A tiny bit of quantum mechanics

Before we begin, we need a few concepts from functional analysis.

- Δ Weak derivatives in $\mathbb{R}^n$, in the L^2-sense. Let $(\omega_1, \ldots, \omega_n)$ or $x = (x_1, \ldots, x_n)$ be the variable in $\mathbb{R}^n$. Let $C_0^\infty(\mathbb{R}^n)$ denote the space of C^∞-functions with compact support in $\mathbb{R}^n$.

Defn A function $f \in L^2(\mathbb{R}^n)$ is weakly differentiable with respect to x_i (in the L^2-sense) if there exists a function $f_i \in L^2(\mathbb{R}^n)$ such that

$$(*) \qquad \int_{\mathbb{R}^n} f_i \phi = -\int_{\mathbb{R}^n} f \frac{\partial \phi}{\partial x_i}$$

for all $\phi \in C_0^\infty(\mathbb{R}^n)$.

Such f_i is unique if it exists, and it is called the weak derivative of f. If f is classically differentiable, then its classical derivative satisfies $(*)$, and thus is equal to the weak derivative of f. This function f_i is also denoted by $\partial_{x_i} f$ or $\partial f / \partial x_i$.

To see how this definition is motivated, observe that, if $\frac{\partial f}{\partial x_i}$ exists in the classical sense, then for each $\phi \in C_0^\infty(\mathbb{R}^n)$, we have the identity

$$0 = \int_{\mathbb{R}^n} \frac{\partial (f\phi)}{\partial x_i} = \int_{\mathbb{R}^n} \left(\frac{\partial f}{\partial x_i}\right) \phi + \int f \frac{\partial \phi}{\partial x_i}.$$

I should have inserted discussion of $H^2(\mathbb{R}^n)$ of twice weakly diff'ble fcns, etc.

The subspace of $L^2(\mathbb{R}^n)$ of functions that are weakly differentiable with respect to $x^1, \ldots, x^n$ is called the Sobolev space $W^{1,2}(\mathbb{R}^n)$. It is also denoted by $H^1(\mathbb{R}^n)$ because it is a Hilbert space with norm given by

$$\|f\|_{H^1} = \|f\|_{L^2} + \sum_{i=1}^{n} \|f_i\|_{L^2} \,,$$

An equivalent norm is $\left[\|f\|_{L^2}^2 + \sum_{i=1}^{n} \|f_i\|_{L^2}^2 \right]^{1/2}$.

- The Fourier transform

The FT and the inverse FT are defined as follows, whenever the integrals exist:

$$[\mathcal{F}(f)](\omega) = \check{f}(\omega) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} f(x)\, e^{-i x \cdot \omega}\, dV(x)$$

$$[\mathcal{F}^{-1}(g)](x) = \check{g}(x) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} g(\omega)\, e^{i x \cdot \omega}\, dV(\omega)$$

The space of Schwartz-class functions $\mathcal{S}(\mathbb{R}^n)$ consists of all functions f on $\mathbb{R}^n$ such that

$$\sup_{x \in \mathbb{R}^n} \left| x^\alpha \frac{\partial^{|\beta|} f}{\partial x^\beta}(x) \right| < \infty$$

for all $\alpha = (\alpha_1, \ldots, \alpha_n)$, $\beta = (\beta_1, \ldots, \beta_n)$, where

$$x^\alpha = x_1^{\alpha_1} \cdots x_n^{\alpha_n} \,,$$

$$\frac{\partial^\beta f}{\partial x^\beta} = \frac{\partial^{|\beta|} f}{\partial x_1^{\beta_1} \cdots \partial x_n^{\beta_n}} \,.$$

There is a huge number of references for this material. Two rather concise treatments are

Reed/Simon Vol II

G. Folland, Chapter 0

Theorem $\mathcal{F}$ is defined on $\mathcal{S}(\mathbb{R}^n)$ through the integrals given above. It is an L^2-isometric isomorphism from $\mathcal{S}(\mathbb{R}^n)$ to itself with inverse $\mathcal{F}^{-1}$ (as defined above). $\mathcal{S}(\mathbb{R}^n)$ is dense in $L^2(\mathbb{R}^n)$, and therefore $\mathcal{F}$ and $\mathcal{F}^{-1}$ extend uniquely to a unitary operator from $L^2(\mathbb{R}^n)$ to itself (denoted again by $\mathcal{F}$ with inverse $\mathcal{F}^{-1}$).

