1. The Laplace operator as a self adjoint operator

For $f \in \mathcal{S}(\mathbb{R}^d)$ we define, as usual,

$$\Delta f(x) = \sum_{j=1}^{d} \frac{\partial^2 f}{\partial x_j^2}(x) \ .$$

Thus we can consider Δ as a linear operator with $D(\Delta) = \mathcal{S}(\mathbb{R}^d)$. It is easy to see that for any $f, g \in \mathcal{S}(\mathbb{R}^d)$

$$\langle \Delta f, g\rangle = \langle f, \Delta g\rangle \ ,$$

and since $\mathcal{S}(\mathbb{R}^d)$ is dense in $L^2(\mathbb{R}^d)$ we see that Δ with domain $D(\Delta)$ is a symmetric operator. The operator Δ is not closed. This is easy to see. E.g., take any function $f \in C^2(\mathbb{R}^d)$ which decays including its derivatives faster than any inverse polynomial at infinity. It is not hard to construct a sequence of functions $f_n \in \mathcal{S}(\mathbb{R}^d)$ so that $f_n \to f$ and $\Delta f_n \to \Delta f$ in $L^2(\mathbb{R}^d)$. The goal of this note is to find a self adjoint extension of Δ.

Using the Fourier Transform we find that

$$|2\pi k|^2 \widehat{f}(k) = \int_{\mathbb{R}^d} e^{-2\pi i k\cdot x} (-\Delta f)(x) dx$$

so that

$$-\Delta f(x) = \mathcal{F}^{-1} |2\pi k|^2 \mathcal{F} f = \mathcal{F}^* |2\pi k|^2 \mathcal{F} f \tag{1}$$

We use this formula to find a self adjoint extension of Δ or rather $-\Delta$.

Lemma 1.1. *On*

$$D(A) := \{\widehat{f} \in L^2(\mathbb{R}^d) : \int_{\mathbb{R}^d} |2\pi k|^4 |\widehat{f}(k)|^2 dk < \infty\}$$

define the operator

$$A\widehat{f}(k) := |2\pi k|^2 \widehat{f}(k) \ .$$

Then A is self adjoint.

Proof. Clearly, A is symmetric. Pick any $\widehat{f} \in D(A^*)$. Then for all $g \in D(A)$ we have that

$$|\langle \widehat{f}, A\widehat{g}\rangle| \le C \|\widehat{g}\|_2 \ ,$$

where the constant C depends only on $\widehat{f}$. Pick

$$\widehat{g}(k) = |2\pi k|^2 \widehat{f}(k) \chi_{|k|<R} \chi_{\{k : |\widehat{f}(k)| < R\}}$$

where $\chi_A(k)$ denotes the characteristic function of the set A, i.e., $\chi_A(k) = 1$ if $k \in A$ and $\chi_A(k) = 0$ if $k \notin A$. Note that this function is in $D(A)$. Now

$$|\langle \widehat{f}, A\widehat{g}\rangle| = \int_{\{|k|<R\}\cap\{k:|\widehat{f}(k)|<R\}} |\widehat{f}(k)|^2 |2\pi k|^4 dk \le C \left[\int_{\{|k|<R\}\cap\{k:|\widehat{f}(k)|<R\}} |\widehat{f}(k)|^2 |2\pi k|^4 dk\right]^{1/2}$$

so that

$$\int_{\{|k|<R\}\cap\{k:|\widehat{f}(k)|<R\}} |\widehat{f}(k)|^2 |2\pi k|^4 dk \le C^2 \ .$$

Letting $R \to \infty$ and using the monotone convergence theorem we find that $\widehat{f} \in D(A)$ and hence A is self adjoint. □

Corollary 1.2. *The operator*

$$H_0 := \mathcal{F}^* |2\pi k|^2 \mathcal{F} \tag{2}$$

on the domain $D(H_0)$ *which consists of all functions* $f \in L^2(\mathbb{R}^d)$ *whose Fourier Transform* $\widehat{f}(k)$ *satisfies*

$$\int_{\mathbb{R}^d} |2\pi k|^4 |\widehat{f}(k)|^2 dk < \infty$$

is selfadjoint. Moreover, H_0 *is an extension of* $-\Delta$ *on*

Proof. H_0 is unitarily equivalent to A and hence self adjoint. For $f \in \mathcal{S}(\mathbb{R}^d)$ we have that

