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- Δ_s is unbounded:
  - This is easy to see using the spectral representation $\hat{\Delta}_s$, which is given by multiplication by an unbounded function $-\omega^2$ on $\mathbb{R}$ (recall Problem Set 2).
  - It is also instructive to see why Δ_s is unbounded directly. Let ϕ be a function in C_0^∞ (such functions exist; see Folland Ch. 0 p. 12, for example) such that $\int_{\mathbb{R}} |\phi(x)|^2 dx = 1$. Define the sequence

$$f_n(x) = n^{1/2} \phi(nx)$$

We calculate $\int |f_n(x)|^2 dx = \int |\phi(nx)|^2 d(nx) = \int |\phi(y)|^2 dy = 1$, so that

$$\|f_n\|_{L^2} = 1 \quad \forall \ n.$$

Now let's examine the L^2-norms of $\Delta_s f_n = f_n''$. We have $f_n'' = n^{5/2} \phi''(nx)$, and thus

$$\int |f_n''(x)|^2 dx = n^4 \int |\phi''(nx)|^2 d(nx) = n^4 \int |\phi''(y)|^2 dy,$$

so

$$\|f''_n\|_{L^2} \to \infty \quad \text{as} \quad n \to \infty,$$

and we see that Δ_s is unbounded.

- $\underline{\Delta_S \text{ is symmetric}}$. By "symmetric", we mean that

$$\langle \Delta_S f, g \rangle = \langle f, \Delta_S g \rangle \quad \text{for all } f, g \in \mathcal{S} = \mathcal{D}(\Delta_S)$$

(Notice that symmetry does not imply self-adjointness because, for the latter, the domains of the operator and its adjoint must coincide.)

* It is easy to show symmetry of Δ_S by showing symmetry of $\hat{\Delta}_S$. For each $g, f \in \mathcal{S}$, we have

$$\langle \hat{\Delta}_S f, g \rangle = \int_{\mathbb{R}} -\omega^2 f(\omega)\, \overline{g(\omega)}\, d\omega$$

$$= \int_{\mathbb{R}} f(\omega) \overline{\left(-\omega^2 g(\omega)\right)}\, d\omega = \langle f, \hat{\Delta}_S g \rangle.$$

* To see the symmetry of Δ_S directly, we use "integration by parts" twice. For $f, g \in \mathcal{S}$,

$$\langle \Delta_S f, g \rangle = \int_{\mathbb{R}} f''(x)\, \overline{g(x)}\, dx =$$

$$= -\int_{\mathbb{R}} f'(x) \overline{g'(x)}\, dx + \underbrace{\lim_{y \to \infty} \left[f'(y)\overline{g(y)} - f'(-y)\overline{g(-y)} \right]}_{=0}$$

$$= -\int_{\mathbb{R}} f'(x) \overline{g'(x)}\, dx$$

$$= \int_{\mathbb{R}} f(x) \overline{g''(x)}\, dx - \underbrace{\lim_{y \to \infty} \left[f(y) \overline{g'(y)} - f(-y) \overline{g'(-y)} \right]}_{=0}$$

$$= \int_{\mathbb{R}} f(x) \overline{g''(x)}\, dx$$

$$= \langle f, \Delta_S g \rangle.$$

- <u>The spectrum of Δ</u>

Before understanding the spectrum of an operator, it is technically necessary to specify its domain. So far, we have dealt with Δ_S, whose domain is the Schwartz class $\mathcal{S}(\mathbb{R})$. We will use the representation of Δ_S under the Fourier transform (which we call $\hat{\Delta}_S$) to determine how to enlarge the domain in order to extend Δ_S to a self-adjoint operator, which we will denote simply by Δ.

<u>Recap</u>: $\mathcal{F}: \mathcal{S} \to \mathcal{S}$ extends to unitary $\mathcal{F}: L^2(\mathbb{R}) \to L^2(\mathbb{R})$

$$\mathcal{D}(\Delta_S) = \mathcal{S} \xrightarrow{\mathcal{F}} \mathcal{S} = \mathcal{D}(\hat{\Delta}_S)$$

$$\Delta_S = \partial_{xx} \text{ on } \mathcal{S} \longrightarrow \hat{\Delta}_S = \mathcal{F}\hat{\Delta}_S\mathcal{F}^{-1} = T_{-\omega^2}\big|_{\mathcal{S}}$$

$$= \text{multiplication by } -\omega^2\text{, restricted to } \mathcal{S}.$$

As we have seen in Problem Set 2, $T_{-\omega^2}$, defined on its natural domain

$$\mathcal{D}(T_{-\omega^2}) = \{ f \in L^2(\mathbb{R}, d\omega) : -\omega^2 f(\omega) \in L^2(\mathbb{R}, d\omega) \}$$

is <u>self-adjoint</u>. Thus we extend $\hat{\Delta}_S$ to $\hat{\Delta}$ by extending the domain!

$$\hat{\Delta} = T_{-\omega^2} \quad \left(\mathcal{D}(\hat{\Delta}) = \mathcal{D}(T_{-\omega^2}) \right)$$

$$\Delta = \mathcal{F}^{-1}\hat{\Delta}\mathcal{F}, \quad \mathcal{D}(\Delta) = \mathcal{F}^{-1}(\mathcal{D}(\hat{\Delta}))$$

Since $\mathcal{F}$ is unitary, <u>Δ is self adjoint on its domain</u>

$$\mathcal{D}(\Delta) = \left\{ \mathcal{F}^{-1} f : f \text{ and } -\omega^2 f \text{ are in } L^2(\mathbb{R}) \right\}.$$

There is a nice characterization of $\mathcal{D}(\Delta)$ in terms of weak derivatives.

