Fernando Falceto
Theoretical Physics Department.
University of Zaragoza

Anomalous Heisenberg equation and related issues

Policeta, June 27th, 2018.

Based on joint work with José G. Esteve

Aim of the talk

How should we modify the equations of quantum mechanics when dealing with observables that do not preserve the domain of the Hamiltonian?

Plan

- Motivation.
- Self-adjoint extensions of symmetric operators.
- Anomalous Heisenberg equation.
- Hellmann-Feynman theorem.
- Virial theorem.
- Quantum quench dynamics.

Motivation

- $\mathcal{H}$ infinite dimensional Hilbert space.
- H unbounded self-adjoint Hamiltonian with dense domain D_H.
- B bounded observable.

The equation for the evolution of B in the Heisenberg picture is

$$\frac{\mathrm{d}}{\mathrm{d}t}B = \mathrm{i}[H, B]$$

This expression makes sense in D_H if $B(D_H) \subset D_H$,

but what, if this does not happen?

Motivation. Example.

$\mathcal{H} = L^2([0,1])$, $\quad H_\alpha = -\dfrac{1}{2}\partial_x^2$ with

$$D_\alpha = \{\psi \in AC^2([0,1]) \mid \psi(1) = \mathrm{e}^{i\alpha}\psi(0),\, \psi'(1) = \mathrm{e}^{i\alpha}\psi'(0)\}$$

Consider the *parity* operator $P\psi(x) = \psi(1-x)$

$$P(D_\alpha) = D_{-\alpha}$$

For $\alpha \neq 0, \pi$ the domain is not preserved.

And the Heisenberg equation

$$\frac{\mathrm{d}}{\mathrm{d}t} P = \mathrm{i}(H_\alpha P - P H_\alpha)$$

does not make sense in D_α

Self-adjoint extensions of symmetric operators

$\tilde{H}$ closed symmetric operator with dense domain $D_{\tilde{H}} \subset \mathcal{H}$

$$\langle \chi_1 | \tilde{H} \chi_2 \rangle = \langle \tilde{H} \chi_1 | \chi_2 \rangle$$

The adjoint operator $\tilde{H}^\dagger$ has domain

$$D_{\tilde{H}^\dagger} = \{ \psi \in \mathcal{H} |\, \langle \psi | H \cdot \,\rangle : D_{\tilde{H}} \to \mathbb{C},\ \text{bounded} \}$$

Riesz rep. thm.: there is a $H^\dagger \psi \in \mathcal{H}$ s. t.

$$\langle \psi | \tilde{H} \cdot \,\rangle = \langle \tilde{H}^\dagger \psi | \cdot \,\rangle$$

Obviously:

$D_{\tilde{H}} \subset D_{\tilde{H}^\dagger}$ and

$\tilde{H}^\dagger|_{D_{\tilde{H}}} = \tilde{H} \quad$ or equiv. $\quad \tilde{H} \subset \tilde{H}^\dagger$

Boundary values.

The abstract space of boundary values is the quotient

$$\mathcal{B} = D_{\tilde{H}^\dagger}/D_{\tilde{H}}$$

Example:

$H_0 = -\frac{1}{2}\partial_x^2$ with domain $D_0 = \{\chi \in AC^2([0,1]) \mid 0, 1 \notin \mathrm{supp}(\chi)\}$

H_0 is symmetric but not closed.

Its closure is $\tilde{H} = -\frac{1}{2}\partial_x^2$ with domain

$D_{\tilde{H}} = \{\chi \in AC^2([0,1]) \,|\, \chi(0) = \chi(1) = \chi'(0) = \chi'(1) = 0\}$

$D_{\tilde{H}^\dagger} = AC^2([0,1])$

$$\mathcal{B} \sim \mathbb{C}^4$$

$$D_{\tilde{H}^\dagger}/D_{\tilde{H}} \ni [\psi] \mapsto (\psi(0), \psi(1), \psi'(0), \psi'(1)) \in \mathbb{C}^4$$

Boundary conditions.

Extensions of $\tilde{H}$ are obtained through the choice of boundary conditions i. e. a subspace of the boundary values

$$\mathcal{C} \subset \mathcal{B}.$$

The extension $H \supset \tilde{H}$ is

$$H = \tilde{H}^\dagger|_{D_H}$$

with

$$D_H = \pi^{-1}(\mathcal{C})$$

and π is the projection

$$\pi : D_{\tilde{H}^\dagger} \to D_{\tilde{H}^\dagger}/D_{\tilde{H}}$$

Relation between boundary conditions of H and its adjoint?

