1]} \, d\mu = 0$

· but there are improper well-defined Riemann integrals that do not make sense as Lebesgue integrals

Important theorems about Lebesgue integration:

$\boxed{\text{Monotone Convergence:}}$ If $(f_n)_n$ with $f_n \geq 0$ and f_n measurable is such that $f_n(x) \leq f_{n+1}(x)$ $\forall n \in \mathbb{N}$ $\forall x \in \mathbb{R}$, then $\lim_{n\to\infty} \int f_n \, d\mu = \int \underbrace{\lim_{n\to\infty} f_n}_{\text{pointwise limit}} d\mu$

$\boxed{\text{Dominated Convergence:}}$ If $(f_n)_n$ with f_n measurable $\forall n$ and $\lim_{n\to\infty} f_n(x) = f(x)$ is such that $|f_n(x)| \leq g(x)$ $\forall n \in \mathbb{N}$ $\forall x \in \mathbb{R}$ for some measurable g with $\int |g| < \infty$, then $\lim_{n\to\infty} \int f_n \, d\mu = \int f \, d\mu$.

Note: Dominated Convergence still holds if $f_n(x) \to f(x)$ and $|f_n(x)| \leq g(x)$ holds $\forall n \in \mathbb{N}$ for $\underbrace{\text{almost all } x}_{\text{"almost everywhere"}}$, i.e., for all x except those in $\underbrace{\text{some set of measure zero.}}_{\text{e.g., finitely many points}}$

note: we often abbreviate:
- almost all x = a.a. x
- almost everywhere = a.e.

$\boxed{\text{Fubini:}}$ If f is measurable with $\iint_{\mathbb{R}\times\mathbb{R}} |f(x,y)| \, dx\,dy < \infty$, then

$$\iint_{\mathbb{R}\times\mathbb{R}} f(x,y)\,dx\,dy = \int_{\mathbb{R}} \left(\int_{\mathbb{R}} f(x,y)\,dy \right) dx = \int_{\mathbb{R}} \left(\int_{\mathbb{R}} f(x,y)\,dx \right) dy.$$

From now on, all integrals are meant in the Lebesgue sense, and we use the usual notations $\int f \, d\mu \equiv \int f(x)\,dx \equiv \int dx \, f(x)$.