Theorem For $f \in \mathcal{S}(\mathbb{R}^n)$,

$$\left(\partial_\beta = \frac{\partial^{|\beta|}}{\partial x^\beta}\right) \qquad (i\omega)^\alpha \partial_\beta \mathcal{F}(f(\omega)) = \mathcal{F}\left[\partial_\alpha\left((-ix)^\beta f(x)\right)\right]$$

Theorem For $f, g \in \mathcal{S}(\mathbb{R}^n)$,

- $(fg)^\wedge = (2\pi)^{-\frac{n}{2}} \hat{f} * \hat{g}$
- $\hat{f}\hat{g} = (2\pi)^{-\frac{n}{2}} (f*g)^\wedge$,

where the convolution $f*g$ is defined by

$$(f*g)(x) = \int_{\mathbb{R}^n} f(y)\, g(x-y)\, d\lambda(y) .$$

The <u>Laplacian</u> is the second-order differential operator

$$\Delta = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}$$

The "Hamiltonian" in quantum mechanics is the operator

$$H = -\frac{\hbar^2}{2m}\Delta + V(x)$$

$$\begin{cases} -\frac{\hbar^2}{2m}\Delta & : \text{ the free propagator} \\ V(x) & : \text{ the potential} \end{cases}$$

The dynamics of a <u>wave function</u> $\psi(x;t)$ is defined through

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi,$$

which is an ODE for $\psi \in L^2(\mathbb{R}^n)$.

In contrast to the finite-dimensional case, the treatment of this ODE in the infinite-dimensional case is very delicate, requiring understanding of the domain of H and the precise meaning of a solution to the equation.

We will see that H is self-adjoint, which will allow a simple approach to understanding the dynamics, in contrast to the more general situation of closed operators, in which this ODE is the origin of the study of <u>semigroups</u>. Local expert: F. Neubrander.

One excellent reference for the concrete mathematics of QM is Gustafson/Sigal. Vol II of Reed/Simon is also good.

We begin with some analysis of Δ and V separately. We will restrict attention to the 1D case $n=1$.

- Analysis of $\Delta = \frac{\partial^2}{\partial x^2} = \partial_x^2$ in $L^2(\mathbb{R})$.

Let us first restrict attention to Δ acting on Schwartz-class functions, where Δ is defined (in the classical sense) and such that $\Delta f \in \mathcal{S}(\mathbb{R})$ for all $f \in \mathcal{S}(\mathbb{R})$:

$\Delta_S = \Delta$ with domain $\mathcal{S}(\mathbb{R})$

$$\Delta_S : \mathcal{S}(\mathbb{R}) \to \mathcal{S}(\mathbb{R})$$

By a theorem on p. 42, we see that Δ_S carries over to multiplication by $-\omega^2$ under the Fourier transform:

$$\ast\rightarrow \qquad (\Delta_S f(x))^{\wedge} = -\omega^2 \hat{f}(\omega).$$

This fact facilitates greatly the study of Δ.

Let us look at some properties of Δ_S both directly (in x-space) and in its representation in frequency space (ω) through the Fourier transform.

Let us denote $\mathcal{F}^{-1} \circ \Delta \circ \mathcal{F} = -\omega^2$ on $\mathcal{S}(\mathbb{R})$ by $\hat{\Delta}_S$

$$(\hat{\Delta}_S g)(\omega) = -\omega^2 g(\omega).$$

$\hat{\Delta}_S$ is a spectral representation of Δ_S. . . .