Boundary flux.

We introduce the *boundary flux*

$$A(\psi_1, \psi_2) = \mathrm{i}\,\langle \tilde{H}^\dagger \psi_1, \psi_2 \rangle - \mathrm{i}\,\langle \psi_1, \tilde{H}^\dagger \psi_2 \rangle\,, \quad \psi_1, \psi_2 \in D_{\tilde{H}^\dagger}$$

which is a symmetric sesquilinear form

$$\overline{A(\psi_1, \psi_2)} = A(\psi_2, \psi_1)$$

A is degenerate, actually

$$A(\psi, \chi) = 0 \text{ for any } \psi \in D_{\tilde{H}^\dagger} \iff \chi \in D_{\tilde{H}}$$

therefore $\ker A = D_{\tilde{H}}$ and A is a boundary term.

It projects to a non degenerate, sesquilinear, symmetric form in the space of boundary values

$$A : \mathcal{B} \times \mathcal{B} \to \mathbb{C}$$

Example

$$\tilde{H}^\dagger = -\tfrac{1}{2}\partial_x^2, \quad D_{\tilde{H}^\dagger} = AC^2([0,1])$$

$$A(\psi_1,\psi_2) = \frac{1}{2}(\overline{\psi}_1(0), \overline{\psi}'_1(0), \overline{\psi}_1(1), \overline{\psi}'_1(1)) \begin{pmatrix} 0 & -\mathrm{i} & 0 & 0 \\ \mathrm{i} & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathrm{i} \\ 0 & 0 & -\mathrm{i} & 0 \end{pmatrix} \begin{pmatrix} \psi_2(0) \\ \psi'_2(0) \\ \psi_2(1) \\ \psi'_2(1) \end{pmatrix}$$

$$= \frac{1}{2}(\overline{\phi}_1^+(0), \overline{\phi}_1^-(0), \overline{\phi}_1^+(1), \overline{\phi}_1^-(1)) \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \phi_2^+(0) \\ \phi_2^-(0) \\ \phi_2^+(1) \\ \phi_2^-(1) \end{pmatrix}$$

with $\phi_i^\pm = \frac{1}{\sqrt{2}}(\psi_i \pm \mathrm{i}\,\psi'_i)$

Boundary flux

A is important for the theory of self-adjoint extensions, because for any H s.t.

$$\tilde{H} \subset H \subset \tilde{H}^\dagger$$

the domain of its adjoint is the A-orthogonal of D_H,

$$D_{H^\dagger} = D_H^{\perp_A}$$

Proof:

$$\begin{aligned} \psi \in D_{H^\dagger} \quad &\Longleftrightarrow \quad \langle \psi | H \cdot \rangle \text{ bounded in } D_H \\ &\Longleftrightarrow \quad \langle \psi | H \cdot \rangle - \langle H^\dagger \psi | \cdot \rangle = 0 \text{ in } D_H \\ &\Longleftrightarrow \quad A(\psi, \cdot) = 0 \text{ in } D_H \\ &\Longleftrightarrow \quad \psi \in D_H^{\perp_A} \end{aligned}$$

Then H is self-adjoint $(D_H = D_{H^\dagger})$ if and only if $D_H^{\perp_A} = D_H$

or, in other words, iff D_H is an A-*Lagrangian* subspace.

Lagrangian subspaces

A way to produce A-Lagrangian subspaces $\mathcal{L} \subset \mathcal{B}$ is as follows.

- Introduce a Hermitian product $(\cdot, \cdot)$ in $\mathcal{B}$ s. t.

$$\mathcal{B} = \mathcal{B}_+ \perp \mathcal{B}_- \text{ and } A([\psi_1], [\psi_2]) = ([\psi_1^+], [\psi_2^+]) - ([\psi_1^-], [\psi_2^-])$$

- The previous is not canonical but $n_+ = \dim \mathcal{B}_+$, $n_- = \dim \mathcal{B}_-$ are invariant (default indices).

- If $n_+ \neq n_-$ there are not A-Lagrangian subspaces.

