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3. The Schrödinger Equation with Potential

Next, we want to understand the Schrödinger equation

$$i\partial_t \psi(t,x) = -\frac{\Delta}{2}\psi(t,x) + V(x)\psi(t,x) = H\psi(t,x) \qquad (\text{here: } V \text{ time-independent})$$

Note: • Fourier transformation turns V into convolution $\Rightarrow$ not easy to find solutions for $V \not\equiv 0$.

• Since $|\psi(t,x)|^2$ is a probability density, we want to understand the SE on L^2. (For the free SE we had $\|\psi(t)\|_{L^2} = \|\psi(0)\|_{L^2}$ if $\psi(0) \in L^2$, and that should also hold for $V \not\equiv 0$.)

Ideas that we will develop in this chapter:

- As we have done for the free SE, we try to make sense of e^{-iHt} for a large class of V, s.t. we can define $\psi(t) = e^{-iHt}\psi(0)$.
- We regard L^2 as a subspace of S', s.t. the SE holds in the sense of distributions; but hopefully it also holds on L^2, at least for some initial data.

First, we want to embed the free SE in the L^2 framework, so we discuss Hilbert spaces (and operators on them) in general, and then how to define $\mathcal{F}: L^2 \to L^2$.

3.1 Hilbert and Banach Spaces

Recall: • Banach space = $\overbrace{\text{complete}}^{\text{every Cauchy sequence converges}}$ normed vector space

• Hilbert space = Banach space with scalar product $\langle\cdot,\cdot\rangle : \mathcal{H}\times\mathcal{H} \to \overbrace{\mathbb{C}}^{\text{or any other field}}$ s.t. $\|\psi\| = \sqrt{\langle\psi,\psi\rangle}$.

Convention: $\langle\lambda\psi,\varphi\rangle = \bar{\lambda}\langle\psi,\varphi\rangle$. "antilinearity in the first argument"

Examples: • $\mathbb{C}^n$ with $\langle x,y\rangle_{\mathbb{C}^n} = \sum_{j=1}^{n} \overline{x_j} y_j$

• ℓ^2 with $\langle x,y\rangle_{\ell^2} = \sum_{j=1}^{\infty} \overline{x_j} y_j$

• $L^2(M,\mu)$ for some measure space (M,μ), with $\langle \psi,\varphi\rangle_{L^2} = \int_M \overline{\psi(x)}\varphi(x)\,d\mu$

Let us first prove some standard properties.

In the following, let $\mathcal{H}$ be a Hilbert space.

$\boxed{\text{Definition 3.3: A sequence } (\varphi_j)_j \text{ in } \mathcal{H} \text{ is called orthonormal sequence (ONS) if } \langle \varphi_i,\varphi_j\rangle = \delta_{ij} \ \forall i,j.}$

The following properties hold:

• orthonormal decomposition: $\forall \psi \in \mathcal{H}$: $\psi = \underbrace{\sum_{j=1}^{n} \langle \varphi_j,\psi\rangle \varphi_j}_{=:\psi_n} + \underbrace{\left(\psi - \sum_{j=1}^{n} \langle \varphi_j,\psi\rangle\varphi_j\right)}_{=:\psi_n^\perp}$

with $\langle \psi_n,\psi_n^\perp\rangle = \langle \psi_n,\psi-\psi_n\rangle = \langle\psi_n,\psi\rangle - \langle\psi_n,\psi_n\rangle = \sum_{j=1}^{n} \overline{\langle\varphi_j,\psi\rangle}\langle\varphi_j,\psi\rangle - \sum_{i,j=1}^{n} \overline{\langle\varphi_j,\psi\rangle}\underbrace{\langle\varphi_j,\varphi_i\rangle}_{=\delta_{ij}}\langle\varphi_i,\psi\rangle$

$= 0$

$\Rightarrow \langle\psi,\psi\rangle = \langle\psi_n+\psi_n^\perp,\psi_n+\psi_n^\perp\rangle = \langle\psi_n,\psi_n\rangle + \langle\psi_n^\perp,\psi_n^\perp\rangle$

• $\boxed{\text{Bessel inequality: } \|\psi\|^2 \geq \sum_{j=1}^{n} |\langle\varphi_j,\psi\rangle|^2}$ $\forall \psi\in\mathcal{H}, n\in\mathbb{N}$, follows directly from orthonormal decomposition ($\langle\psi,\psi\rangle \geq \langle\psi_n,\psi_n\rangle$).

