Classical self-adjoint extension schemes, modern applications, and open problems.

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Start with a very, very classical question in modern mathematics

(stemming from PDE theory, operator and spectral theory, stochastic equations theory, moment problems, theory of orthogonal polynomials, number theory, ...)

and also in modern physics

(ergodic theory, quantum mechanics, quantum field theory, ...)

which has very, very classical and complete answers

Consider an (infinite-dim) Hilbert space $\mathcal{H}$ on $\mathbb{C}$

scalar product: $\langle\cdot,\cdot\rangle$ (anti-linear in the *first* entry),
norm: $\|\cdot\|$,

and consider a densely defined symmetric operator S acting in $\mathcal{H}$,

i.e.,

➠ domain $\equiv \mathcal{D}(S)$ is a dense linear subspace of $\mathcal{H}$,
➠ $S:\mathcal{D}(S)\subset\mathcal{H}\to\mathcal{H}$ is a linear operator with *real expectations*

$$\langle\psi,S\psi\rangle \in \mathbb{R} \qquad \forall\psi\in\mathcal{D}(S)$$

equivalently (by polarisation),

$$\langle\psi_1,S\psi_2\rangle = \langle S\psi_1,\psi_2\rangle \qquad \forall\psi_1,\psi_2\in\mathcal{D}(S)$$

(non-trivial case in the following: when S is *unbounded*) problem:

① to find **conditions** under which S does or does not admit **self-adjoint extensions**

② in the affirmative, to identify **all self-adjoint extensions** of S

Recall: a linear operator S on $\mathcal{H}$ is **self-adjoint** when $S = S^*$
where $S^* \equiv$ the Hilbert adjoint of S, i.e.,

$$\mathcal{D}(S^*) = \{\phi \in \mathcal{H} \,|\, \exists\, \xi_\phi \in \mathcal{H} \text{ with } \langle \xi_\phi, \psi \rangle = \langle \phi, S\psi \rangle \ \forall \psi \in \mathcal{D}(S)\},$$

$$S^*\phi = \xi_\phi .$$

Symmetry is *less* than self-adjointness:

if S is densely defined and symmetric, then

$$S \subset S^*\,, \qquad \text{i.e.,} \qquad \begin{cases} \mathcal{D}(S) \subset \mathcal{D}(S^*)\,, \\ S\psi = S^*\psi \quad \forall \psi \in \mathcal{D}(S)\,. \end{cases}$$

Example:

➠ On $\mathcal{H} = L^2(0,1)$, the operator $\begin{cases} \mathcal{D}(S) = C_c^\infty(0,1) \\ Sf = -\mathrm{i}f' \end{cases}$

is symmetric, but not self-adjoint;

➠ the adjoint of S is $\begin{cases} \mathcal{D}(S^*) = H^1(0,1) \\ S^*g = -\mathrm{i}g'\,; \end{cases}$

➠ for any $\theta \in [0, 2\pi)$, the operator $\begin{cases} \mathcal{D}(S_\theta) = \left\{ \begin{array}{c} g \in H^1(0,1) \text{ s.t.} \\ g(1) = e^{\mathrm{i}\theta} g(0) \end{array} \right\} \\ S_\theta\, g = -\mathrm{i}g' \end{cases}$

is self-adjoint, and in fact is a self-adjoint extension of S:

$$S \subset S_\theta \subset S^*\,.$$

The **self-adjoint extension problem** has very complete, classical answers.

It was fully understood first by von Neumann in 1928-1930

Mathematische Annalen. 102.

Allgemeine Eigenwerttheorie Hermitescher Funktionaloperatoren.

Von

J. v. Neumann in Berlin.

Together with precursors by [Cayley, 1846] and [Weyl, 1910], additional results by [Calkin, 1940] and [Krasnosel'skiĭ and Kreĭn, 1947], and re-visitations by [Dunford and Schwartz, 1958], it constitutes von Neumann's theory of self-adjoint extensions.

VON NEUMANN'S EXTENSION THEORY:

① A densely defined and symmetric operator S on $\mathcal{H}$ admits self-adjoint extensions *if and only if* the two cardinal numbers

$$d_-(S) := \dim\ker(S^* - z\mathbb{1})\,, \qquad d_+(S) := \dim\ker(S^* - \overline{z}\mathbb{1})$$

are equal for one, hence for all $z \in \mathbb{C}^+$.
$d_\pm(S) \to$ the "deficiency indices" of S,
$\ker(S^* - z\mathbb{1})$, $\ker(S^* - \overline{z}\mathbb{1}) \to$ the "deficiency spaces" of S.