Theorem (Theorem IX. 27 of Reed/Simon, Vol II)
Let Δ be defined as above, with the domain $\mathcal{D}(\Delta)$ as specified. Then $\mathcal{D}(\Delta) = H^2(\mathbb{R})$, and Δ is self-adjoint on this domain.

Here are the steps in a proof:

$\boxed{1}$ As we have seen (Prob. Set 2), the operator $T_{-\omega^2}$ of multiplication by $-\omega^2$, with its natural domain defined above, is self-adjoint. Since Δ is unitarily equivalent to $\hat{\Delta} = T_{-\omega^2}$ through the Fourier transform, Δ is self-adjoint on $\mathcal{D}(\Delta) = \mathcal{F}^{-1}(\mathcal{D}(T_{-\omega^2}))$.

$\boxed{2}$ Not only is $\hat{\Delta}$ a self-adjoint extension of $\hat{\Delta}_S$ (by extending the domain from Schwartz class to all of $\mathcal{D}(T_{-\omega^2})$), but it is actually the <u>closure of $\hat{\Delta}_S$</u>, that is, the graph of $\hat{\Delta}$ is the closure in $L^2 \oplus L^2$ of the graph of $\hat{\Delta}_S$:

$$\Gamma(\hat{\Delta}) = \overline{\Gamma(\hat{\Delta}_S)} .$$

This takes some proving, but it is not too hard (Try it.).
<u>Notes</u>: In Problem Set 2, you saw that <u>all adjoints are closed</u> (a similar proof is valid in general, not just for multiplication operators), so $\hat{\Delta}$ is closed. Since the closure of $\hat{\Delta}_S$ is self-adjoint, we say that $\hat{\Delta}_S$ is <u>essentially self-adjoint</u> (more on this later).

$\boxed{3}$ We deduce by unitary equivalence through $\mathcal{F}$, that Δ is self adjoint and is the closure of Δ_S. Let's see what this means:

This means that

$$\Gamma(\Delta) = \overline{\Gamma(\Delta_S)}.$$

In other words, the set of pairs $(f, \Delta f)$, where $f \in \mathcal{D}(\Delta)$ is equal to the closure in $L^2 \oplus L^2$ of the set of pairs $(g, \Delta g)$, where g is of Schwartz class. Thus, $f \in \mathcal{D}(\Delta)$ if and only if there exists a sequence $\{g_n\}$ from $\mathcal{S}$ such that $g_n \to f$ in L^2 and Δg_n converges in L^2 (to the function we call Δf). This can be said in yet another way. Define the graph norm $|||\cdot|||_{\Delta_S}$ for Δ_S on $\mathcal{S}$ by

$$|||g|||_{\Delta_S} = \|g\|_{L^2} + \|\Delta g\|_{L^2} \quad \text{for } g \in \mathcal{S}.$$

Then we see that $\{g_n\}$ is Cauchy in $|||\cdot|||_{\Delta_S}$ if and only if both $\{g_n\}$ and $\{\Delta g_n\}$ converge in L^2. We conclude that $\mathcal{D}(\Delta)$ is the completion of $\mathcal{S}$ in the graph norm of Δ_S:

$$\mathcal{D}(\Delta) = \text{completion of } \mathcal{S} \text{ with respect to } |||\cdot|||_{\Delta_S}.$$

We may then extend $|||\cdot|||_{\Delta_S}$ from $\mathcal{S}$ to $\mathcal{D}(\Delta)$ to obtain the graph norm of Δ, called $|||\cdot|||_\Delta$. Now we see that

$$\mathcal{D}(\Delta) = \text{closure of } \mathcal{S} \text{ with respect to } |||\cdot|||_\Delta.$$

$\boxed{4}$ One proves in the theory of Sobolev spaces that the norm $|||f||| = \|f\| + \|f''\|$ is equivalent to the Sobolev norm $\|f\|_{H^2(\mathbb{R})} = \|f\|_{L^2} + \|f'\|_{L^2} + \|f''\|_{L^2}$ (on $\mathcal{S}$, say), and since $H^2(\mathbb{R})$ is a Hilbert space in this norm, we conclude that

$$\mathcal{D}(\Delta) = H^2(\mathbb{R}).$$

it is complete and $\mathcal{S}$ is dense in it

- Analysis of the operator $\overset{T_V}{\swarrow}$ of multiplication by $V(x)$ in $L^2(\mathbb{R})$.

