MATHEMATICAL COMPLEMENT to QUANTUM MECHANICS (MA4A7)

I. Spaces of Functions

The Lebesgue space $L^2(\mathbb{R}^d)$ is the linear space of all measurable functions $f : \mathbb{R}^d \to \mathbb{C}$ such that

$$\int |f(x)|^2 dx < \infty .$$

This is a Hilbert space with the inner product

$$(f,g) = \int \overline{f(x)}\, g(x)\, dx .$$

$L^2(\mathbb{R}^d)$ is separable, and many nice sets of functions are dense. For instance, the set of C^∞ functions with compact support. Another useful space is the Schwartz space.

Definition 1. A function $f \in C^\infty(\mathbb{R}^d)$ is Schwartz if $\forall \alpha \in \mathbb{N}^d$, $\forall k \in \mathbb{N}$, we have

$$\sup_{x \in \mathbb{R}^d} \|x\|^k \left| \frac{\partial^{\alpha_1 + \dots + \alpha_d}}{\partial x_1^{\alpha_1} \dots \partial x_d^{\alpha_d}} f(x) \right| < \infty .$$

The Fourier transform plays a central rôle in quantum mechanics.

Definition 2. The Fourier transform $\hat{f}$ of $f \in L^1(\mathbb{R}^d)$ is

$$\hat{f}(k) = \int e^{-ikx} f(x)\, dx .$$

The inverse Fourier transform $f^\vee$ of $f \in L^1$ is

$$f^\vee(x) = \frac{1}{(2\pi)^d} \int e^{ikx} f(k)\, dk .$$

If $f, \hat{f}$ both belong to L^1, we have $f = (\hat{f})^\vee = \widehat{f^\vee}$. Further, we have Plancherel theorem:

$$\|f\| = \frac{1}{(2\pi)^{d/2}} \|\hat{f}\| .$$

(Unless specified otherwise, $\|\cdot\|$ denotes the L^2 norm.) The theorem also applies to the inner product:

$$(f,g) = \frac{1}{(2\pi)^d} (\hat{f}, \hat{g}) .$$

Recall that the Fourier transform of L^1 functions, defined above, can be extended to all L^2 functions by continuity. Indeed, let $\mathcal{F} : L^2 \to L^2$ denote the map $f \mapsto \hat{f}$. It is defined on a dense set of functions in L^2 by the integral above. $\mathcal{F}$ is linear, and $\underset{\text{op. norm}}{\|\mathcal{F}\|} = (2\pi)^{d/2} < \infty$ so $\mathcal{F}$ is continuous and it can be extended to all of $L^2(\mathbb{R}^d)$. The inverse map $\mathcal{F}^{-1}$ exists for the same reason.

Definition 3. The weak derivative of f in the direction $j = 1, \dots, d$, noted $\frac{\partial f}{\partial x_j}$, is the function that satisfies

$$\int \phi(x) \frac{\partial f}{\partial x_j} dx = -\int \frac{\partial \phi}{\partial x_j} f\, dx \quad \forall \text{ Schwartz fct } \phi .$$

If this function exists, it is unique.

<u>Definition 4.</u> The <u>Sobolev space</u> $H^1 = H^1(\mathbb{R}^d)$ is the space of all $f \in L^2$ such that $\frac{\partial f}{\partial x_j}$ exists and belongs to L^2, for all $j = 1, \dots, d$. It is a Hilbert space with the Sobolev inner product

$$(f,g)_{H^1} = (f,g)_{L^2} + \sum_{j=1}^{d} \left(\frac{\partial f}{\partial x_j}, \frac{\partial g}{\partial x_j} \right)_{L^2} = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} (1 + \|k\|^2) \overline{\hat{f}(k)} \hat{g}(k) \, dk$$

II. <u>Operator theory</u>

We review essential notions about operators in infinite-dimensional Hilbert spaces. The Laplacian is an interesting and useful example. The main complication of unbounded operators is that they are only defined on a subspace of the Hilbert space.

<u>Definition 5.</u> A <u>densely-defined operator</u> on $\mathcal{H}$ is a pair $(T, D(T))$ where the <u>domain</u> $D(T)$ is a dense linear subspace of $\mathcal{H}$, and T is a linear map $D(T) \to \mathcal{H}$.

For example, $\mathcal{H} = L^2(\mathbb{R}^d)$, $T = \Delta = \sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2}$ and $D(T) = S(\mathbb{R}^d)$ (the Schwartz space), or $D(T) = L^2 \cap C^2, \dots$ Exercise: check that Δ is unbounded.

Any operator T has an adjoint T^*. In words, T^* is an operator $D(T^*) \to \mathcal{H}$ such that $(Tf, g) = (f, T^*g)$ $\forall f \in D(T)$, $\forall g \in D(T^*)$, and the domain of T^* is the largest possible. Notice that $D(T^*)$ is not necessarily dense.

<u>Definition 6.</u> Let $T: D(T) \to \mathcal{H}$ where $D(T)$ is dense in $\mathcal{H}$. The <u>domain of the adjoint</u> is

$$D(T^*) = \{ f \in \mathcal{H} : \exists g \in \mathcal{H} \text{ s.t. } (Th, f) = (h, g) \; \forall h \in D(T) \}.$$

If such g exists, it is unique because $D(T)$ is dense. Then the <u>adjoint</u> is the operator T^* that assigns $T^*f = g$ to each $f \in D(T^*)$.

In the case where T is bounded, Riesz representation theorem implies that $D(T^*) = \mathcal{H}$. And if $\dim \mathcal{H} < \infty$, the adjoint of a matrix is the hermitian conjugate.

<u>Definition 7.</u>

An operator $T: D(T) \to \mathcal{H}$ is <u>symmetric</u> if $(Tf, g) = (f, Tg)$ $\forall f, g \in D(T)$.

An operator $T: D(T) \to \mathcal{H}$ is <u>self-adjoint</u> if $T^* = T$.

One can check that T is symmetric if T^* is an extension of T, i.e. if $D(T^*) \supset D(T)$ and $T^*f = Tf$ $\forall f \in D(T)$.