• If $d_-(S) = d_+(S) = 0$, then $\overline{S}$, the operator closure of S, is self-adjoint, and is the *only* self-adjoint extension of S. It satisfies

$$\overline{S} = S^*\,,$$

in which case S is said to be essentially self-adjoint.

• If $d_-(S) = d_+(S) \geqslant 1$, then $\overline{S}$ is not self-adjoint (nor is S), and S admits an infinite multiplicity of distinct self-adjoint extensions.

A quick detour: the *operator closure*.

A densely defined and symmetric operator S on $\mathcal{H}$ is always *closable*, i.e., it admits closed extensions. In particular, the operator

$$\begin{aligned} \mathcal{D}(\overline{S}) &:= \left\{ \psi \in \mathcal{H} \,\middle|\, \begin{array}{c} \exists\, (\psi_n)_{n\in\mathbb{N}} \subset \mathcal{D}(S) \text{ such that } \psi_n \xrightarrow{n\to\infty} \psi \\ \text{and } (S\psi_n)_{n\in\mathbb{N}} \text{ converges in } \mathcal{H} \end{array} \right\}, \\ \overline{S}\psi &:= \lim_{n\to\infty} S\psi_n \end{aligned}$$

exists, and is called operator closure of S.

$\overline{S}$ is a closed operator, it extends S, i.e., $S \subset \overline{S}$, and it is the <u>smallest closed extension</u> (in the sense of domain) of S. Moreover, $\overline{S} = S^{**}$.

Recall: an operator T in $\mathcal{H}$ is *closed* when its graph $\Gamma(T) := \{(\psi, T\psi) \in \mathcal{H} \oplus \mathcal{H}\}$ is a closed subspace of $\mathcal{H} \oplus \mathcal{H}$.
If $\mathcal{D}(T)$ is dense in $\mathcal{H}$, then T^* is always closed.
$\Rightarrow$ Self-adjoint operators are closed.

VON NEUMANN'S EXTENSION THEORY – CONT.

② For a densely defined and symmetric operator S on $\mathcal{H}$ for which $d_+(S) = d_-(S)$, and for fixed $z \in \mathbb{C}^+$, there is a one-to-one correspondence

$$\left\{\begin{matrix}\text{self-adjoint}\\ \text{extensions}\\ S_U \text{ of } S\end{matrix}\right\} \overset{1:1}{\longleftrightarrow} \left\{\begin{matrix}\text{unitary maps}\\ U : \ker(S^* - z\mathbb{1}) \xrightarrow{\cong} \ker(S^* - \overline{z}\mathbb{1})\end{matrix}\right\}.$$

Each self-adjoint extension S_U is of the form $S_U = S^* \restriction \mathcal{D}(S_U)$ with

$$\begin{aligned}\mathcal{D}(S_U) &:= \mathcal{D}(\overline{S}) \dotplus (\mathbb{1} - U)\ker(S^* - z\mathbb{1})\\ &= \left\{ g = f + v_- - Uv_- \;\middle|\; \begin{matrix} f \in \mathcal{D}(\overline{S})\\ v_- \in \ker(S^* - z\mathbb{1})\end{matrix} \right\}.\end{aligned}$$

Thus,

$$S_U\big(f + v_- - Uv_-\big) = \overline{S}\, f + z\, v_- - \overline{z}\, Uv_-\,.$$

Previous example continued (on $\mathcal{H} = L^2(0,1)$):

.

We picked $\begin{cases} \mathcal{D}(S) = C_c^\infty(0,1) \\ Sf = -\mathrm{i}f' \end{cases}$ whose adjoint is $\begin{cases} \mathcal{D}(S^*) = H^1(0,1) \\ S^*g = -\mathrm{i}g' . \end{cases}$

Fix $z = \mathrm{i}$ (for concreteness).

- Deficiency spaces: $\mathcal{K}_\pm := \ker(S^* \mp \mathrm{i}\mathbb{1}) = \mathrm{span}\{\, e^{\mp x}\,\}$
  (indeed, e.g. for $\mathcal{K}_+$ case: $-\mathrm{i}g' = \mathrm{i}g$ is solved by $g = c\, e^{-x}$, $c \in \mathbb{C}$).

- Thus, deficiency indices $d_-(S) = d_+(S) = 1$.
  $\Rightarrow$ S not essentially self-adj. and admits self-adjoint extensions.