All of this analysis was done in Problem Set 2, where you analyzed the most general multiplication operators in $L^2(\mathbb{R})$. We will typically take V to be bounded and real-valued. We have

$$\sigma(T_V) = \text{ess range}(V)$$
$$\|T_V\| = \|V\|_\infty$$
$$T_V \text{ is self-adjoint (if } V \text{ is real-valued)}$$
$$\sigma_p(T_V) = \{ y : m\{x : V(x) = y\} > 0 \}$$

Now let's come back to our Hamiltonian

$$H = -\frac{\hbar^2}{2m}\Delta + T_V \quad \Big[\underbrace{= -\frac{\hbar^2}{2m}\Delta + V(x)}_{\text{People use this notation.}} \Big].$$

We now know precisely how Δ and T_V are defined: we have stipulated their domains and how they act on these domains. They are both self-adjoint and we have explicit spectral representations (i.e., representations as multiplication operators) for each. Δ is spectrally represented through the Fourier transform by multiplication by $-\omega^2$ in ω-space (frequency space), and T_V is already a multiplication operator in x-space.

But what about the sum of these two self-adjoint operators? If V is bounded, then it is ~~evident~~ true that we can take

$$\mathcal{D}(H) = \mathcal{D}(\Delta),$$

and that, on this domain, H is self-adjoint. Let's prove it:

<u>Fact</u> Suppose that A is a self-adjoint operator on a Hilbert space $\mathcal{H}$, with domain $\mathcal{D}(A)$, and that B is a bounded linear operator on $\mathcal{H}$. Then the operator $A+B$ defined by

$$\mathcal{D}(A+B) = \mathcal{D}(A)$$
$$(A+B)x = Ax + Bx \quad \text{for all } x \in \mathcal{D}(A+B)$$

is <u>self-adjoint</u>.

<u>Proof</u> Suppose that $y \in \mathcal{H}$ is such that the functional

$$\mathcal{D}(A+B) \to \mathbb{C} :: x \mapsto \langle (A+B)x, y\rangle$$

is bounded, that is, $y \in \mathcal{D}((A+B)^*)$. Then by the density of $\mathcal{D}(A+B)$ in $\mathcal{H}$, there exists $z \in \mathcal{H}$ such that

$$\langle (A+B)x, y\rangle = \langle x, z\rangle \quad \forall \ x \in \mathcal{D}(A+B).$$

Since B is bounded and self adjoint, $\mathcal{D}(B) = \mathcal{H}$, and we obtain

$$\langle Ax, y\rangle = \langle x, z\rangle - \langle Bx, y\rangle = \langle x, z - By\rangle \quad \forall \ x \in \mathcal{D}(A+B).$$

This equality implies that $y \in \mathcal{D}(A^*) = \mathcal{D}(A) = \mathcal{D}(A+B)$, and we obtain

$$\mathcal{D}((A+B)^*) \subset \mathcal{D}(A+B).$$

On the other hand, if $y \in \mathcal{D}(A+B) = \mathcal{D}(A)$, then for all $x \in \mathcal{D}(A+B)$, $\langle (A+B)x, y\rangle = \langle Ax, y\rangle + \langle Bx, y\rangle = \langle x, Ay\rangle + \langle x, By\rangle$ $= \langle x, (A+B)y\rangle$, so $y \in \mathcal{D}((A+B)^*)$ with $(A+B)^*y = (A+B)y$.

In conclusion,
$$\mathcal{D}((A+B)^*) = \mathcal{D}(A+B),$$
$$(A+B)^* y = (A+B)y \quad \forall \ y \in \mathcal{D}(A+B).$$

Therefore $A+B$ is self-adjoint.

Let's examine the <u>spectrum</u> of $H = -\frac{\hbar}{2m}\Delta + T_V$.

<u>Question</u> Can Δ and V be represented as multiplication operators on the same L^2-space? That is, does there exist a measure space $(X, d\mu)$, a unitary operator $U: L^2(X, d\mu) \to L^2(\mathbb{R}, dx)$, and two μ-measurable functions g_1 and g_2 on X such that $T_{g_1} = U^{-1}\Delta U$ and $T_{g_2} = U^{-1} T_V U$? If so, then Δ and T_V would commute because $T_{g_1} T_{g_2} = T_{g_2} T_{g_1} = T_{g_1 g_2}$. However, Δ and T_V do not commute because

$$\Delta T_V f - T_V \Delta f = (Vf)'' - Vf'' = V''f + 2V'f' \neq 0.$$

<u>Note</u>: The converse question is answered in the theory of commutative operator algebras. The basic answer is that commuting operators can be represented by multiplication operators on a common L^2-space — they are "<u>simultaneously diagonalizable</u>". For unbounded operators, the issue of commutativity is tricky, so such statements must be formulated with great care. We will not pursue this subject at this point.

What we do know is that H is self-adjoint, with $\mathcal{D}(H) = H^2(\mathbb{R})$, so it does have a spectral representation, i.e., it is unitarily equivalent to a multiplication operator on some L^2-space.