The Touchy Business of Formal Computations

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Introduction

"No theorist in his right mind would have invented quantum mechanics unless forced by data"

– Craig Hogan

From Axioms:

- **Phase space:** Complex Hilbert space ($\mathcal{H} = L^2(\mathbb{R}^3, dx)$)
- **Observables:** Self-adjoint operators on $\mathcal{H}$
- **Time evolution:** Unitary 1-parameter group generated by Schrödinger equation

Unboundedness

Unboundedness is **unavoidable** in Quantum Mechanics:
Heisenberg's uncertainty principle:

$$[X, P] = \mathrm{i}$$

Proof:

$$[X^n, P] = \mathrm{i}nX^{n-1} \qquad \Rightarrow \qquad \|[X^n, P]\| = n\|X^{n-1}\|$$

$$\|[X^n, P]\| = \|X^nP - PX^n\| \leq 2\|X^n\|\|P\| \leq 2\|X^{n-1}\|\|X\|\|P\|$$

$$\frac{n}{2} \leq \|X\|\|P\| \qquad \forall n \in \mathbb{N}$$

Scientists in the '20-'30 need to develop the theory of **unbounded operators** (von Neumann, Stone, ...)

Unbounded operators

Unbounded operator

An unbounded (= not necessarily bounded) operator is a linear map

$$T : \mathcal{D}(T) \subset \mathcal{H} \to \mathcal{H}$$

The assignment of the domain is **crucial**!

Different domains assigned to the same formal operator define **different operators:**

- eigenvalues
- scattering properties
- invertibility
- ...

What can go wrong? (1/2)

Statement

Time evolution associated to $\mathrm{i}\partial_t\psi = -\partial_x^2\psi$ is unitary (e.g. $\|\psi(t,x)\|_{L^2(\mathcal{I},dx)} = \|\psi(0,x)\|_{L^2(\mathcal{I},dx)}$) ($\mathcal{I} = (0,1) \subset \mathbb{R}$)

$$\begin{cases} \mathrm{i}\partial_t\psi(t,x) = -\partial_x^2\psi(t,x) \\ \psi(0,x) = e^{\frac{\mathrm{i}+1}{\sqrt{2}}x} \quad \in L^2(\mathcal{I},dx) \end{cases}$$

Look for solutions $\psi(t,x) = e^{\omega t}e^{kx}$:

Solution: $\psi(t,x) = e^{-t}e^{\frac{\mathrm{i}+1}{\sqrt{2}}x}$

$$\|\psi(t,x)\|^2_{L^2(\mathcal{I},dx)} = e^{-2t}\|\psi(0,x)\|^2_{L^2(\mathcal{I},dx)} \overset{t\to+\infty}{\longrightarrow} 0$$

Source of problem: $\psi(0,x) \notin$ domain of self-adjointness!

What can go wrong? (2/2)

Statement

Eigenfunctions associated to different eigenvalues are orthogonal

$$-\mathrm{i}\frac{d}{dx}\psi_k(x) = k\psi_k(x) \qquad L^2(\mathcal{I}, dx)$$

If $k \in \mathbb{C}$, $\psi_k(x) = e^{\mathrm{i}kx} \in L^2(\mathcal{I}, dx)$ is an eigenfunction.
To see if they are orthogonal we need to evaluate

$$\langle \psi_k, \psi_j \rangle_{L^2(\mathcal{I},dx)} = \int_0^1 e^{-\mathrm{i}kx} e^{\mathrm{i}jx}\, dx$$

$$\langle \psi_j, \psi_k \rangle_{L^2(\mathcal{I},dx)} = \begin{cases} \frac{\mathrm{i}-\mathrm{i}e^{\mathrm{i}(j-k)}}{j-k} & j \neq k \\ 1 & j = k \end{cases}$$

Handbook of Definitions

Closed. T is closed iff $\mathcal{D}(T)$ with the *operatorial scalar product*:

$$\langle \psi, \varphi \rangle_T := \langle T\psi, T\varphi \rangle_{\mathcal{H}} + \langle \psi, \varphi \rangle_{\mathcal{H}}$$

is a Hilbert space (it is a Banach space).

Closable/Closure. $\overline{T}$, $\mathcal{D}(\overline{T}) = \overline{\mathcal{D}(T)}^{\|\cdot\|_T}$

Adjoint T^* If $\mathcal{D}(T)$ is dense in $\mathcal{H}$ then one defines

$$\mathcal{D}(T^*) := \{f \in \mathcal{H} \,|\, \exists \eta \in \mathcal{H} \text{ s.t. } \langle f, T\varphi \rangle_{\mathcal{H}} = \langle \eta, \varphi \rangle_{\mathcal{H}}, \forall \varphi \in \mathcal{D}(T)\}$$

$$T^* f := \eta$$

Symmetric. $\langle \varphi, T\psi \rangle_{\mathcal{H}} = \langle T\varphi, \psi \rangle_{\mathcal{H}}$ $\forall \varphi, \psi \in \mathcal{D}(T)$. (equiv. $T \subset T^*$)

Self-adjoint. $T = T^*$ and $\mathcal{D}(T) = \mathcal{D}(T^*)$

Essentially self-adjoint. $\overline{T}$ is self-adjoint.