- Generic unitary $U : \mathcal{K}_+ \xrightarrow{\cong} \mathcal{K}_-$ is $\quad \frac{\sqrt{2}\,e}{\sqrt{e^2-1}}\, e^{-x} \longmapsto e^{\mathrm{i}\alpha} \frac{\sqrt{2}}{\sqrt{e^2-1}}\, e^{x}$
  for some $\alpha \in [0, 2\pi)$

$$\Rightarrow \quad \mathcal{D}(S_U) = \left\{ g = f + c\,\frac{\sqrt{2}\,e}{\sqrt{e^2-1}}\, e^{-x} - e^{\mathrm{i}\alpha}\, c\,\frac{\sqrt{2}}{\sqrt{e^2-1}}\, e^{x} \,\middle|\, \begin{array}{l} f \in \mathcal{D}(\overline{S}) \\ c \in \mathbb{C} \end{array} \right\} .$$

Re-write $\mathcal{D}(S_U)$ conveniently:

$$\mathcal{D}(S_U) \ni g = f + c\,\frac{\sqrt{2}\,e}{\sqrt{e^2-1}}\,e^{-x} - e^{\mathrm{i}\alpha}\,c\,\frac{\sqrt{2}}{\sqrt{e^2-1}}\,e^{x}$$

$$\Downarrow$$

$$g(0) = \frac{e\,c\sqrt{2}}{\sqrt{e^2-1}} - e^{\mathrm{i}\alpha}\,\frac{c\sqrt{2}}{\sqrt{e^2-1}}\,, \qquad g(1) = \frac{c\sqrt{2}}{\sqrt{e^2-1}} - e^{\mathrm{i}\alpha}\,\frac{c\,e\sqrt{2}}{\sqrt{e^2-1}}$$

$$\Downarrow$$

$$\frac{g(1)}{g(0)} = \frac{1-e^{\mathrm{i}\alpha}\,e}{e-e^{\mathrm{i}\alpha}} \quad\Rightarrow\quad \left|\frac{g(1)}{g(0)}\right| = 1 \quad\Rightarrow\quad \boxed{\frac{g(1)}{g(0)} = e^{\mathrm{i}\theta}}\,, \quad \theta\in[0,2\pi)$$

Therefore, $(S_\theta)_{\theta\in[0,2\pi)}$ with $\begin{cases} \mathcal{D}(S_\theta) = \left\{ \begin{array}{c} g\in H^1(0,1)\ \text{s.t.} \\ g(1) = e^{\mathrm{i}\theta}g(0) \end{array} \right\} \\ S_\theta\, g = -\mathrm{i}g' \end{cases}$

is the family of *<u>all</u>* self-adjoint extensions of S.

VON NEUMANN'S EXTENSION THEORY – **RECAP**

A densely defined an symmetric S on $\mathcal{H}$ admits self-adjoint extensions $\Leftrightarrow$ S has equal deficiency indices, i.e.,

$$\dim\ker(S^* - z\mathbb{1}) \;=\; \dim\ker(S^* - \overline{z}\mathbb{1})\,, \qquad z \in \mathbb{C}^+\,,$$

in which case the self-adjoint extensions of S
are in one-to-one correspondence $S_U \leftrightarrow U$
with the unitaries $\quad U : \ker(S^* - z\mathbb{1}) \xrightarrow{\cong} \ker(S^* - \overline{z}\mathbb{1}) \quad$ via

$$\begin{aligned}\mathcal{D}(S_U) \;&:= \mathcal{D}(\overline{S}) \dotplus (\mathbb{1} - U)\ker(S^* - z\mathbb{1}) \\ &= \left\{ g \;=\; f + v_- - Uv_- \;\middle|\; \begin{array}{c} f \in \mathcal{D}(\overline{S}) \\ v_- \in \ker(S^* - z\mathbb{1}) \end{array} \right\}\end{aligned}$$

$$S_U\Big(f + v_- - Uv_-\Big) \;:= \overline{S}\,f + z\,v_- - \overline{z}\,Uv_-\,.$$

In the two decades after [von Neumann, 1928-1930] the main focus of self-adjoint extension theory was on the class of densely defined and symmetric operators that are (*lower*) *semi-bounded*, i.e., with

$$\mathfrak{m}(S) \;:=\; \inf_{\substack{\psi\in\mathcal{D}(S)\\ \psi\neq 0}} \frac{\langle\psi, S\psi\rangle}{\|\psi\|^2} \;>\; -\infty\,.$$

($\rightarrow$ crucial relevance of such operators in quantum mechanics).