$$H_0 f = \mathcal{F}^* |2\pi k|^2 \mathcal{F} f = -\Delta f$$

using (1) and hence H_0 is an extension of $-\Delta$. □

Note that $D(H_0)$ is not really accessible. It is difficult to decide whether any given function is in $D(H_0)$ or not. So, while it is very important to know that H_0 is self adjoint, for computational purposes, H_0 is useless. One might argue that H_0 is an extension of $-\Delta$ defined on $\mathcal{S}(\mathbb{R}^d)$ and on this space one can inded compute. The problem, however, is that there might be other self adjoint extensions of $-\Delta$ on $\mathcal{S}(\mathbb{R}^d)$. Which one should one choose? We shall show that $-\Delta$ on $\mathcal{S}(\mathbb{R}^d)$ specifies the self adjoint extension uniquely, i.e, there are no others. This is the source of the following definition.

Definition 1.3. *An operator* A *with domain* $D(A)$ *is* **essentially self adjoint** *if the closure* $\overline{A}$ *is self adjoint. In this case we call* $D(A)$ *a* **core** *of* $\overline{A}$.

Here is a simple of what can go wrong. Consider the Hilbert space $L^2(0,1)$ and consider the operator

$$Af(x) = \frac{1}{i}\frac{df}{dx}(x)$$

with domain $C_c^\infty(0,1)$, i.e., all infinitely differentiable functions that have compact support in the interval $(0,1)$. It is easy to see that A is symmetric. One can also compute $\overline{A}$, the closure of the operator A. Its domain is the set

$$\{f \text{ absolutely continuous on } (0,1)\ , f(0) = f(1) = 0\}\ .$$

Take any smooth function g with $g(1), g(0)$ not necessarily equals to zero and compute

$$\langle \overline{A} f, g\rangle = \langle f, \frac{1}{i}\frac{dg}{dx}\rangle\ .$$

There are no boundary terms since $f(0) = f(1) = 0$ Thus, clearly ,$\overline{A}$ is not self adjoint. We shall see later that the operator A has infinitely many self adjoint extensions, depending on the **boundary conditions** one imposes. Boundary conditions are an important part of the physical description of a process. E.g., if and considers the heat equation on a bounded domain, one can fix the temparature on the boundary to be zero or one could choose insulating boundary conditions, which means the the normal derivative of the temperature function vanishes on the boundary.

We shall now prove that $-\Delta$ on $\mathcal{S}(\mathbb{R}^d)$ is essentially self adjoint, in fact we shall show more.

Theorem 1.4. *Define*

$$Bf(x) = -\Delta f(x)$$

with

$$D(B) = C_c^\infty(\mathbb{R}^d)\ .$$

Then B is essentially self adjoint, in fact $\overline{B} = H_0$.

Proof. For any given $f \in D(H_0)$ we have to produce a sequence of functions $f_n \in C_c^\infty(\mathbb{R}^d)$ such that $f_n \to f$ and $-\Delta f_n \to H_0 f$.

Let $\phi \in C_c^\infty(B(0,1))$ where $B(0,1)$ is the unit ball centered at the origin. Assume that $\phi \geq 0$, $\int_{\mathbb{R}^d} \phi(x)dx = 1$. Such functions do exists, e.g., set

$$\phi(x) = \text{const.} e^{-\frac{1}{1-|x|^2}} \text{ if } x \neq 0$$

and set $\phi(x) = 0$ for all x with $|x| > 1$. It is a standard exercise to see that $\phi \in C_c^\infty(B(0,1))$ and the constant in front of the function can be adjusted so that the function integrates to one.

Now, consider

$$\phi_\delta(x) = \delta^{-d}\phi(\frac{x}{\delta})$$

which is now a smooth function with support in the ball $B(0,\delta)$ and whose integral over the whole space is again one. Now pick any $f \in D(H_0)$ and consider

$$f_\delta(x) = \int_{\mathbb{R}^d} \phi_\delta(x-y)f(y)dy \ .$$

It is very easy to see that f_δ is $C^\infty(\mathbb{R}^d)$ and that

$$-\Delta f_\delta(x) = -\int_{\mathbb{R}^d} \Delta\phi_\delta(x-y)f(y)dy \ .$$

Since for every fixed x the function $\phi_\delta \in D(H_0)$ we can rewrite the above expression as

$$-\Delta f_\delta(x) = -\langle H_0\phi_\delta(x-\cdot), f\rangle \ ,$$

and since $f \in D(H_0)$ and H_0 is symmetric this equals

$$-\langle \phi_\delta(x-\cdot), H_0 f\rangle = -(H_0 f)_\delta \ .$$

It is a general fact from real analysis that for any $g \in L^2(\mathbb{R}^d)$

$$\lim_{\delta\to 0} \|g_\delta - g\| = 0 \ .$$

Once more, this fact is closely related to the outer regularity of Lebesgue measure.