- If $n_+ = n_-$, the A-lagrangian subspaces $\mathcal{L}$ are of the form:

$$\mathcal{L} = (I + U)\mathcal{B}_+ \text{ with } U : \mathcal{B}_+ \to \mathcal{B}_- \text{ unitary w.r.t. } (\cdot, \cdot)$$

. There are several ways of accomplishing this program

Lagrangian subspaces. Examples

i) von Neumann

$$(\psi_1, \psi_2) = \langle \psi_1 | \psi_2 \rangle + \langle \tilde{H}^\dagger \psi_1 | \tilde{H}^\dagger \psi_2 \rangle$$

Define $\mathcal{H}_\pm = \ker(\tilde{H}^\dagger \pm \mathrm{i})$, then $D_{\tilde{H}^\dagger} = D_{\tilde{H}} \perp \mathcal{H}_+ \perp \mathcal{H}_-$

$D_{\tilde{H}^\dagger}/D_{\tilde{H}} \sim \mathcal{H}_+ \perp \mathcal{H}_-$ and

$A(\psi_1^+ + \psi_1^-, \psi_1^+ + \psi_1^-) = (\psi_1^+, \psi_2^+) - (\psi_1^-, \psi_2^-)$

ii) Asorey-Ibort-Marmo

$\tilde{H}^\dagger = -\frac{1}{2}\partial_x^2$, $\mathcal{B} \sim \mathbb{C}^4$ with standard scalar product $(\cdot, \cdot)$

$\mathcal{B}_+ = \mathrm{span}\{(1, \mathrm{i}, 0, 0), (0, 0, 1, -\mathrm{i})\}$
$\mathcal{B}_- = \mathrm{span}\{(1, -\mathrm{i}, 0, 0), (0, 0, 1, \mathrm{i})\}$.

$$A(w_1, w_2) = \frac{1}{2}(w_1^+, w_2^+) - \frac{1}{2}(w_1^-, w_2^-)$$

Anomalous Heisenberg equation

Let $H : D_H \to \mathcal{H}$ be a self-adjoint extension of $\tilde{H}$.

B bounded observable s. t. $B(D_H) \not\subset D_H$,

but $B(D_{\tilde{H}}) \subset D_{\tilde{H}}$ and $B(D_{\tilde{H}^\dagger}) \subset D_{\tilde{H}^\dagger}$.

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} \langle \psi_1 | B \psi_2 \rangle &= -\mathrm{i} \langle \psi_1 | B H \psi_2 \rangle + \mathrm{i} \langle H \psi_1 | B \psi_2 \rangle \\
&= -\mathrm{i} \langle \psi_1 | B \tilde{H}^\dagger \psi_2 \rangle + \mathrm{i} \langle \psi_1 | \tilde{H}^\dagger B \psi_2 \rangle \\
&\quad + \mathrm{i} \langle \tilde{H}^\dagger \psi_1 | B \psi_2 \rangle - \mathrm{i} \langle \psi_1 | \tilde{H}^\dagger B \psi_2 \rangle \\
&= \mathrm{i} \langle \psi_1 | [\tilde{H}^\dagger, B] \psi_2 \rangle + A(\psi_1, B\psi_2)
\end{aligned}$$

For time dependent B:

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle \psi_1 | B \psi_2 \rangle = \langle \psi_1 | \left(\frac{\partial}{\partial t} B + \mathrm{i} [\tilde{H}^\dagger, B] \right) \psi_2 \rangle + A(\psi_1, B\psi_2)$$

Anomalous Heisenberg equation. Example.

$H_\alpha = -\frac{1}{2}\partial_x^2$,
$D_\alpha = \{\psi \in AC^2([0,1]) \mid \psi(1) = \mathrm{e}^{\mathrm{i}\alpha}\psi(0),\ \psi'(1) = \mathrm{e}^{\mathrm{i}\alpha}\psi'(0)\}$

$\tilde{H}^\dagger = -\frac{1}{2}\partial_x^2$, $D_{\tilde{H}^\dagger} = AC^2([0,1])$

$$P\psi(x) = \psi(1-x), \quad P(D_\alpha) = D_{-\alpha}$$

$[\tilde{H}^\dagger, P] = 0$ then

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle\psi_1|P\psi_2\rangle &= A(\psi_1, P\psi_2) \\ &= 2(\overline{\psi}_1(0)\psi_2'(0) - \overline{\psi}_1'(0)\psi_2(0))\sin\alpha \end{aligned}$$

Anomaly cancels for $\alpha = 0$ and $\alpha = \pi$, when D_α is P-invariant.

