Diagonalization of Quadratic Operators via Non-Autonomous Evolution Equations

joint work with V. Bach

J.-B. Bru

University of the Basque Country - Ikerbasque Basque Foundation for Science

Outline

One–Particle Hilbert Space

- $\mathfrak{h} := L^2(\mathcal{M}, \mathfrak{a})$ is a separable complex Hilbert space of square–integrable functions on a measure space $(\mathcal{M}, \mathfrak{a})$. The scalar product on $\mathfrak{h}$ is given by

$$\langle f|g\rangle := \int_{\mathcal{M}} \overline{f(x)} g(x) \, \mathrm{d}\mathfrak{a}(x) \ .$$

- For any operator X on $\mathfrak{h}$, we define its transpose X^{t} and its complex conjugate $\bar{X}$ by $\langle f|X^{\mathrm{t}}g\rangle := \langle \bar{g}|X\bar{f}\rangle$ and $\langle f|\bar{X}g\rangle := \overline{\langle \bar{f}|X\bar{g}\rangle}$, for $f, g \in \mathfrak{h}$, respectively. Note that

$$X^* = \overline{X^{\mathrm{t}}} = \overline{X}^{\mathrm{t}}.$$

- $\mathcal{B}(\mathfrak{h})$ is the Banach space of bounded operators acting on $\mathfrak{h}$ and $\mathcal{L}^2(\mathfrak{h})$ is the Hilbert spaces of Hilbert–Schmidt operators defined from the scalar product

$$(X, Y)_2 := \mathrm{trace}(X^* Y) \quad \text{with} \quad \|X\|_2 := \mathrm{trace}(X^* X).$$

- Condition A1: Let $\Omega_0 = \Omega_0^* \geq 0$ be a positive (possibly unbounded) operator on $\mathfrak{h}$.
- Condition A2: Let $B_0 = B_0^{\mathrm{t}} \in \mathcal{L}^2(\mathfrak{h})$ be a (non–zero) Hilbert–Schmidt operator.

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Many–particle Hilbert Space: The Boson Fock Space

- The boson Fock space is the Hilbert space

$$\mathcal{F}_b := \bigoplus_{n=0}^{\infty} \mathcal{S}_n \left(\mathfrak{h}^{\otimes n} \right) .$$

Here, $\mathcal{S}_n$ is the orthogonal projection onto the subspace of totally symmetric n–particle wave functions in $\mathfrak{h}^{\otimes n}$, the n–fold tensor product of $\mathfrak{h}$.

- Annihilation/Creation operators $\{a(f), a^*(f)\}$ are unbounded operators on $\mathcal{F}_b$ defined for $f \in \mathfrak{h}$ by

$$\begin{aligned} (a(f)\Psi)^{(n)}(x_1,\ldots,x_n) &:= \sqrt{n+1} \left\langle f \middle| (\Psi)^{(n+1)}(\cdot,x_1,\ldots,x_n) \right\rangle \\ (a^*(f)\Psi)^{(n)}(x_1,\ldots,x_n) &:= \mathcal{S}_n \left(f(x)(\Psi)^{(n-1)}(x_1,\ldots,x_{n-1}) \right) \end{aligned}$$

They satisfy the Canonical Commutation Relation (CCR):

$$[a(f), a(g)] = [a^*(f), a^*(g)] = 0 \quad \text{whereas} \quad [a(f), a^*(g)] = \langle f|g \rangle .$$

Here

$$[A, B] := AB - BA.$$

Quadratic Boson Operators

- Condition A1: Let $\Omega_0 = \Omega_0^* \geq 0$ with domain $\mathcal{D}(\Omega_0) \subseteq \mathfrak{h}$.
- Condition A2: Let $B_0 = B_0^{\mathrm{t}} \in \mathcal{L}^2(\mathfrak{h})$ be a (non–zero) Hilbert–Schmidt operator.
- Take some orthonormal basis $\{\varphi_k\}_{k=1}^{\infty} \subset \mathcal{D}(\Omega_0) \subseteq \mathfrak{h}$ and let $a_k := a(\varphi_k)$.
- Then, for any fixed $C_0 \in \mathbb{R}$, the quadratic boson operator is defined by

$$\mathrm{H}_0 := \sum_{k,\ell} \{\Omega_0\}_{k,\ell}\, a_k^* a_\ell + \{B_0\}_{k,\ell}\, a_k^* a_\ell^* + \left\{\bar{B}_0\right\}_{k,\ell} a_k a_\ell + C_0$$

with $\{X\}_{k,\ell} := \langle \varphi_k | X \varphi_\ell \rangle$. ($\int \mathrm{d}k\ \mathrm{d}\ell$ could also replace $\sum_{k,\ell}$.)