Another useful fact is the inequality

$$\|g_\delta\| \leq \|g\| \ . \tag{3}$$

This fact follows essentially from an integral version of the triangle inequality, which is called Minkowski's inequality, i.e.,

$$\left[\int_{\mathbb{R}^d} |\int_{\mathbb{R}^d} \phi_\delta(x-y)g(y)dy|^2 dx\right]^{1/2} = \left[\int_{\mathbb{R}^d} |\int_{\mathbb{R}^d} \phi_\delta(y)g(x-y)dy|^2 dx\right]^{1/2}$$

$$\leq \int \phi_\delta(y)\left[\int_{\mathbb{R}^d} |g((x-y)|^2 dx\right]^{1/2} dy \ ,$$

and since

$$\int_{\mathbb{R}^d} |g((x-y)|^2 dx = \int_{\mathbb{R}^d} |g((x)|^2 dx$$

we find the bound

$$\int \phi_\delta(y)dy \left[\int_{\mathbb{R}^d} |g((x)|^2 dx\right]^{1/2} = \|g\|$$

With these facts at our disposal we can now advance our argument, namely

$$\|f_\delta - f\| \to 0 \ , \ \|H_0 f - (-\Delta f_\delta)\| \to 0$$

as $\delta \to 0$. The sequence of functions f_δ is in $C^\infty(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$ and does not have compact support, so we are not quite there yet.

Pick any function $w \in C_c^\infty(\mathbb{R}^d)$ such that $w(x) = 1$ on the unit ball $B(0,1)$. For $\delta > 0$ fixed consider the sequence

$$f_{n,\delta}(x) = w(\frac{x}{n}) f_\delta(x) \ .$$

Clearly, for any fixed δ, n this function is in $C_c^\infty(\mathbb{R}^d)$. Using the monotone convergence theorem,

$$\lim_{n\to\infty} \|f_\delta - f_{n,\delta}\|^2 = \lim_{n\to\infty} \int_{\mathbb{R}^d} |(1 - w(\frac{x}{n})|^2 |f_\delta(x)|^2 dx \le \lim_{n\to\infty} \int_{|x|>n} |f_\delta(x)|^2 dx = 0 \ .$$

Next we compute

$$\Delta f_{n,\delta}(x) = \frac{1}{n^2}(\Delta w)(\frac{x}{n}) f_\delta(x) + 2\frac{1}{n}(\nabla w)(\frac{x}{n}) \cdot \nabla f_\delta(x) + w(\frac{x}{n}) \Delta f_\delta(x) \ ,$$

so that

$$\|\Delta f_{n,\delta} - \Delta f_\delta\| \le \frac{1}{n^2}\|(\Delta w)(\frac{\cdot}{n}) f_\delta\| + 2\frac{1}{n}\|(\nabla w)(\frac{\cdot}{n}) \cdot \nabla f_\delta\| + \|(1 - w(\frac{x}{n}))\Delta f_\delta\| \ .$$

Since w including its derivatives is bounded we find

$$\|\Delta f_{n,\delta} - \Delta f_\delta\| \le C\frac{1}{n^2}\|f_\delta\| + 2C\frac{1}{n}\|\nabla f_\delta\| + \|(1 - w(\frac{x}{n}))\Delta f_\delta\|$$

where C is some constant independent of n, δ. Since

$$\lim_{n\to\infty} \|(1 - w(\frac{x}{n}))\Delta f_\delta\| = 0$$

we have that

$$\lim_{n\to\infty} \|\Delta f_{n,\delta} - \Delta f_\delta\| = 0 \ .$$

Pick any $\varepsilon > 0$. There exists $\delta > 0$ so that

$$\left[\|f - f_\delta\|^2 + \|H_0 f - (-\Delta f_\delta\|^2\right]^{1/2} < \frac{\varepsilon}{2}$$

Next for this particular value of δ pick n so that

$$\left[\|f_\delta - f_{n,\delta}\|^2 + \|\Delta f_\delta - \Delta f_{n,\delta}\|\right]^{1/2} < \frac{\varepsilon}{2}$$

and hence

$$\left[\|f - f_{n,\delta}\|^2 + \|H_0 f - (-\Delta f_{n,\delta}\|^2\right]^{1/2} < \varepsilon$$

which is precisely what we wanted to show. □