C^*-algebras and Geometric Integration

Time Independent Quantum Mechanics

Let $\mathcal{H}$ be a separable Hilbert space. Let H be a densely defined, unbounded, self adjoint operator on $\mathcal{H}$ i.e. H may be the one dimensional Hamiltonian on $L^2(\mathbb{R})$ thus

$$Hf(x) = -\frac{1}{2}f''(x) + V(x)f(x).$$

Question: How do we compute $\sigma(H)$ the spectrum of H?

Algorithm for computing the spectrum

- Define an appropriate one parameter family $H_\tau \in \mathcal{B}(\mathcal{H})$.
- Find a sequence of finite dimensional Hilbert spaces $\{\mathcal{H}_n\}$, $\mathcal{H}_n \subset \mathcal{H}$ with corresponding projections P_n such that $P_n \to I$ strongly and $\bigcup_{n\geq 1} \mathcal{H}_n$ is dense in $\mathcal{H}$ with respect to the norm topology.
- Compute the eigenvalues of $A_n = P_n H_\tau \big|_{\mathcal{H}_n}$.

Divide the problem into two parts:

- Find the one-parameter family $H_\tau \in \mathcal{B}(\mathcal{H})$.
- Computations of the spectrum of elements in $\mathcal{B}(\mathcal{H})$.

Let $A \in \mathcal{B}(\mathcal{H})$ and let $A_n = P_n A\big|_{\mathcal{H}_n}$. Defi ne

$$\Lambda = \{\lambda \in \mathbb{R} : \exists \lambda_n \in \sigma(A_n), \lambda_n \to \lambda\}.$$

For every set S of real numbers let $N_n(S)$ denote the number of eigenvalues (counting mult.) of A_n which belong to S.

Definition 1 *(1) A point $\lambda \in \mathbb{R}$ is called essential if, for every open set U containing λ, we have*

$$\lim_{n\to\infty} N_n(U) = \infty.$$

The set of essential points is denoted Λ_e

(2) $\lambda \in \mathbb{R}$ is called transient if there is an open set U containing λ such that

$$\sup_{n\geq 1} N_n(U) < \infty.$$

Theorem 1 *(Arveson) Let $A_1, A_2, \ldots$ be as discussed. Then $\sigma(A) \subset \Lambda$ and $\sigma_e(A) \subset \Lambda_e$.*

- Examples show that the inclusions can be proper, i.e. one may experience convergence to points not in the desired spectrum.
- We need to impose some restrictions.

Definition 2 *(1) A filtration of $\mathcal{H}$ is a sequence $\mathcal{F} = \{\mathcal{H}_1, \mathcal{H}_2, \ldots\}$ of finite dimensional subspaces of $\mathcal{H}$ such that $\mathcal{H}_n \subset \mathcal{H}_{n+1}$ and*

$$\overline{\cup_{n\geq 1}\mathcal{H}_n} = \mathcal{H}$$

(2) Let $\mathcal{F} = \{\mathcal{H}_n\}$ be a filtration of $\mathcal{H}$ and let P_n be the projection onto $\mathcal{H}_n$. The degree of an operator $A \in \mathcal{B}(\mathcal{H})$ is defined by

$$deg(A) = \sup_{n\geq 1} rank(P_nA - AP_n).$$

Let $D(\mathcal{F})$ denote the set of all operators $A \in \mathcal{B}(\mathcal{H})$ such that

$$A = \sum_{k=1}^{\infty} A_k, \quad deg(A_K) < \infty$$

and

$$s = \sum_{k=1}^{\infty}(1 + deg(A_K)^{1/2})\|A_k\| < \infty \tag{1}$$

Defining $|A|_{\mathcal{F}}$ to be the infimum of all such sums s which arise from representations of A as in (1). Then $(D(\mathcal{F}), |\cdot|_{\mathcal{F}})$ is a Banach *-algebra.

Theorem 2 *(Arveson) Assume $A = A^* \in D(\mathcal{F})$. Then*

(i) $\sigma_e(A) = \Lambda_e$.

(ii) Every point of Λ is either transient or essential.

Open problems

- Closing the gap $\sigma(A) \subset \Lambda$.
- Detect “false” eigenvalues.
- Definition of convergence.
- Rate of convergence.
- Error bounds in terms of n and possibly $\mathcal{H}_n$.
- Can the algorithm be improved?

The art of choosing H_τ

Consider the Hamiltonian H on $\mathcal{H} = L^2(\mathbb{R})$ defined by

$$H = \frac{1}{2}P^2 + v(Q),$$

where $P = -i\frac{d}{dx}$, $Q =$ multiplication by x and v is continuous. We want to find

$$P_\tau, Q_\tau \in \mathcal{B}(\mathcal{H}) \quad \text{and define} \quad H_\tau = \frac{1}{2}P_\tau^2 + v(Q_\tau).$$

Define

$$V_t f(x) = f(x-t) \quad \text{then} \quad P = \lim_{t\to 0}\frac{1}{it}(V_t - I)$$

so P is the infinitesimal generator of V_t i.e. $V_t = e^{itP}$ (Stone's Thrm).