Hellmann-Feynman theorem

The previous also applies to the Hellmann-Feynman theorem:

Consider an α-dependent Hamiltonian H_α with domain D_α,

$$H_\alpha \psi_\alpha = E_\alpha \psi_\alpha, \qquad \langle \psi_\alpha | \psi_\alpha \rangle = 1$$

Then the **Hellmann-Feynman** theorem says

$$\frac{\mathrm{d}E_\alpha}{\mathrm{d}\alpha} = \langle \psi_\alpha | \frac{\partial H_\alpha}{\partial \alpha} \psi_\alpha \rangle$$

But: $H_\alpha = -\frac{1}{2}\partial_x^2$

$D_\alpha = \{\psi \in AC^2([0,1]) \mid \psi(1) = \mathrm{e}^{\mathrm{i}\alpha}\psi(0),\ \psi'(1) = \mathrm{e}^{\mathrm{i}\alpha}\psi'(0)\}$.

Then $E_\alpha = (2\pi n + \alpha)^2$ and

$$\frac{\partial H_\alpha}{\partial \alpha} = 0 \text{ while } \frac{\partial E_\alpha}{\partial \alpha} = 4\pi(2\pi n + \alpha)$$

The problem is that ψ_α is not in the domain of $H_{\alpha'}$

Hellmann-Feynman theorem. A closer look.

Take $\tilde{H}_\alpha \subset H_\alpha \subset \tilde{H}_\alpha^\dagger$ and assume $\psi_\alpha \in D_{\tilde{H}^\dagger_{\alpha'}}, \text{ for any } \alpha, \alpha'$

Then $E_\alpha = \langle \psi_\alpha | \tilde{H}_\alpha^\dagger \, \psi_\alpha \rangle$ and the following holds

$$\frac{\mathrm{d}E_\alpha}{\mathrm{d}\alpha} = \langle \frac{\partial \psi_\alpha}{\partial \alpha} | \tilde{H}_\alpha^\dagger \, \psi_\alpha \rangle + \langle \psi_\alpha | \frac{\partial \tilde{H}_\alpha^\dagger}{\partial \alpha} \psi_\alpha \rangle + \langle \psi_\alpha | \tilde{H}_\alpha^\dagger \frac{\partial \psi_\alpha}{\partial \alpha} \rangle$$

But given that $\tilde{H}_\alpha^\dagger \, \psi_\alpha = E_\alpha \psi_\alpha$ and $\langle \psi_\alpha | \psi_\alpha \rangle = 1$ we have

$$\langle \frac{\partial \psi_\alpha}{\partial \alpha} | \tilde{H}_\alpha^\dagger \, \psi_\alpha \rangle = \langle \tilde{H}_\alpha^\dagger \psi_\alpha | \frac{\partial \psi_\alpha}{\partial \alpha} \rangle = 0$$

Then the generalization of Hellmann-Feynman theorem reads.

$$\frac{\mathrm{d}E_\alpha}{\mathrm{d}\alpha} = \langle \psi_\alpha | \frac{\partial \tilde{H}_\alpha^\dagger}{\partial \alpha} \psi_\alpha \rangle + \mathrm{i} A(\psi_\alpha, \frac{\partial \psi_\alpha}{\partial \alpha})$$

Virial theorem

A similar anomalous disease infects the virial theorem.

Take $\mathcal{H} = L^2([0,1])$ and $H = T + V(x)$ with $T = -\frac{1}{2}\partial_x^2$, then for any stationary state, the virial theorem says

$$2\langle\psi_n|T|\psi_n\rangle = \langle\psi_n|x\partial_x V|\psi_n\rangle$$

But: Take $V = 0$ and periodic boundary conditions, then $\psi_n(x) = \mathrm{e}^{2\pi\mathrm{i}nx}$

$$\langle\psi_n|T|\psi_n\rangle = 2\pi^2 n^2 \qquad \text{while} \qquad \langle\psi_n|x\partial_x V|\psi_n\rangle = 0$$

In this occasion both expectation values are well defined with the operators correctly acting in their domains.

Where is the problem?

Virial theorem. A closer look.

In order to prove the virial theorem we introduce the virial operator $G = x\partial_x$, such that in the appropriate domain

$$[H, G] = 2T - x\partial_x V(x).$$

But $G\psi_n \notin D_H$ and $\langle \psi_n | [H, G] | \psi_n \rangle$ does not make sense.