Self-adjoint extension. T symmetric, $T \subset \overline{T} \subset T_{\text{s.a.}} \subset T^*$.

Beyond toy examples

For differential and multiplicative operators, non-self-adjointness is due to

- boundary conditions
- singular points of the operator

In principle one can choose a lot of domains for unbounded operators. If we want to model nature there are some **natural** choices.

Natural domains

Formal operator $T = \sum_j c_j(\mathrm{i}\nabla)^j + V(x)$, Hilbert space $\mathcal{H} = L^2(\Omega)$, $\Omega \subset \mathbb{R}^n$ open:

- **Minimal domain:** $\mathcal{D}(T_{min}) = C_c^\infty(\Omega \setminus \Gamma)$.
  $\Gamma = \{x \in \Omega \mid V(x) \text{ is 'too singular'}\}$
- **Maximal domain:** $\mathcal{D}(T_{max}) = \{f \in \mathcal{H} | Tf \in \mathcal{H}\}$.
  T acts *distributionally*.

$\rightarrow$ **Minimal operator** T_{min}**:** $(T, \mathcal{D}(T_{min}))$

$\rightarrow$ **Maximal operator** T_{max}**:** $(T, \mathcal{D}(T_{max}))$

$$T_{min} \subset T_{max}$$

$$\begin{cases} T_{min} \text{ symmetric} \\ \mathcal{D}(T_{min}) \text{ is dense in } \mathcal{H} \end{cases} \quad \Longrightarrow \quad T_{max} = T_{min}^*$$

Relativistic Quantum Mechanics

Dirac found the right equation to describe the motion of a $\frac{1}{2}$-spin particle in the relativistic regime:

$$i\hbar\partial_t \Psi(t,x) = H\Psi(t,x)$$

$$H_{free} = -ic\hbar\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta mc^2$$

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}$$

$\Psi(t,x)$ is a **spinor**, i.e. $\Psi(t,x) \in L^2(\mathbb{R}^3, \mathbb{C}^4)$. This means

$$\Psi(t,x) = \begin{pmatrix} \Psi_1(t,x) \\ \Psi_2(t,x) \\ \Psi_3(t,x) \\ \Psi_4(t,x) \end{pmatrix} \qquad \begin{array}{l} e^- \text{ spin up} \\ e^- \text{ spin down} \\ ??? \\ ??? \end{array}$$

Relativistic Hydrogen Atom

Model of the hydrogen atom with relativistic kinetic energy

$$H_\nu = -\mathrm{i}\hbar c\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta mc^2 + \frac{\nu}{|x|}\mathbb{1}$$

It has been used to compute bond states energies:

$$E_n = mc^2\left(1 + \frac{\nu^2/c^2}{(n+\sqrt{1-(\nu^2/c^2)})^2}\right)^{-1/2}$$

- Correct non-relativistic limit

$$E_n - mc^2 \overset{c\to\infty}{\longrightarrow} -\frac{m\nu^2}{2(n+1)^2}$$

- Correct experimental prediction (fine-structure corrections)
- **Break-down of the formula:** If $|\nu| > c^2$ ($Z \approx 137$) we have **imaginary eigenvalues!**

History of the problem

$\underline{c = \hbar = 1}$

1948 - 1955: *Rellich* and *Kato* proved independently essentially self-adjointness for $|\nu| < \frac{1}{2}$

1970: *Rejtö* proved essentially self-adjointness for $|\nu| < \frac{3}{4}$

1971-1972: *Weidmann*, *Schmincke*, *Rejtö* and *Gustafsson* proved

- Essential-self adjointness for $|\nu| \leq \frac{\sqrt{3}}{2}$ (well-posedness)
- Non essential self-adjointness for $|\nu| > \frac{\sqrt{3}}{2}$ (ill-posedness)

2007: *Voronov*, *Gitman*, *Tyutin* classification 'a la von Neumann' of the extensions (abstract)

2013: *Hogreve* attempt of classification in terms of boundary conditions at $r = 0$

(M. Gallone, *Self-adjoint extensions of Dirac Operator with Coulomb Potential*, Advances in Quantum Mechanics, Springer, 2017)

