Lecture 1. Mathematical Physics SS 2013

Note Title 4/14/2013

I. Some mathematical preliminaries

I.1 The Schrödinger equation

In quantum mechanics, the state of a particle is described by a wave function $\psi : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{C}$ with the interpretation that for fixed $t \in \mathbb{R}$

$|\psi(\cdot, t)|^2$ is the prob. distribution for the position of the particle.

The state space (for one particle) is the Hilbert-space $L^2(\mathbb{R}^3) = \{ \psi : \mathbb{R}^3 \to \mathbb{C} \,/\, \int |\psi(x)|^2 dx < \infty \}$ with scalar product

$$\langle \psi, \phi \rangle = \int_{\mathbb{R}^3} \overline{\psi(x)}\, \phi(x)\, dx$$

The Schrödinger equation is given by

$$(1) \quad \begin{cases} i\hbar \dfrac{\partial}{\partial t} \psi = H\psi \\ \psi(0) = \psi_0 \in L^2(\mathbb{R}^3) \end{cases}$$

$$(\text{i.e., } \psi(x,0) = \psi_0(x))$$

(2) $$H\psi(x,t) = -\frac{\hbar^2}{2m}\Delta_x \psi(x,t) + V(x)\psi(x,t)$$

Potential.

Laplace $\Delta_x = \sum_{j=1}^{3} \frac{\partial^2}{\partial x_j^2}$

Note that (1) yields an initial value problem, also called Cauchy problem.

$\hbar$ = Planck's constant $= \frac{h}{2\pi}$

Domain $\mathcal{D}(H) \subset L^2(\mathbb{R}^3)$ is unspecified at the moment (it usually is the Sobolev space H^2 of functions having square integrable second derivatives)

<u>Remark</u>: From the interpretation of Q.M. we need that

$$\langle \psi(t), \psi(t)\rangle = \int |\psi(x,t)|^2 dx = \int |\psi(x,0)|^2 dx \quad \forall t \in \mathbb{R}$$

(conservation of probability).

This is the case if H is symmetric, i.e., if for all $\psi, \phi \in \mathcal{D}(H)$ one has

$$\langle \psi, H\phi\rangle = \langle H\psi, \phi\rangle$$

Indeed, if $\psi(t)$ solves the Cauchy problem (1), with $\psi(0) = \psi_0 \in \mathcal{D}(H)$

then, with $\dot{\psi} = \frac{\partial}{\partial t} \psi$

$$\frac{d}{dt} \langle \psi(t), \psi(t) \rangle = \langle \dot{\psi}, \psi \rangle + \langle \psi, \dot{\psi} \rangle$$

$$= \langle \tfrac{1}{i\hbar} H \psi, \psi \rangle + \langle \psi, \tfrac{1}{i\hbar} H \psi \rangle$$

$$= \frac{1}{i\hbar} \left(\langle \psi, H\psi \rangle - \langle H\psi, \psi \rangle \right) = 0$$

if H is symmetric (and if $\psi(0) \in \mathcal{D}(H)$)

Note that we implicitly assumed here that things are nice: we needed a) $\psi_0 \in \mathcal{D}(H) \Rightarrow \psi(t) \in \mathcal{D}(H)$ $\forall t$

b) The Cauchy problem (1) has a solution !

In the following we consider the Cauchy-problem for an abstract linear operator H on a Hilbert-space $\mathcal{H}$.

<u>Definition 1:</u> We say the dynamics exists, if for all $\psi_0 \in \mathcal{H}$ the Cauchy problem (1) has a unique solution which conserves probability.

<u>Theorem 2:</u> The dynamics exists iff H is self-adjoint.

We want to prove this, but first we need to give meaning of most of the above words.

I.2 Some mathematical supplements

I.2.1 Spaces, norms, scalar products etc.

Vector spaces: A vector space V is a collection of elements for which the operations of addition, $(u,v) \mapsto u+v$ and multiplication by a (real or complex) number, $\mathbb{F} \times V \ni (\alpha, v) \mapsto \alpha v$ $\quad \mathbb{F} = \mathbb{R}$ or $\mathbb{C}$ are defined such that

$$u+v = v+u \quad \text{(commutativity)}$$

$$u+(v+w) = (u+v)+w \quad \text{(associativity)}$$

$$u+0 = 0+u = u \quad \text{(existence of zero vector)}$$

$$\alpha(\beta u) = (\alpha\beta) u$$

$$(\alpha+\beta) u = \alpha u + \beta u$$

$$\alpha(u+v) = \alpha u + \alpha v$$

$$0 \cdot v = 0, \quad 1 \cdot v = v$$

hold. We also denote $-v = (-1) \cdot v$

Elements of a vector space are called vectors

Examples

a) $\mathbb{R}^d = \{x = (x_1, \dots, x_d) \mid x_j \in \mathbb{R} \quad j = 1, \dots, d\}$