The choice of P_τ

Possible choices of P_τ

$$(1)\, P_\tau = \frac{1}{i\tau}(V_\tau - I) \quad \text{or} \quad (2)\, P_\tau = \frac{1}{2i\tau}(V_\tau - V_{-\tau}).$$

(1) is not self-adjoint, but (2) is. Choosing $P_\tau = \frac{1}{2i\tau}(V_\tau - V_{-\tau})$ and since $V_t = e^{itP}$ we have

$$P_\tau = \frac{1}{\tau}\sin(\tau P).$$

Recalling the Spectral Mapping Theorem

$$\sigma(f(a)) = f(\sigma(a))$$

and since $f(x) = \frac{1}{\tau}\sin(\tau x)$ approximates x when τ is small suggest that P_τ could be a good choice.

The choice of Q_τ

Now P and Q satisfy the Weyl relation

$$V_t U_s = e^{ist} U_s V_t, \quad \text{where} \quad V_t = e^{itP}, U_t = e^{itQ} \tag{2}$$

which implies the “uncertainty principle”

$$PQ - QP = \frac{1}{i} I. \tag{3}$$

Now (2) cannot be achieved for P_τ, Q_τ by the Stone-von Neumann Theorem but (3) is true if

$$P = F^{-1} Q F, \quad \text{where} \quad F \quad \text{is the Fourier transform.}$$

$$Q_\tau = F P_\tau F^{-1} = F \frac{1}{\tau} \sin(\tau P) F^{-1} = \frac{1}{\tau} \sin(\tau Q).$$

Simplification using representations

Theorem 3 *(Arveson) Let* $\mathcal{A}$ *be the* C^**-algebra generated by* P_τ^2 *and* Q_τ *and let* K *be a Hilbert space spanned by a bilateral orthonormal set* $\{e_n : n \in \mathbb{Z}\}$*. Then there is a faithful representation* $\pi : \mathcal{A} \to \mathcal{B}(K)$ *such that* $\pi(H_\tau)$ *has the form*

$$\pi(H_\tau) = aT + bI$$

where $a = 1/8\tau^2$*,*$b = -1/4\tau^2$*, and* T *is the tridiagonal operator*

$$Te_n = e_{n-1} + 8\tau^2 v(\frac{1}{\tau}\sin(2n\tau))e_n + e_{n+1},$$

$n = 0, \pm 1, \pm 2, \ldots.$

Open problems

- Definition of convergence.
- Rate of convergence.
- How the structure preservation affects the computational result.
- Error bounds in terms of τ.
- Final open Problem: Error bounds in terms of τ, n and $\mathcal{H}_n$.

Computational Chemistry

The key problem is to compute the ground state of a molecule given by

$$E_0 = \inf\{\langle\psi, H\psi\rangle, \psi \in \mathcal{H}, \|\psi\| = 1\}. \quad (4)$$

- Problems: E_0 may not be attained and $\mathcal{H}$ may be huge.
- Solution: Born-Oppenheimer approximation, leads to the problem

  $$\inf\{\langle\psi, \hat{H}\psi\rangle, \psi \in \hat{\mathcal{H}}, \|\psi\| = 1\}, \quad (5)$$

  where $\hat{H}$ and $\hat{\mathcal{H}}$ are different from (4), and (5) is attained in most cases.
- State of the art method: Born-Oppenheimer-Hartree-Fock approximation which leads to a large number of nonlinear partial differential equations.
- Possible solution: Born-Oppenheimer approximation together with the Arveson method.

Operator theory

We consider Barry Simon's 15 open problems in connection with Schrödinger operators. Given the operator on $l^2(\mathbb{Z})$ defined by

$$(h_{\alpha,\lambda,\theta}u)(n) = u(n+1) + u(n-1) + \lambda\cos(\pi\alpha + \theta)u(n),$$

where $\alpha, \lambda \in \mathbb{R}$ and $\theta \in [0, 2\pi]$

- (Problem 4)(Ten Martini) Prove that for all $\lambda \neq 0$ and all irrational α that $\sigma(h_{\alpha,\lambda,\theta})$ is a Cantor set.
- (Problem 5) Prove that for all irrational α and $\lambda = 2$ that $\sigma(h_{\alpha,\lambda,\theta})$ has measure zero.
- (Problem 6) Prove that for all irrational α and $\lambda < 2$ that the spectrum is purely continuous.