Quadratic Forms, Unbounded Self-Adjoint Operators and Self-Adjoint Extensions of the Laplace-Beltrami Operator

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- Introduction to the geometrical description of quantum observables
- Unbounded self-adjoint operators
- Quadratic Forms
- Motivating Example: Laplace-Beltrami operator

- Quantum Phase Space
  - Projective Hilbert Space $\mathcal{PH}$
  - Complex Struture $J^2_{[\Psi]} = -\mathbb{I}_{[\Psi]}$
  - Riemannian metric $g_{[\Psi]}(\cdot,\cdot)$
  - Symplectic Form $\omega_{[\Psi]}(\cdot,\cdot)$
- Compatibility Conditions

$$g_{[\Psi]}(Ju, Jv) = g_{[\Psi]}(u, v)$$

$$\omega_{[\Psi]}(u, v) = g_{[\Psi]}(Ju, v)$$

- Observables $\Rightarrow$ Kählerian functions

$f \in C^\infty(\mathcal{PH}, \mathbb{R})$ $\quad X_f$ Hamiltonian Vector Field $\quad \omega(X_f, \cdot) = df(\cdot)$

$$\mathcal{L}_{X_f}\omega = 0$$

$$\mathcal{L}_{X_f}\, \mathrm{g} = 0$$

- f is a real Kählerian function iff it exists a bounded, self--adjoint, linear operator A such that

$$f([\Psi]) = \frac{\langle \Psi\, , A\Psi \rangle}{||\Psi||^2}$$

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- Linear Operators on a complex Hilbert space $\mathcal{H}$.

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

- Dense Domains $\overline{\mathcal{D}(T)} = \mathcal{H}$
- Bounded Operator

$$\exists M \text{ s.t. } ||T\Phi|| \leq M||\Phi|| \;\; \forall \Phi \in \mathcal{D}(T)$$

- Bounded operators are continuous operators

$$\lim_{n\to\infty} \Phi_n = \Phi \qquad \lim_{n\to\infty} T\Phi_n = T\Phi$$

- Elements of the domain must satisfy

$$||T\Phi|| < \infty$$

- The operator can be densely defined. But you can not extend it to the whole Hilbert space

$$\{\Phi_n\} \text{ is Cauchy } \not\Rightarrow \{T\Phi_n\} \text{ is Cauchy}$$

$$\mathcal{H} = \mathcal{L}^2[0,1] \qquad P := i\frac{d}{dx}$$

$\sqrt{x} \in \mathcal{L}^2[0,1]$ **but** $P(\sqrt{x}) = \dfrac{i}{2\sqrt{x}} \notin \mathcal{L}^2[0,1]$

- Continuity is not completely lost

$$\text{if } \{\Phi_n\} \text{ is Cauchy } \text{ and } \{T\Phi_n\} \text{ is Cauchy}$$

$$\lim \Phi_n = \Phi \qquad\qquad \lim T\Phi_n =: T\Phi$$

- The graph norm

$$|||\cdot||| = \sqrt{||\cdot||^2 + ||T\cdot||^2}$$

- Closed operator

$$\overline{\mathcal{D}(T)}^{|||\cdot|||} = \mathcal{D}(T)$$

- Extensions

$$\tilde{T} \text{ extends } T \ (\tilde{T} \supset T) \text{ if}$$

$$\mathcal{D}(\tilde{T}) \supset \mathcal{D}(T)$$

$$\tilde{T} \mid_{\mathcal{D}(T)} = T$$

- T is closable if it has closed extensions
- In general there are infinitely many extensions

- Equivalent for bounded operators
- T is symmetric if $T \subset T^\dagger$

$$\Rightarrow \ T \text{ is closable}$$

- T is self-adjoint if $T = T^\dagger$

$$\Rightarrow \ T \text{ is closed}$$

- Symmetric operators may have no self-adjoint extensions

- T is a symmetric differential operator on a riemannian manifold Ω
- $\mathcal{H} = \mathcal{L}^2(\Omega)$
- Integration by parts

$$\langle \Psi\,, T\Phi \rangle - \langle T\Psi\,, \Phi \rangle = \Sigma\big(\Psi, \Phi\big)$$

$$\Psi, \Phi \in \mathcal{D}(T^\dagger)$$

- S.a. extensions are in correspondence with maximally isotropic subspaces of $\Sigma(\cdot,\cdot)$ if T has equal deficiency indices

Ref: M. Asorey, A. Ibort, G. Marmo. Int. J. Mod. Phys. A 20, 1001-1026 (2005)