Euclidian space of dimension d.

b) $\mathcal{C}(\Omega)$ = space of continuous functions on Ω

(real or complex valued)

c) $\mathcal{C}^k(\Omega)$ = space of k times cont. diff. f'cts on Ω

($\Omega \subset \mathbb{R}^d$ open)

Norms: A norm on a vector space V is a map

$V \ni u \mapsto \|u\| = \|u\|_V \in \mathbb{R}_+ = [0, \infty)$ s.t.

a) $\|\alpha u\| = |\alpha| \, \|u\|$

b) $\|u+v\| \le \|u\| + \|v\|$ (Δ-ineq.)

c) $\|u\| = 0 \iff u = 0$.

Ex: • $V = \mathbb{R}^d$ $\|x\| = |x| = \left(\sum_{j=1}^{d} x_j^2\right)^{d}$

• $\|f\|_\infty := \sup_{x \in \Omega} |f(x)|$, $f \in \mathcal{C}(\Omega)$.

• $\|f\|_{C^k} := \max_{0 \le |\alpha| \le k} \left\| \frac{d^\alpha}{dx^\alpha} f \right\|_\infty$ on $\mathcal{C}^k(\Omega)$

- $\|f\|_p = \|f\|_{L^p} := \left(\int_\Omega |f(x)|^p \, d\mu \right)^{1/p}$

A <u>normed vector space</u> is a vector space equipped with a norm.

<u>Examples</u>
- $\mathbb{R}^d$ with $\|x\| = |x|$
- $\mathcal{C}_b(\Omega) \subset \mathcal{C}(\Omega)$, cont. bounded fcns on $\Omega \subset \mathbb{R}^d$ with norm $\|f\|_\infty$.
- $\mathcal{C}^k(\Omega)$ with $\|f\|_{\mathcal{C}^k}$ or $\|f\|_p$.

<u>Banach spaces</u>: A normed vector space is complete, if Cauchy sequences converge, i.e., if $(u_n) \subset V$ with $\lim_{l,m \to \infty} \|u_l - u_m\| = 0$, then $\exists\, u \in V$ with

$$\lim_{l \to \infty} \|u - u_l\| = 0.$$

A complete normed vector space is called Banach space

<u>Ex</u>:
- $\mathbb{R}^d$ with norm $\|x\| = |x|$
- $\mathcal{C}_b(\Omega)$ with norm $\|f\|_\infty$
- $\mathcal{C}^k(\Omega)$ with norm $\|f\|_{\mathcal{C}^k}$.

- $1 \le p < \infty$. $L^p(\Omega) := \{ f : \Omega \to \mathbb{C} \mid \int_\Omega |f(x)|^p dx < \infty \}$

with norm $\|f\|_p$

(also $L^\infty(\Omega) = \{ f : \Omega \to \mathbb{C} \mid \operatorname{ess\,sup}_\Omega |f(x)| < \infty \}$

with

$$\|f\|_\infty := \operatorname{ess\,sup}_{x \in \Omega} |f(x)| =$$

$$= \inf (M \mid |f(x)| \le M \text{ almost every } x).$$

Dual space

1) A <u>bounded linear</u> functional on a normed Vector space $(V, \|.\|)$ is a map $\ell : V \to \mathbb{C}$ (or $V \to \mathbb{R}$ if V is a real vector space) s.t. it is linear

$$\ell(\alpha u + \beta v) = \alpha \ell(u) + \beta \ell(v)$$

$\forall\, u, v \in V$, $\alpha, \beta \in \mathbb{C}$ (or $\mathbb{R}$) and there is $C < \infty$ s.t. $|\ell(u)| \le C\|u\|$ $\forall u \in V$.

2) $V^* =$ dual space of V

$:=$ space of all bounded lin. funct. on V.

Note that V^* has a canonical norm given by

$$\|\ell\|_{V^*} := \sup_{\substack{u\in V\\ \|u\|=1}} |\ell(u)|$$

and $(V^*, \|\cdot\|_{V^*})$ is always a Banach-space.

One often writes $\langle \ell, u\rangle := \ell(u)$.