Proposition (Berezin (66) – Bruneau-Derezinski (07))

Under Conditions A1–A2, H_0 *is essentially self–adjoint on the domain*

$$\mathcal{D}(\mathrm{H}_0) := \bigcup_{N=1}^{\infty} \left(\bigoplus_{n=0}^{N} \mathcal{S}_n \left(\mathcal{D}(\Omega_0)^{\otimes n} \right) \right) \subset \mathcal{F}_b \ .$$

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A2 Let $B_0 = B_0^{\mathrm{t}} \in \mathcal{L}^2(\mathfrak{h})$ be a (non–zero) Hilbert–Schmidt operator.

A3 $\Omega_0 \geq 4 B_0 (\Omega_0^{\mathrm{t}})^{-1} \bar{B}_0$.

B4 $\Omega_0^{-1-\varepsilon} B_0 \in \mathcal{L}^2(\mathfrak{h})$ and $\mathbf{1} \geq (4+\mathrm{r})\, B_0 (\Omega_0^{\mathrm{t}})^{-2} \bar{B}_0$ for some constant $\mathrm{r}, \varepsilon > 0$.

B5 $\Omega_0 \geq 4 B_0 (\Omega_0^{\mathrm{t}})^{-1} \bar{B}_0 + \mu \mathbf{1}$ for some constant $\mu > 0$.

Theorem (Bach-B (11))

Under A1–A3 and either B4 or B5, there are $\Omega_\infty = \Omega_\infty^* \geq 0$ on $\mathfrak{h}$, $C_\infty \in \mathbb{R}$ and a unitary operator U_∞ on $\mathcal{F}_b$ such that

$$\mathrm{U}_\infty \mathrm{H}_0 \mathrm{U}_\infty^* = \mathrm{H}_\infty := \sum_{k,\ell} \{\Omega_\infty\}_{k,\ell}\, a_k^* a_\ell + C_\infty$$

Then H_∞ can be diagonalized by a unitary operator acting on $\mathfrak{h}$, only.

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Historical Overview on Diagonalization of Such Operators

- 1947, Bogoliubov: Ω_0 and B_0 are 2×2 real matrices satisfying A1–A2, B5 and
$$\Omega_0 B_0 = B_0 \Omega_0 \ .$$
Ω_∞ and C_∞ are explicitly known. Assumptions stronger than A1, A2, and B5.

- 1953, Friedrichs - 1966, Berezin: $\Omega_0 \in \mathcal{B}(\mathfrak{h})$ and $B_0 \in \mathcal{L}^2(\mathfrak{h})$ are both real symmetric operators satisfying $\Omega_0 \pm 2B_0 \geq \mu \mathbf{1}, \ \mu > 0$.
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Ω_∞ and C_∞ not explicitly known and $\Omega_0, \Omega_0^{-1} \in \mathcal{B}(\mathfrak{h})$ are bounded operators.

- 2011, Bach-B: Ω_0 and B_0 satisfy A1–A3 and either B4 or B5: $\Omega_0, \Omega_0^{-1} \notin \mathcal{B}(\mathfrak{h})$.
Ω_∞ and C_∞ are generally not known, but we have proven that:
$$\mathrm{trace}\left(\Omega_\infty^2 - \Omega_0^2 + 4B_0\bar{B}_0\right) = 0 \quad \text{and} \quad C_\infty = C_0 + \frac{1}{2}\mathrm{trace}\left(\Omega_0 - \Omega_\infty\right).$$
Furthermore, if $\Omega_0 B_0 = B_0 \Omega_0^t$ then
$$\Omega_\infty = \{\Omega_0^2 - 4B_0\bar{B}_0\}^{1/2} \quad \text{and} \quad C_\infty = C_0 + \frac{1}{2}\mathrm{trace}\left(\Omega_0 - \{\Omega_0^2 - 4B_0\bar{B}_0\}^{1/2}\right)$$