[von Neumann, 1928-1930] conjectured the existence of an extension of such S with precisely the same largest lower bound $\mathfrak{m}(S)$, showing that there are extensions with lower bound $\mathfrak{m}(S)-\varepsilon\;\forall\,\varepsilon>0$

[Stone, 1932]: existence of self-adjoint extension(s) with same $\mathfrak{m}(S)$

[Friedrichs, 1934] (and in much simplified form [Freudenthal, 1936]): explicit construction of a s.a. extension S_{F} of S with $\mathfrak{m}(S_{\mathsf{F}})=\mathfrak{m}(S)$
$\rightarrow$ the 'Friedrichs extension'

The FRIEDRICHS EXTENSION
Inherently a *quadratic form construction*.

Let S be densely defined and symmetric, with $\mathfrak{m}(S) > -\infty$.
Then, the completion of $\mathcal{D}(S)$ w.r.t. the norm

$$\psi \;\mapsto\; \sqrt{\langle\psi, S\psi\rangle + (1-\mathfrak{m}(S))\|\psi\|^2} \qquad (\geqslant\; \|\psi\|\,)$$

is a subspace $\mathcal{D}[S] \subset \mathcal{H}$, and it is non-ambiguous to set, $\forall \psi, \varphi \in \mathcal{D}[S]$,

$$S[\psi,\varphi] \;:=\; \lim_{n\to\infty} \langle\psi_n, S\varphi_n\rangle\,, \qquad S[\psi] \;:=\; S[\psi,\psi]$$

irrespectively on the approximants $\mathcal{D}(S) \ni \psi_n \to \psi$, $\mathcal{D}(S) \ni \varphi_n \to \varphi$.

The quadratic form $(S[\cdot], \mathcal{D}[S])$ is <u>lower semi-bounded</u> and <u>closed</u>
$\Rightarrow$ there exists a unique self-adjoint operator $(S_{\mathsf{F}}, \mathcal{D}(S_{\mathsf{F}}))$ such that

$$S[\varphi,\psi] = \langle\varphi, S_{\mathsf{F}}\psi\rangle \qquad \forall\varphi \in \mathcal{D}[S]\,,\,, \forall\psi \in \mathcal{D}(S_{\mathsf{F}})$$

By construction, $\langle\varphi, S_{\mathsf{F}}\psi\rangle = \langle\varphi, S\psi\rangle$ $\forall\psi,\varphi \in \mathcal{D}(S)$, meaning that $S \subset S_{\mathsf{F}}$.
$S_{\mathsf{F}} \equiv$ the Friedrichs extension of S.

The FRIEDRICHS EXTENSION – distinguished properties:

.

- $\mathfrak{m}(S_{\mathsf{F}}) \;=\; \mathfrak{m}(S)$

- S_{F} is the *only* self-adjoint extension of S
whose operator domain $\mathcal{D}(S_{\mathsf{F}})$ is contained in $\mathcal{D}[S]$

- For any other self-adjoint extension $\widetilde{S}$ of S: $\quad S_{\mathsf{F}} \geqslant \widetilde{S}$
in the usual sense of expectations, i.e.,

$$\mathcal{D}[S_{\mathsf{F}}] \subset \mathcal{D}[\widetilde{S}] \qquad \text{and} \qquad S_{\mathsf{F}}[\varphi] \;\geqslant\; \widetilde{S}[\varphi] \qquad \forall \psi, \varphi \in \mathcal{D}[S_{\mathsf{F}}]\,.$$

- S only having the self-adjoint extension S_{F}
is equivalent to S being essentially self-adjoint ($\overline{S} = \overline{S}^* = S^*$)

The FRIEDRICHS EXTENSION – Two examples.

1. On $\mathcal{H} := L^2(\mathbb{R})$ consider $\begin{cases} \mathcal{D}(S) = C_c^\infty(\mathbb{R}) \\ Sf = -f''. \end{cases}$

S is symmetric and positive, and $\begin{cases} \mathcal{D}(S_{\mathsf{F}}) = H^2(\mathbb{R}) \\ S_{\mathsf{F}}f = -f''. \end{cases}$

2. On $\mathcal{H} := L^2(0,1)$ consider $\begin{cases} \mathcal{D}(S) = C_c^\infty(0,1) \\ Sf = -f'' \end{cases}$

S is symmetric (integration by parts), with $\mathfrak{m}(S) = \pi^2$, indeed:

Poincaré inequality: $\displaystyle\int_0^1 |f'(x)|^2\,\mathrm{d}x \geqslant \pi^2 \int_0^1 |f(x)|^2\,\mathrm{d}x \quad \forall f \in C_c^\infty(0,1)\,.$

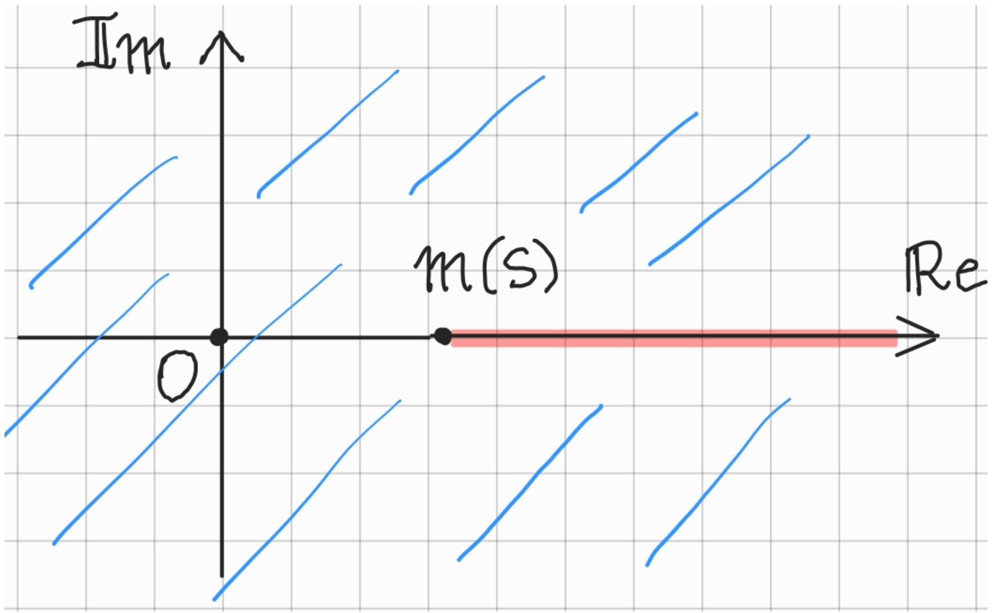
Its Friedrichs extension is $\begin{cases} \mathcal{D}(S_{\mathsf{F}}) = \left\{\begin{matrix} f \in H^2(0,1) \text{ with} \\ f(0) = 0 = f(1) \end{matrix}\right\} \\ S_{\mathsf{F}}f = -f'', \end{cases}$

i.e., S_{F} is the *Dirichlet* Laplacian.

Thus, densely defined symmetric operators S on $\mathcal{H}$
that are lower semi-bounded always admit self-adjoint extensions
(they at least have the *highest* one, S_{F})

and actually ([Krasnosel'skiĭ and Kreĭn, 1947])

$$\dim\ker(S^* - z\mathbb{1}) = \text{constant} \qquad \forall z \in \mathbb{C} \setminus [\mathfrak{m}(S), +\infty)$$

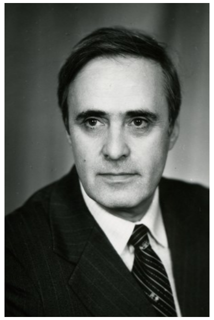


whence indeed $d_-(S) = d_+(S)$.

The study of the family of self-adjoint extensions of a lower semi-bounded S was completed in three seminal works by

[Kreĭn, 1946] *The theory of self-adjoint extensions of semi-bounded Hermitian transformations and its applications. I*, Rec. Math. [Mat. Sbornik] N.S., 20(62) (1947), pp. 431-49
$\rightarrow$ limited to the case of finite $d_\pm(S)$

[Višik, 1952] *On general boundary problems for elliptic differential equations*, Trudy Moskov. Mat. Obšč., 1 (1952), pp. 187-246
$\rightarrow$ applied to elliptic boundary value problems on domain
$\rightarrow$ focus, more gen., on closed extensions of a closed operator



[Birman, 1954] *On the theory of self-adjoint extensions of positive definite operators*, Mat. Sb. N.S., 38(80) (1956), pp. 431450.
$\rightarrow$ full generality, $d_-(S) = d_+(S) \leqslant +\infty$

➠ The Kreĭn-Višik-Birman (KVB) self-adjoint extension theory.