Scalar products and Hilbert spaces

Let $\mathcal{H}$ be a (complex) vector space and assume that $\mathcal{H}$ has an inner-product (scalar product) $\langle \cdot,\cdot\rangle$

i.e., $\langle\cdot,\cdot\rangle : \mathcal{H}\times\mathcal{H} \to \mathbb{C}$ obeys

a) $\langle v, \alpha w + \beta z\rangle = \alpha\langle v,w\rangle + \beta\langle v,z\rangle$

linearity $\forall\, v,w,z \in \mathcal{H},\ \alpha,\beta\in\mathbb{C}$.

b) $\langle w,v\rangle = \overline{\langle v,w\rangle}$ (conjugate symmetry)

c) pos. definite $\langle v,v\rangle \geq 0$ for all $v\in\mathcal{H}$

$$\langle v,v\rangle = 0 \Rightarrow v = 0.$$

Note: • Cauchy Schwarz ineq.: For $u,w\in\mathcal{H}$

$$|\langle u,w\rangle| \leq \|u\|\,\|w\|$$

with $\|u\| := \sqrt{\langle u,u\rangle}$.

- Because of Cauchy-Schwarz, $\|u\|$ is a norm on $\mathcal{H}$.

If $\mathcal{H}$ is complete under $\|\cdot\| := \sqrt{\langle \cdot, \cdot \rangle}$, then $\mathcal{H}$ is called Hilbert space.

Ex:

- $$L^2(\mathbb{R}^d) := \{ \psi : \mathbb{R}^d \to \mathbb{C} \mid \int_{\mathbb{R}^d} |\psi(x)|^2 dx < \infty \}$$

with $\langle \psi, \phi \rangle := \int_{\mathbb{R}^d} \overline{\psi} \phi \, dx = \int \overline{\psi} \phi$

- Sobolev space of order n, $n \in \mathbb{N}$:

$$H^n(\mathbb{R}^d) = \{ \psi \in L^2(\mathbb{R}^d) \mid \partial^\alpha \psi \in L^2(\mathbb{R}^d) \ \forall \alpha, |\alpha| \leq n \}$$

$\alpha = (\alpha_1, .., \alpha_d) \in \mathbb{N}_0^d$ multiindex

$|\alpha| := \sum_{j=1}^{d} \alpha_j$.

$$\partial^\alpha \psi = \partial_1^{\alpha_1} \partial_2^{\alpha_2} \dots \partial_d^{\alpha_d} \psi$$

with inner product

$$\langle \psi, \phi \rangle_{H^n} := \sum_{0 \leq |\alpha| \leq n} \langle \partial^\alpha \psi, \partial^\alpha \phi \rangle$$

With the help of the Fourier transform one can characterize the Sobolev space

$$\psi \in H^n(\mathbb{R}^d) \iff \int_{\mathbb{R}^d} (1+|\xi|^2)^n |\hat{\psi}(\xi)|^2 d\xi < \infty$$

$$\iff \int_{\mathbb{R}^d} (1+|\xi|^{2n}) |\hat{\psi}(\xi)|^2 d\xi < \infty .$$

Parseval relation

A set $\{v_n \mid n \in \mathbb{N}\} \subset \mathcal{H}$ is orthonormal if

$\|v_n\| = 1$ all n, $\langle v_n, v_m \rangle = 0$ if $n \neq m$.

It is a complete orthonormal set (or a basis) if in addition

$$\overline{\mathrm{Span}(v_n \mid n \in \mathbb{N})} = \mathcal{H}$$

where $\overline{A}$ = closure of $A \subset \mathcal{H}$.

= set of all limit points

$\mathrm{Span}(v_n \mid n \in \mathcal{H})$ = set of finite linear combinations of the v_n.

Parseval relation: If $\{v_n\}_n$ is a complete orthonormal set, then $\forall w \in \mathcal{H}$

$$\|w\|^2 = \sum_n |\langle w, v_n \rangle|^2$$

For physicists:

$$= \sum_n \langle w, v_n \rangle \langle v_n, w \rangle$$

$$= \langle w | \sum_n |v_n\rangle \langle v_n | w \rangle$$

so $\sum_n |v_n\rangle\langle v_n| =$ identity on $\mathcal{H}$.

Riesz representation

If $\mathcal{H}$ is a Hilbert space, then its dual $\mathcal{H}^*$ can be identified with $\mathcal{H}$ itself via the map

$$\mathcal{H} \ni u \mapsto l_u := \langle u, \cdot \rangle \in \mathcal{H}^*$$

$$l_u(v) = \langle u, v \rangle \quad \forall v \in \mathcal{H}.$$

Thm (Riesz) The above map is onto, i.e., for any $l \in \mathcal{H}^*$ exists $u \in \mathcal{H}$ s.t. $l = l_u = \langle u, \cdot \rangle$.