A way to proceed is to extend H to $\tilde{H}^\dagger$ so that $G\psi_n \in D_{\tilde{H}^\dagger}$ and

$$\langle \psi_n | [\tilde{H}^\dagger, G] | \psi_n \rangle = \langle \psi_n | 2T - x\partial_x V(x) | \psi_n \rangle \,.$$

Now using $\langle \psi_n | G\tilde{H}^\dagger | \psi_n \rangle = \langle \tilde{H}^\dagger \psi_n | G | \psi_n \rangle = E_n \langle \psi_n | G | \psi_n \rangle$,

$$\langle \psi_n | 2T - x\partial_x V(x) | \psi_n \rangle = \mathrm{i} A(\psi_n, G\psi_n)$$

Quantum quench dynamics

Take $\psi_0 \in D_{H_0}$ and suddenly change H_0 to H, then the state evolves with the new Hamiltonian, but ψ_0 is not in its domain...

We define the unitary operator $U_H(t) = \mathrm{e}^{\mathrm{i}Ht}$ in D_H (by functional calculus for instance) and then it is continuously extended to the full Hilbert space.

$$\psi(t) = U_H(t)\psi_0$$

$\psi(t)$ is strongly continuous but, in general, it is not differentiable.

Also $\psi(t) \notin D_{H_0}$ and even considering the extension $\tilde{H}^\dagger \supset H, H_0$

$$\psi(t) \notin D_{\tilde{H}^\dagger}$$

.

Quantum quench dynamics. Example

Let us consider an example in $L^2(\mathbb{R})$.

$$\tilde{H} = -\mathrm{i}\partial_x, \qquad D_{\tilde{H}} = \{\psi \in AC(\mathbb{R}) \mid \psi(0) = 0\}$$

$$\tilde{H}^\dagger = -\mathrm{i}\partial_x, \qquad D_{\tilde{H}^\dagger} = AC(\mathbb{R}^-) \oplus AC(\mathbb{R}^+)$$

Self-adjoint extensions H_α are parametrized by a phase $\mathrm{e}^{\mathrm{i}\alpha}$ such that $D_\alpha = \{\psi \in D_{\tilde{H}^\dagger} | \psi(0^+) = \mathrm{e}^{\mathrm{i}\alpha}\psi(0^-)\}$

They can be understood as the insertion of a δ-function.

$$H_\alpha \psi(x) = -\mathrm{i}\partial_x \psi(x) + a\delta(x)\,(\psi(0^+) + \psi(0^-)), \qquad \mathrm{e}^{\mathrm{i}\alpha} = \frac{a - \mathrm{i}}{a + \mathrm{i}}$$

Then, a quench that changes α is like changing the strength of the δ potential.

Quantum quench dynamics. Example

In this example it is easy to compute the evolution.

For $t > 0$ one has

$$U_\alpha(t)\psi(x) = \begin{cases} \psi(x-t) & x \notin (0,t) \\ \mathrm{e}^{i\alpha}\psi(x-t) & x \in (0,t) \end{cases}$$

- Observe that for $\psi \in D_{\tilde{H}^\dagger}$ we have

$$U_\alpha(t)\psi(0^+) = \mathrm{e}^{i\alpha}\psi(-t^+) = \mathrm{e}^{i\alpha}\psi(-t^-) = \mathrm{e}^{i\alpha}U_\alpha(t)\psi(0^-)$$

That is, the boundary conditions are fulfilled

- If $\psi(0^+) \neq \mathrm{e}^{\mathrm{i}\alpha}\psi(0^-)$ evolution produces a singularity in $x = t$.

$$U_\alpha(t)\psi(t^+) = \psi(0^+), \quad U_\alpha(t)\psi(t^-) = \mathrm{e}^{\mathrm{i}\alpha}\psi(0^-)$$

Conclusions

The introduction of observables that do not preserve the domain of the Hamiltonian induces the appearance of anomalous boundary terms.

These terms modify several equation of quantum mechanics like Heisenberg equation, Hellmann-Feynman theorem or the virial theorem.

When the initial state is not in the domain of the Hamiltonian (like it could happen in a quench) the evolution may drive the system outside the domain of $\tilde{H}^\dagger$.

In some cases the boundary conditions are instantaneously restored while in the bulk there appear singularities.