- Spectral Theorem

Let A be a self-adjoint operator. Then it exists a spectral decomposition of the identity, $\mathrm{E}(\lambda)$, such that:

$$A = \int_{\sigma(A)} \lambda \ \mathrm{dE}(\lambda)$$

- Stone's Theorem

A is the generator of a strongly continuous one parameter unitary group, U_t, if and only if A is a self-adjoint operator

$$U_t = e^{itA}$$

- Kähler isomorphism

A Kähler isomorphism is a smooth diffeomorphism $\Theta : \mathcal{PH} \to \mathcal{PH}$, such that

$$\Theta^* \omega = \omega \qquad \Theta^* g = g$$

- Because of Stone's Theorem any self-adjoint operator A (not necessarily bounded) defines a strongly continuous one parameter group of Kähler isomorphisms

$$\Theta_t([\Psi]) := [\exp(itA)\Psi]$$

If A is bounded $\Leftrightarrow$ $(\Theta_t)_{t\in\mathbb{R}}$ is smooth

- $Q(\Phi) := Q(\Phi, \Phi)$ is a quadratic form with domain $\mathcal{D}(Q)$
- Expectation value functions are quadratic forms
- To every s.a. operator T one can associate a quadratic form Q_T

$$\mathcal{D}(Q_T) = \left\{\Phi \in \mathcal{H} \middle| \int_{\sigma(T)} |\lambda| \langle \Phi \,, dE_\lambda \Phi \rangle \leq \infty \right\}$$

$$Q_T(\Phi) = \int_{\sigma(T)} \lambda \langle \Phi \,, dE_\lambda \Phi \rangle$$

- Closed Quadratic Form
  - Q is semibounded

$$Q(\cdot) \geq -M||\cdot||^2$$

  - Q is complete if $\mathcal{D}(Q)$ is complete in the graph norm

$$|||\cdot||| = \sqrt{(M+1)||\cdot||^2 + Q(\cdot)}$$

- Closable Quadratic Form

- Representation Theorem of Quadratic Forms. The following statements are equivalent:
  - Q is the form arising from a semibounded self-adjoint operator
  - $Q : \mathcal{H} \to \mathbb{R}$ is a lower semicontinuous function.

$$\liminf_{n\to\infty} Q(\Phi_n) \geq Q(\Phi)$$

  - The domain $\mathcal{D}$ of the quadratic form is complete with respect to the graph norm

Ref: Davies, E.B. *Spectral Theory and Differential Operators, 1995*

- Real lower semicontinuous functions
  - Lower semibounded

$$Q(\cdot) \geq -M$$

  - Satisfy the "parallelogram identity"

$$Q(\Psi + \Phi) + Q(\Psi - \Phi) = 2\Big(Q(\Psi) + Q(\Phi)\Big)$$

Closable Operator

- Symmetric Operators are always closable
- The minimal extension doesn't need to be s.a. operator
- It is possible that none of the extensions is s.a.

Closable Quadratic Forms

- Hermitian quadratic forms are not always closable
- If they are closable the minimal extension is always associated with a s.a. Operator (Friedrichs' extension)

- No information is required about the adjoint operator
- It is not necessary to compute the deficiency indices
- They contain information of the spectrum of the operator
  - min-max Principle
- They are more suitable for numerics
  - They are explicitly Hermitian
  - Their domains are bigger $\mathcal{D}(Q_T) \supset \mathcal{D}(T)$

- Laplace-Beltrami operator on a compact riemannian manifold (Ω, η)

$$\Delta_\eta = \sum_{j,k} \frac{1}{\sqrt{|\eta|}} \frac{\partial}{\partial x^j} \sqrt{|\eta|}\eta^{jk} \frac{\partial}{\partial x^k}$$

- Single integration by parts leads to

$$\langle \Phi \,, -\Delta_\eta \Phi \rangle = \langle d\Phi \,, d\Phi \rangle - \langle \varphi \,, \dot{\varphi} \rangle_{\mathcal{L}^2(\partial\Omega)} =: Q(\Phi)$$

$$\Phi \in \mathcal{C}^\infty(\Omega)$$

$$\varphi := \Phi\big|_{\partial\Omega} \qquad \dot{\varphi} := \frac{d\Phi}{d\vec{n}}\bigg|_{\partial\Omega}$$

- Hermitian Domains for Q

$$\langle \varphi \,, \dot\varphi \rangle \neq \langle \dot\varphi \,, \varphi \rangle$$