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Strategy of the Proof

- We use a (quadratically) nonlinear first–order differential equation:

$$\forall t \geq 0 : \quad \partial_t \mathrm{H}_t = [\mathrm{H}_t, [\mathrm{H}_t, A]] \,, \quad \mathrm{H}_{t=0} := \mathrm{H}_0, \quad A = N := \sum_k a_k^* a_k .$$

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- Then explicit computations using the CCR to study the commutators show formally that

$$\mathrm{H}_t := \sum_{k,\ell} \{\Omega_t\}_{k,\ell} a_k^* a_\ell + \{B_t\}_{k,\ell} a_k^* a_\ell^* + \{\bar{B}_t\}_{k,\ell} a_k a_\ell + C_0 + 8 \int_0^t \|B_\tau\|_2^2 \, \mathrm{d}\tau,$$

where the operators $\Omega_t = \Omega_t^*$ and $B_t = B_t^{\mathrm{t}}$ satisfy a system of (quadratically) nonlinear first–order differential equations

$$\forall t \geq 0: \quad \begin{cases} \partial_t \Omega_t = -16 B_t \bar{B}_t, & \Omega_{t=0} := \Omega_0, \\ \partial_t B_t = -2 \left(\Omega_t B_t + B_t \Omega_t^{\mathrm{t}} \right), & B_{t=0} := B_0, \end{cases}$$

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- The map $t \mapsto \|B_t\|_2$ must be, at least, square–integrable on $[0, \infty)$. Then in the strong resolvent sense,

$$\mathrm{H}_\infty := \sum_{k,\ell} \{\Omega_\infty\}_{k,\ell} a_k^* a_\ell + C_\infty = \lim_{t \to \infty} \mathrm{H}_t$$

Flow Equations for Operators

1. Let the unitary operator $U_{t,s}$ on a Hilbert space $\mathfrak{h}$ be the solution of the non-autonomous evolution equation

$$\forall t \geq s \geq 0 : \quad \partial_t U_{t,s} = -iG_t U_{t,s}, \quad U_{s,s} := \mathbf{1},$$

with self-adjoint (s.a.) generator G_t. Here $U_t := U_{t,0}$.

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2. Let $H_0 = H_0^*$ acting on $\mathfrak{h}$. Then $H_t := U_t H_0 U_t^*$ satisfies

$$\forall t \geq 0: \quad \partial_t H_t = i\,[H_t, G_t] := i(H_t G_t - G_t H_t), \quad H_{t=0} := H_0.$$

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1. Let the unitary operator $U_{t,s}$ on a Hilbert space $\mathfrak{h}$ be the solution of the non-autonomous evolution equation

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with self-adjoint (s.a.) generator G_t. Here $U_t := U_{t,0}$.

Remark: There is no unified theory of such Cauchy problem for unbounded generators G_t in spite of its long history starting 60 years ago.

2. Let $H_0 = H_0^*$ acting on $\mathfrak{h}$. Then $H_t := U_t H_0 U_t^*$ satisfies

$$\forall t \geq 0 : \quad \partial_t H_t = i\,[H_t, G_t] := i(H_t G_t - G_t H_t), \quad H_{t=0} := H_0.$$

Question: find G_t depending on a fixed operator A such that in the limit $t \to \infty$,

$$H_\infty = U_\infty H_0 U_\infty^* \quad \text{with} \quad [A, H_\infty] := AH_\infty - H_\infty A = 0.$$

- Assume that $H_0 = H_0^*$ and $A = A^*$ are two self-adjoint matrices.
- Let

$$\forall t \geq 0 : \quad f(t) := \mathrm{trace}((H_t - A)^2) = \|H_t - A\|_2^2 \geq 0$$

and observe that

$$\begin{aligned} \partial_t f(t) &= \partial_t \left\{ \mathrm{trace} \left(H_t^2 - 2H_t A + A^2 \right) \right\} = \partial_t \left\{ \mathrm{trace} \left(-2H_t A \right) \right\} \\ &= -2\mathrm{trace} \left(i \left[H_t, G_t \right] A \right) = -2\mathrm{trace} \left(i \left[A, H_t \right] G_t \right), \end{aligned}$$

by using $\partial_t H_t = i [H_t, G_t]$ and the cocyclicity of the trace.

