Reading: Woit Chapter 21.1, 21.3, Chapter 22.1, 22.2

The main aim of this assignment is to build on the material on Hilbert spaces from Assignment 3 to explain the kinds of operators which occur in quantum mechanics. The key idea is that of self-adjointness.

1. Facts about Sobolev spaces

The *Sobolev space* of order n is a generalization of L^2; it is the Hilbert space of complex-valued functions all of whose derivatives up to and including n are in L^2.

$$H^n(\mathbb{R}) = \{\psi \in L^2(\mathbb{R}) \mid \psi', \psi'', \ldots, \psi^{(n)} \in L^2(\mathbb{R})\}$$

The inner product making this into a Hilbert space is

$$\langle \psi_1, \psi_2 \rangle_{H^n} = \sum_{k=1}^{n} \langle \psi_1^{(k)}, \psi_2^{(k)} \rangle.$$

So, although H^n is a proper linear subspace of L^2, the inner product which makes it into a Hilbert space is different from the L^2 norm. In fact, H^n is not closed as a subspace of L^2, but is actually dense. The Sobolev spaces have a very nice description in terms of the Fourier transform $\mathcal{F}(\psi) = \hat{\psi}$:

$$\psi \in H^n(\mathbb{R}) \Leftrightarrow \int_{\mathbb{R}} (1 + |k|^2)^n |\hat{\psi}(k)|^2 dk < \infty.$$

All of this also holds for functions on S^1, and we have a similar characterization in terms of the Fourier transform $\mathcal{F}(\psi) = (a_k)_{k\in\mathbb{Z}} \in \ell^2(\mathbb{Z})$:

$$\psi \in H^n(S^1) \Leftrightarrow \sum_{k\in\mathbb{Z}} (1 + |k|^2)^n |a_k|^2 < \infty.$$

The remarkable lemma of Sobolev then states that if $\psi \in H^n$ on a bounded interval (or on the circle), then ψ is automatically $n-1$-times continuously differentiable; furthermore the pointwise norm of these derivatives is bounded above by the Sobolev norm of ψ. For example, if $\psi \in H^1(S^1)$, then it is automatically a continuous function, whose value at any point may not exceed $\langle \psi, \psi \rangle_{H^1}$.

2. Facts about self-adjointness

An operator on the Hilbert space $\mathcal{H}$ is a pair $(A, D(A))$ (usually denoted just A) where $D(A) \subset \mathcal{H}$ is a dense linear subspace and $A : D(A) \to \mathcal{H}$ is a linear map. An extension $\tilde{A}$ of A is an operator such that $D(A) \subset D(\tilde{A})$ and which agrees with A on $D(A)$.

Definition 1. Let A be an operator on $\mathcal{H}$. The adjoint A^* is the operator with domain $D(A^*) \subset \mathcal{H}$ given by

$$D(A^*) = \{y \in \mathcal{H} \mid \text{ there is a } z \in \mathcal{H} \text{ with } \langle Ax, y \rangle = \langle x, z \rangle \text{ for all } x \in D(A)\}.$$

If $y \in D(A^*)$, we define $A^*y = z$, where z is the unique element such that $\langle Ax, y \rangle = \langle x, z \rangle$ for all $x \in D(A)$. Finally, We say that the operator A is *self-adjoint* when it coincides with A^*, meaning that $D(A) = D(A^*)$ and on this subspace $A = A^*$.

Exercise 1. When an operator A satisfies $\langle Ax, y\rangle = \langle x, Ay\rangle$ for all $x, y \in D(A) \subset \mathcal{H}$, we say that it is *symmetric*. Show that A is symmetric if and only if A^* is an extension of A.

Exercise 2. Let $A = -i\frac{d}{d\theta}$, the differentiation operator on $\mathcal{H} = L^2(S^1)$.

1. Apply A to the Fourier basis and, using the above facts, show that A is not defined on all of L^2 (give an example of an L^2 function which must not lie in the domain of A)

2. Show that the largest possible domain of A must be $H^1(S^1) \subset L^2(S^1)$, and define A on this domain [use the Fourier transform again].

3. Compute the adjoint of A by first determining $D(A^*)$ and then defining A^*. Conclude by establishing that A is self-adjoint.

4. How is the above affected if we consider the differential operator A^2? Is A^2 also self-adjoint?

Exercise 3. Let $v : S^1 \to \mathbb{R}$ be a real-valued function and let $V : \psi \mapsto v\psi$ be the operator on $\mathcal{H} = L^2(S^1)$ defined by multiplication by v.

1. If v is a continuous function on the circle, prove that V is a bounded operator defined on all of $\mathcal{H}$, that is $D(V) = \mathcal{H}$ and there exists $M \in \mathbb{R}$ positive such that for all $\psi \in \mathcal{H}$, $||V\psi|| \leq M||\psi||$.

2. Let $v = 1/\sin\theta$, a function with singularities at $\theta = 0$ and $\theta = \pi$. Show that V is self-adjoint if we take $D(V)$ to be all functions ψ such that $\psi/\sin\theta \in L^2(S^1)$.

Exercise 4. For this exercise, we work in $\mathcal{H} = L^2([0,1])$, the square-integrable complex-valued functions on the interval $[0,1]$. The Sobolev spaces $H^n([0,1])$ are defined exactly as for the real line, and we have the following useful description of them. A *test function* is any smooth function on $[0,1]$ which vanishes outside some sub-interval $[\epsilon, 1-\epsilon]$ for $\epsilon > 0$. In particular, test functions and all their derivatives vanish at the endpoints of $[0,1]$. A function f in $L^2([0,1])$ is said to have *weak derivative* g when, for all test functions ϕ, we have

$$\int_0^1 g\phi\, dx = -\int_0^1 f\phi'\, dx.$$

(Certainly if f were smooth, then $g = f'$ satisfies the above equation, by integration by parts.) In fact, the Sobolev space $H^n([0,1])$ consists of the functions in L^2 with n weak derivatives in L^2.

Now consider the operator $A\psi = \psi''$, the second derivative operator.

1. First take the domain of A to be $D_0 = H^2([0,1])$, the maximal possible domain. Prove that for $f, g \in D_0$,

   $$\langle Af, g\rangle - \langle f, Ag\rangle = (\overline{f'(1)}g(1) - \overline{f(1)}g'(1)) - (\overline{f'(0)}g(0) - \overline{f(0)}g'(0))$$

   Conclude that A is not symmetric if we take $D(A) = D_0$.

2. Now take the domain of A to be $D_1 = \{f \in H^2([0,1]) \mid f(0) = f(1) = 0\}$.

   Using the above characterization of the Sobolev spaces, the fact that test functions lie in D_1, and the first part of this exercise to prove that (A, D_1) is a self-adjoint operator.