I.2.2 Operators on Hilbert spaces

A linear operator (or short operator) on a Hilbert space $\mathcal{H}$ is a tuple $(A, D(A))$,

$D(A) =$ domain of $A \subset \mathcal{H}$ linear & dense subset.

and $A : \mathcal{D}(A) \to \mathcal{H}$ s.t. $\forall\, u, v \in \mathcal{D}(A), \alpha, \beta \in \mathbb{C}$

$$A(\alpha u + \beta v) = \alpha A u + \beta A v$$

Ex
- identity $\mathbb{1} = id : \psi \to \psi$ $\quad \mathcal{D}(\mathbb{1}) = \mathcal{H}$

- Multiplication by a coordinate

$$x_j : \psi \mapsto x_j \psi$$

i.e., $(x_j \psi)(x) := x_j \psi(x)$.

$$\mathcal{D}(x_j) = \{\psi \in L^2 \mid \int x_j^2 |\psi(x)|^2 dx < \infty\}$$
$$\subsetneq L^2(\mathbb{R}^2).$$

Note $C_0^\infty(\mathbb{R}^d) =$ set of ∞ often diff. fcns with compact support

is dense in $L^2(\mathbb{R}^d)$ and $C_0^\infty(\mathbb{R}^d) \subset \mathcal{D}(x_j)$

so $\mathcal{D}(x_j)$ is dense in $L^2(\mathbb{R}^d)$.

- Momentum operator

$$p_j : \psi \mapsto -i\hbar\, \partial_j \psi$$

$$\mathcal{D}(p_j) = \{\psi \in L^2 \mid \partial_j \psi \in L^2\}$$
$$= \{\psi \in L^2 \mid \int k_j^2 |\hat{\psi}(k)|^2 dk < \infty\}$$

again $\mathcal{C}_c^\infty(\mathbb{R}^d) \subset \mathcal{D}(p_j)$, so $\mathcal{D}(p_j)$ is dense in L^2.

- Laplace $\quad \Delta : \psi \mapsto \sum_{j=1}^{d} \partial_j^2 \psi$

$$\mathcal{C}_c^\infty \subset \mathcal{D}(\Delta) = \{ \psi \in L^2 \mid \Delta \psi \in L^2 \}$$
$$= \{ \psi \in L^2 \mid \int k^2 |\hat{\psi}(k)|^2 dk < \infty \}$$

- Multiplication by a function $V : \mathbb{R}^d \to \mathbb{R}$.

$$V : \psi \mapsto V\psi \quad , \text{i.e. } (V\psi)(x) := V(x)\psi(x).$$

$$D(V) = \{ \psi \in L^2 \mid \int V(x)^2 |\psi(x)|^2 dx < \infty \}$$
$$\supset \mathcal{C}_c^\infty \text{ if } V \in L^2_{loc}$$

- Schrödinger operator

$$H : \psi \mapsto -\frac{\hbar^2}{2m} \Delta\psi + V\psi$$

$$\mathcal{D}(H) = \mathcal{D}(H) \cap \mathcal{D}(V).$$

- Integral operator

$$K : \psi \mapsto \int k(\cdot, y)\, \psi(y) dy$$

i.e., $\quad (K\psi)(x) := \int k(x,y)\, \psi(y) dy$

$k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$ is called integral kernel of K

Def 3 An operator A on $\mathcal{H}$ is bounded, if

$$\|A\| := \underbrace{\sup\left(\|A\psi\| \,/\, \psi \in \mathcal{D}(A), \|\psi\| = 1 \right)}_{\text{operator norm}} < \infty$$

$$= \sup\left(\|A\psi\| \,/\, \psi \in \mathcal{D}(A), \|\psi\| \leq 1 \right)$$

$$= \sup\left(\|A\psi\| \,/\, \psi \in \mathcal{D}(A), \|\psi\| < 1 \right)$$

$\mathcal{L}(\mathcal{H})\ (= \mathcal{B}(\mathcal{H}))$ = set of all bounded linear operators.

Note ($(\mathcal{L}(\mathcal{H}), \|.\|)$ is a Banach space)

Lemma 4 If an operator A satisfies $\|A\psi\| \leq C\|\psi\|$ for all ψ in a dense domain $D \subset \mathcal{H}$, then its extends uniquely to a bounded operator (also called A) on all of $\mathcal{H}$ with $\|A\psi\| \leq C\|\psi\| \quad \forall \psi \in \mathcal{H}$.

idea of proof: If $u \in \mathcal{H} \Rightarrow \exists\, (u_n)_n \subset D$, $u_n \to u$ (D is dense in $\mathcal{H}$). So, since

$$\|Au_n - Au_m\| \leq C\|u_n - u_m\| \to 0 \quad n,m \to \infty$$

$(Au_n)_n$ is Cauchy in $\mathcal{H}$. So

$$v := \lim_{n\to\infty} Au_n \quad \text{exists}$$

Define $Au := v = \lim_{n\to\infty} Au_n$. Done.

<u>Remark</u>: One needs to check consistency, i.e., if $u_n \to u$ and $\tilde{u}_n \to u$, then $v = \lim Au_n = \lim A\tilde{u}_n$ and that A is bounded with $\|A\| \leq C$.