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1. We then obtain

$$\forall t \geq 0 : \quad \partial_t f(t) = -2\mathrm{trace}\left(G_t G_t^* \right) = -2\|G_t\|_2^2 \leq 0 \ .$$

2. This suggests that $\partial_t f(t) \to 0$ as $t \to \infty$, which implies $i[A, H_t] \to 0$ and that

$$H_t = U_t H_0 U_t^* \to H_\infty = U_\infty H_0 U_\infty^* \quad \text{with} \quad \left[A, H_\infty \right] = 0 \ .$$

Brocket–Wegner Flow for Operators

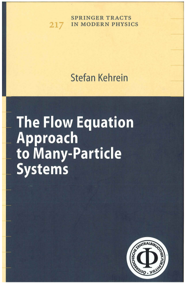
It is the (quadratically) nonlinear first–order differential equation:

$$\forall t \geq 0 : \quad \partial_t H_t = [H_t, [H_t, A]] \, , \quad H_{t=0} := H_0 .$$

R. W. Brockett, *Linear Algebra Appl.* ('91). F. Wegner, *Ann. Phys. Leipzig* ('94).

The Brocket–Wegner flow has successfully been applied to various problems in Condensed Matter Physics including:

- Electron-phonon coupling
- Dissipative quantum systems
- Interacting fermions, Hubbard model
- Impurity problems
- Non-equilibrium systems



A similar idea is also used in quantum chromodynamics and quantum electrodynamics.

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Mathematical difficulties of this idea:

1. Proof of the existence of $(H_t)_{t \geq 0}$ solution of the flow ?
2. Problem of the existence of $(U_t)_{t \geq 0}$ such that $H_t = U_t H_0 U_t^{-1}$ which means that
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Well-posedness of Brocket–Wegner Flow Equations

Theorem (Bach-B ('10 - '11))

Let $\mathfrak{h}$ be any separable Hilbert space.

- **Bounded operators: Global existence.** *Take $H_0 = H_0^*, A = A^* \in \mathcal{B}(\mathfrak{h})$. Then there are two unique solutions $(H_t)_{t\geq 0}, (U_t)_{t\geq 0} \in C^\infty[\mathbb{R}_0^+; \mathcal{B}(\mathfrak{h})]$ respectively of*

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- **Unbounded operators: Local existence.** *The flow has a unique, smooth local unbounded solution $(H_t = U_t H_0 U_t^*)_{t \in [0, T_{\max})}$ under some restricted conditions on iterated commutators.*

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- **Blows up of the Brocket–Wegner flow.** *There are two unbounded self–adjoint $H_0 = H_0^*, A \geq 0$ such that the flow has a (unbounded) local solution $(H_t = U_t H_0 U_t^*)_{t\in[0,T_{\max})}$ which blows up on its domain at a finite time $T_{\max} < \infty$.*

Brocket–Wegner Flow Equations for Quadratic Operators

- We use the Brocket–Wegner flow for any quadratic operators H_0:

$$\forall t \geq 0: \quad \partial_t \mathrm{H}_t = [\mathrm{H}_t, [\mathrm{H}_t, A]], \quad \mathrm{H}_{t=0} := \mathrm{H}_0, \quad A = N := \sum_k a_k^* a_k.$$

- Then explicit computations using the CCR show formally that

$$\mathrm{H}_t := \sum_{k,\ell} \{\Omega_t\}_{k,\ell} a_k^* a_\ell + \{B_t\}_{k,\ell} a_k^* a_\ell^* + \{\bar{B}_t\}_{k,\ell} a_k a_\ell + C_0 + 8 \int_0^t \|B_\tau\|_2^2 \, \mathrm{d}\tau,$$

where the operators $\Omega_t = \Omega_t^*$ and $B_t = B_t^{\mathrm{t}}$ must satisfy a system of (quadratically) nonlinear first–order differential equations

$$\forall t \geq 0: \quad \begin{cases} \partial_t \Omega_t = -16 B_t \bar{B}_t, & \Omega_{t=0} := \Omega_0, \\ \partial_t B_t = -2 \left(\Omega_t B_t + B_t \Omega_t^{\mathrm{t}} \right), & B_{t=0} := B_0, \end{cases}$$