• $\boxed{\text{Cauchy-Schwarz: } |\langle\varphi,\psi\rangle| \leq \|\varphi\|\cdot\|\psi\|}$ $\forall\varphi,\psi\in\mathcal{H}$, follows from Bessel for $n=1$, $\varphi_1 = \frac{\varphi}{\|\varphi\|}$

• $\boxed{\text{Polarisation identity}}$ for complex $\mathcal{H}$:

$$\boxed{\langle \varphi, \psi \rangle = \frac{1}{4}\left(\|\varphi+\psi\|^2 - \|\varphi-\psi\|^2 - i\|\varphi+i\psi\|^2 + i\|\varphi-i\psi\|^2 \right)} \quad \forall \varphi,\psi \in \mathcal{H}$$

(check by direct calculation)

Next: some basic consequences of the concept of orthonormal basis.

Definition 3.7: A sequence $(\varphi_j)_j$ in $\mathcal{H}$ is called orthonormal basis (ONB) if $\psi = \underbrace{\sum_{j=1}^{\infty} \langle \varphi_j, \psi \rangle \varphi_j}$ $\forall \psi \in \mathcal{H}$.

meaning $\|\psi - \sum_{j=1}^{N} \langle \varphi_j, \psi \rangle \varphi_j \|_{\mathcal{H}} \xrightarrow{N\to\infty} 0$

Note: With Zorn's lemma, every vector space has a basis (in the context of infinite dimensional $\mathbb{R}$ or $\mathbb{C}$ vector spaces called Hamel basis), meaning every vector can be written uniquely as a finite linear combination of basis vectors (recall Linear Algebra). Thus, ONBs are a different notion (but obviously it makes a lot of sense to also call them basis).

Consequences (here, $\mathcal{H}$ is a Hilbert space and $(\varphi_j)_j$ an ONB):

The general definition of separability for topological spaces is the existence of a countable dense subset. By this definition, one can show that a Hilbert space is separable iff it has an ONB.

Proof: "$\Leftarrow$" $\left\{ \sum_{j=1}^{N} (a_j + i b_j)\varphi_j : N \in \mathbb{N}, a_j, b_j \in \mathbb{Q} \right\}$ is clearly a countable dense subset (of a complex Hilbert space)

"$\Rightarrow$" If $(\varphi_j)_j$ is any countable dense subset, we can – if necessary – just remove φ_j's such that the remaining $\{\varphi_j\}_{j\in J}$ are still $\underbrace{\text{linearly independent}}$, but still $\underbrace{\overline{\operatorname{span}\{\varphi_j\}_{j\in J}} = \mathcal{H}}$.

recall that for ∞-dim. vector spaces, this means all *finite* linear combinations are linearly independent

meaning $\psi = \sum_{j=1}^{\infty} a_j \varphi_j$ $\forall \psi \in \mathcal{H}$

The remaining basis can be made orthonormal by $\underbrace{\text{Gram-Schmidt}}$. $\square$

recall this from Linear Algebra

Notes: • In this class we are only interested in separable Hilbert spaces

• Examples of non-separable spaces:

↳ more from physics: infinite spin chain : $\overbrace{\bigotimes_{k\in\mathbb{Z}}}^{\text{tensor product (rigorously introduced later)}} \mathbb{C}^2$ (reason: think of the two basis vectors in $\mathbb{C}^2$ as 0 and 1, then basis vectors in the infinite tensor product are all 0,1 sequences; but there are as many such sequences as real numbers)

↳ ℓ^∞ (bounded real sequences) is a non-separable Banach space

↳ more from math: space of almost periodic functions $H = \overline{X}$ (completion of X), where

$X = \{ f : \mathbb{R} \to \mathbb{C},\ f(t) = \sum_{j=1}^{n} c_j e^{i s_j t},\ s_j \in \mathbb{R},\ c_j \in \mathbb{C},\ n \in \mathbb{N} \}$ with scalar product

$\langle f, g \rangle = \lim_{N\to\infty} \frac{1}{2N} \int_{-N}^{N} \overline{f(t)}\, g(t)\, dt$ ($\{e^{ist} : s \in \mathbb{R}\}$ is an uncountable orthonormal set)