Maximally Isotropic Subspaces of

$$\Sigma(\varphi, \dot\varphi) := \langle \varphi \,, \dot\varphi \rangle - \langle \dot\varphi \,, \varphi \rangle$$

- Cayley Transform $\quad \varphi_\pm = \varphi \pm i\dot\varphi$

$$\Sigma(\varphi, \dot\varphi) = \langle \varphi \,, \dot\varphi \rangle - \langle \dot\varphi \,, \varphi \rangle$$

$$\Downarrow$$

$$\tilde\Sigma(\varphi_+, \varphi_-) = i\big[\langle \varphi_+ \,, \varphi_+ \rangle - \langle \varphi_- \,, \varphi_- \rangle\big]$$

$$\varphi_- = U\varphi_+, \quad U \in \mathcal{U}(\mathcal{L}^2(\partial\Omega))$$

$$\varphi - i\dot\varphi = U(\varphi + i\dot\varphi)$$

- Semiboundedness

Assume that $\operatorname{dist}(\sigma(U)/\{-1\},-1) \geq \kappa > 0 \quad \Rightarrow \quad U = \begin{bmatrix} U_0 & 0 \\ 0 & U_1 \end{bmatrix}$

$$\langle \varphi \,, \dot{\varphi} \rangle = \langle \varphi_0 \,, \dot{\varphi}_0 \rangle + \langle \varphi_1 \,, \dot{\varphi}_1 \rangle$$

- Completeness

- Semiboundedness

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$$\langle \varphi \, , \dot{\varphi} \rangle = \underbrace{\cancel{\langle \varphi_0 \, , \dot{\varphi}_0 \rangle}}_{0} + \langle \varphi_1 \, , \dot{\varphi}_1 \rangle \leq ||A_1|| \, ||\varphi||^2$$

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$$\left.\begin{array}{l} \langle \varphi \,, \dot{\varphi} \rangle = \cancel{\langle \varphi_0 \,, \dot{\varphi}_0 \rangle}^{\,0} + \langle \varphi_1 \,, \dot{\varphi}_1 \rangle \leq ||A_1||\,||\varphi||^2 \\ \text{Trace inequality:} \quad ||\varphi|| \leq C||\Phi||_{\mathcal{H}^1} \end{array}\right\} |\langle \varphi \,, \dot{\varphi} \rangle| \leq M||\Phi||^2_{\mathcal{H}^1}$$

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- Completeness

$$|||\cdot||| = \sqrt{(M+1)||\cdot||^2 + Q(\cdot)} \sim ||\cdot||_{\mathcal{H}^1}$$

The quadratic forms

$$Q_U := \langle d\Phi \, , d\Phi \rangle - \langle \varphi \, , \dot{\varphi} \rangle$$

$$\mathcal{D}(Q_U) = \{\Phi \in \mathcal{C}^\infty(\Omega) | \varphi - i\dot{\varphi} = U(\varphi + i\dot{\varphi})\}$$

- Are closable provided that
  - $|\langle \varphi \, , \dot{\varphi} \rangle| \leq M ||\Phi||^2_{\mathcal{H}^1}$ $\qquad M < 1$
- The domains of their closures are

$$\overline{\mathcal{D}(Q_U)}^{\mathcal{H}^1(\Omega)}$$

- They are quadratic forms associated to s.a. extensions of the Laplace-Beltrami Operator

Ref: A. Ibort, F. Lledó, J.M. Pérez-Pardo. Quadratic Forms and General Self--Adjoint Extensions of the Laplace--Beltrami Operator. *In preparation*

- There are self--adjoint extensions of the Laplace-Beltrami operator that are not semibounded.
- They still define quadratic forms
- Another characterization of completeness that does not use semiboundedness

The quadratic form Q is complete iff whenever a sequence $\{\Phi_n\}$ satisfies $\lim \Phi_n = \Phi$ and $Q(\Phi_n - \Phi_m) \to 0$ as $n, m \to \infty$, then $\Phi \in \mathcal{D}$ and $Q(\Phi - \Phi_n) \to 0$.

Ref: T. Kato, *Perturbation theory for linear operators*, 1995

- Even for standard Q.M. one can take advantage of the properties of the quadratic forms. For instance, they contain the information about the spectrum of the operator.

- Quadratic Forms arise as the natural objects to define observables in the Geometrical Picture. However, a characterization for the infinite dimensional case is still missing. A generalized version of the representation theorem that accounts for quadratic forms that are not lower semibounded, but satisfy a weaker condition, might be the guide for a proper characterization.

Thanks for your attention