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- **A blows up of the Brocket–Wegner flow can then be seen by taking**

$$\Omega_0 = 0 \quad \textbf{and} \quad B_0 = \begin{pmatrix} 0 & \mathrm{b} \\ \mathrm{b} & 0 \end{pmatrix} \quad \textbf{with} \quad \mathrm{b} > 0.$$

Diagonalization of Quadratic Operators

1. Under Conditions A1–A3, there is $(\Omega_t, B_t)_{t\in[0,T_{\max})}$ solution of

$$\forall t \in [0, T_{\max}) \subseteq \mathbb{R}_0^+ : \quad \begin{cases} \partial_t \Omega_t = -16 B_t \bar{B}_t \ , & \Omega_{t=0} := \Omega_0 \ , \\ \partial_t B_t = -2\left(\Omega_t B_t + B_t \Omega_t^{\mathrm{t}}\right) \ , & B_{t=0} := B_0 \ . \end{cases}$$

The operators $\Omega_t = \Omega_t^* \geq 0$ and $B_t \in \mathcal{L}^2(\mathfrak{h})$ satisfies:

$$\forall t \in [0, T_{\max}) : \quad \mathrm{trace}\left(\Omega_t^2 - 4B_t\bar{B}_t - \Omega_0^2 + 4B_0\bar{B}_0\right) = 0$$

and if $\Omega_0 B_0 = B_0 \Omega_0^{\mathrm{t}}$ then

$$\forall t \in [0, T_{\max}) : \quad \Omega_t = \{\Omega_0^2 - 4B_0\bar{B}_0 + 4B_t\bar{B}_t\}^{1/2} \ .$$

This is possible to show because

$$\forall t \in [0, T_{\max}) : \quad B_t = B_t^{\mathrm{t}} = W_t B_0 W_t^{\mathrm{t}} \ ,$$

where W_t is a (bounded, positive) operator acting on $\mathfrak{h}$ solution of

$$\forall t \in [0, T_{\max}) : \quad \partial_t W_t = -2\Omega_t W_t \ , \quad W_t := \mathbf{1} \ .$$

So, one only has one equation solved by the contraction mapping principle.

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$$\forall t \in [0, T_{\max}) : \quad \partial_t \mathrm{U}_t = [\mathrm{N}, \mathrm{H}_t]\, \mathrm{U}_t := -i \mathrm{G}_t \mathrm{U}_t, \quad \mathrm{U}_t := \mathbf{1}.$$

Indeed, denoting $\mathcal{Y} := \mathcal{B}(\mathcal{D}(\mathrm{N}))$, the generator $\mathrm{G}_t := i\,[\mathrm{N}, \mathrm{H}_t] = \mathrm{G}_t^*$satisfies

$$\|\mathrm{G}_t\|_{\mathcal{Y}} \leq 11 \|B_0\|_2, \ \|\mathrm{G}_t - \mathrm{G}_s\|_{\mathcal{Y}} \leq 11 \|B_t - B_s\|_2, \ \|\,[\mathrm{N}, \mathrm{G}_t]\,\|_{\mathcal{Y}} \leq 22\,\|B_0\|_2$$

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3. Using resolvents, show next that, for all $t \in [0, T_{\max})$,

$$\mathrm{H}_t := \sum_{k,\ell} \{\Omega_t\}_{k,\ell}\, a_k^* a_\ell + \{B_t\}_{k,\ell}\, a_k^* a_\ell^* + \left\{\bar{B}_t\right\}_{k,\ell} a_k a_\ell + C_t = \mathrm{U}_t \mathrm{H}_0 \mathrm{U}_t^* .$$