Classification of extensions

2018: *M.G.* and *A. Michelangeli* proved that if $\nu \in (\frac{\sqrt{3}}{2}, 1)$ then

- $f \in \mathcal{D}(H^*)$ have asymptotics
  $f = \boldsymbol{a} r^{-\sqrt{1-\nu^2}} + \boldsymbol{b} r^{\sqrt{1-\nu^2}} + o(r^{1/2})$ as $r \to 0$
- The choice of $\gamma \in \mathbb{R} \cup \{\infty\}$ defines a self-adjoint realisation through the boundary condition

$$\boldsymbol{a} = (c_\nu \gamma + d_\nu)\boldsymbol{b}$$

  c_ν and d_ν are explicit (but not very illuminating!)
- Estimate of the ground state

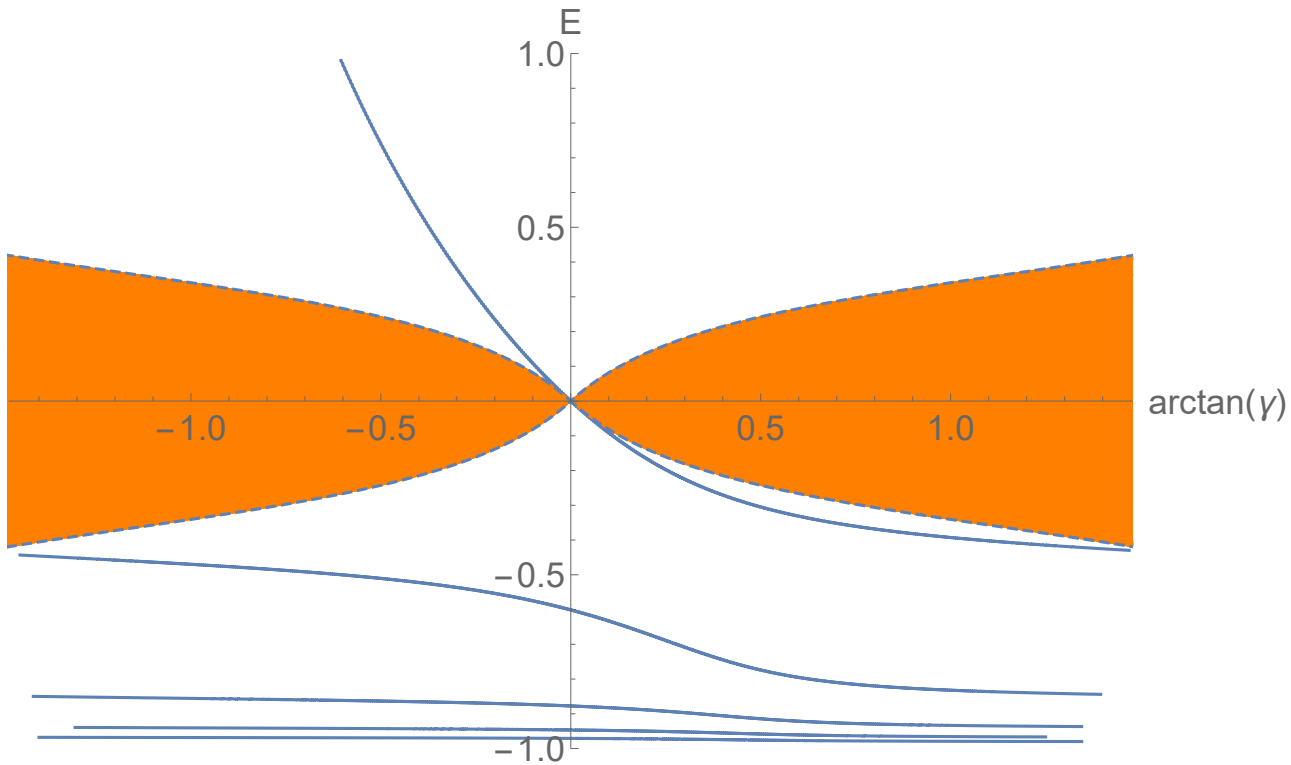
$$|E_0(\gamma)| = \frac{|\gamma|}{|\gamma|\sqrt{1-\nu^2}+1}$$

(M. Gallone and A. Michelangeli, *Self-adjoint realisations of the Dirac-Coulomb Hamiltonian for heavy nuclei*, Analysis and Math Phys, 2018)

Eigenvalues

Boundary condition $\Longrightarrow$ explicit formula for EV

$$\mathfrak{F}(E) = c_\nu \gamma + d_\nu$$



(M. Gallone and A. Michelangeli, *Discrete spectra for critical Dirac-Coulomb Hamiltonians*, Journal Math Phys, 2018)

Thank you for your attention