4. Using an a priori estimate, the assumption $\Omega_0^{-1/2} B_0 \in \mathcal{L}^2(\mathfrak{h})$ exclude blows up, i.e., $T_{\max} = \infty$, and yields the convergence, in the strong resolvent sense, of the family $(\mathrm{H}_t = \mathrm{U}_t \mathrm{H}_0 \mathrm{U}_t^*)_{t \geq 0}$ of unbounded operators to

$$\mathrm{H}_\infty := \sum_{k,\ell} \{\Omega_\infty\}_{k,\ell} \, a_k^* a_\ell + C_0 + 8 \int_0^\infty \|B_\tau\|_2^2 \mathrm{d}\tau \ .$$

In particular, one shows that

$$\mathrm{trace}\left(\Omega_t^2 - \Omega_0^2 + 4 B_0 \bar{B}_0\right) = 4 \|B_t\|_2^2 \Longrightarrow \mathrm{trace}\left(\Omega_\infty^2 - \Omega_0^2 + 4 B_0 \bar{B}_0\right) = 0$$

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Indeed, $\Omega_0^{-1/2} B_0 \in \mathcal{L}^2(\mathfrak{h})$ yields the integrability of $t \mapsto \|B_t\|_2^2$ on $[0, \infty)$ whereas

$$\Omega_t = \Omega_0 - 16 \int_0^t B_\tau \bar{B}_\tau \mathrm{d}\tau \Longrightarrow \Omega_\infty = \Omega_0 - 16 \int_0^\infty B_\tau \bar{B}_\tau \mathrm{d}\tau$$

and

$$\left\| \{(\mathrm{H}_\infty + i\lambda \mathbf{1})^{-1} - (\mathrm{H}_t + i\lambda \mathbf{1})^{-1}\}(\mathrm{N} + \mathbf{1})^{-1} \right\|_{\mathrm{op}} \leq C \left(\int_t^\infty \|B_\tau\|_2^2 \mathrm{d}\tau + \|B_t\|_2 \right) .$$

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$$\mathrm{trace}\left(\Omega_t^2 - \Omega_0^2 + 4 B_0 \bar{B}_0\right) = 4\|B_t\|_2^2 \Longrightarrow \mathrm{trace}\left(\Omega_\infty^2 - \Omega_0^2 + 4 B_0 \bar{B}_0\right) = 0$$

and if $\Omega_0 B_0 = B_0 \Omega_0^{\mathrm{t}}$ then

$$\Omega_t = \{\Omega_0^2 - 4 B_0 \bar{B}_0 + 4 B_t \bar{B}_t\}^{1/2} \Longrightarrow \Omega_\infty = \left\{\Omega_0^2 - 4 B_0 \bar{B}_0\right\}^{1/2} .$$

5. Use Conditions B4 or B5 to obtain the strong convergence of $(\mathrm{U}_t)_{t \geq 0}$ to U_∞ as well as

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Indeed, B4 (or B5), which yields $\Omega_0^{-1/2} B_0 \in \mathcal{L}^2(\mathfrak{h})$, implies the integrability of $t \mapsto \|B_t\|_2$ on $[0, \infty)$ whereas

$$\|(\mathrm{U}_\infty - \mathrm{U}_t)(\mathrm{N} + \mathbf{1})^{-1}\|_{\mathrm{op}} \leq \tilde{C} \int_t^\infty \|B_\tau\|_2 \, \mathrm{d}\tau \ . \qquad (1)$$

4. Using an a priori estimate, the assumption $\Omega_0^{-1/2} B_0 \in \mathcal{L}^2(\mathfrak{h})$ exclude blows up, i.e., $T_{\max} = \infty$, and yields the convergence, in the strong resolvent sense, of the family $(\mathrm{H}_t = \mathrm{U}_t \mathrm{H}_0 \mathrm{U}_t^*)_{t \geq 0}$ of unbounded operators to

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6. Then H_∞ can be diagonalized by a unitary operator acting on $\mathfrak{h}$, using a diagonalization of Ω_∞ to have

$$\{\Omega_\infty\}_{k,\ell} := \langle \varphi_k | \Omega_\infty \varphi_\ell \rangle = \delta_{k,\ell} \lambda_k .$$

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- This example is the first mathematical use of the Brocket–Wegner flow to diagonalize (unbounded) operators.