1956 МАТЕМАТИЧЕСКИЙ СБОРНИК Т. 38 (80), № 4

К теории самосопряженных расширений положительно определенных операторов

М. Ш. Бирман (Ленинград)

A. Michelangeli (ed.), *Mathematical Challenges of Zero-Range Physics*,
Springer INdAM Series 42, https://doi.org/10.1007/978-3-030-60453-0_13

Translation and Adaptation from Russian of M. Sh. Birman, "On the Theory of Self-Adjoint Extensions of Positive Definite Operators", Math. Sb. 38 (1956), 431–450

Mikhail Khotyakov and Alessandro Michelangeli

(+ previous, unpublished translation by S. Albeverio in the 1970's)

KVB EXTENSION THEORY – I

For a densely defined, lower semi-bounded (symmetric) S on $\mathcal{H}$, conventionally with $\mathfrak{m}(S) > 0$, there is a one-to-one correspondence

$$\left\{\begin{array}{c}\text{self-adjoint}\\ \text{extensions}\\ S_T \text{ of } S\end{array}\right\} \stackrel{1:1}{\longleftrightarrow} \left\{\begin{array}{c}\text{self-adjoint operators } T:\mathcal{D}(T)\subset\mathcal{K}\to\mathcal{K}\\ \text{acting in Hilbert subspaces } \mathcal{K}\subset\ker S^*\end{array}\right\}$$

with

$$\begin{aligned} S_T \; &:= \; S^* \upharpoonright \mathcal{D}(S_T) \\ \mathcal{D}(S_T) \; &:= \; \left\{ f + S_{\mathsf{F}}^{-1}(Tv+w)+v \;\middle|\; \begin{array}{l} f\in\mathcal{D}(\overline{S})\,,\;\; v\in\mathcal{D}(T) \\ w\in\ker S^*\cap\mathcal{D}(T)^{\perp} \end{array} \right\}. \end{aligned}$$

The Friedrichs extension corresponds to the choice $\mathcal{K}=\mathcal{D}(T)=\{0\}$ (i.e., "$T=\infty$"): explicitly, $\mathcal{D}(S_{\mathsf{F}}) = \mathcal{D}(\overline{S}) \dotplus S_{\mathsf{F}}^{-1}\ker S^*$.

Example. On $\mathcal{H} := L^2(\mathbb{R}^+)$ consider $\begin{cases} \mathcal{D}(S) = C_c^\infty(\mathbb{R}^+) \\ S = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \mathbb{1}\,. \end{cases}$ Then:

$$
\begin{aligned}
\mathfrak{m}(S) &= 1\,, \\
\mathcal{D}(S^*) &= H^2(\mathbb{R}^+)\,, \qquad S^* = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \mathbb{1}\,, \\
\mathcal{D}(\overline{S}) &= H^2_0(\mathbb{R}^+) = \{f \in H^2(\mathbb{R})\,|\,f(0) = f'(0) = 0\}\,, \\
\mathcal{D}(S_{\mathrm{F}}) &= H^2(\mathbb{R}^+) \cap H^1_0(\mathbb{R}^+) = \{f \in H^2(\mathbb{R})\,|\,f(0) = 0\}\,, \\
\ker S^* &= \mathrm{span}\{e^{-x}\}\,, \text{ i.e., } d_\pm(S) = 1\,, \\
S_{\mathrm{F}}^{-1} e^{-x} &= \frac{1}{2}\, x\, e^{-x}\,.
\end{aligned}
$$

$\Rightarrow$ The generic s.a. extension S_T is of the form S_β, $\beta \in \mathbb{R}$, with

$$
\begin{aligned}
\mathcal{D}(S_\beta) &= \left\{ g = f + S_F^{-1}(\beta\, c\, e^{-x}) + c\, e^{-x} \,\middle|\, \begin{array}{c} f \in H^2_0(\mathbb{R}^+) \\ c \in \mathbb{C} \end{array} \right\} \\
&= \left\{ g \,\middle|\, \begin{array}{l} g(x) = f(x) + c\,(\tfrac{1}{2}\beta x + 1)\, e^{-x} \\ x \in [0,1]\,,\ f \in H^2_0(\mathbb{R}^+)\,,\ c \in \mathbb{C} \end{array} \right\}.
\end{aligned}
$$

Since, for $\mathcal{D}(S_\beta) \ni g$, $g(0) = c$, $g'(0) = c(\frac{1}{2}\beta - 1)$, can re-write

$$
\mathcal{D}(S_\beta) = \{g \in H^2(\mathbb{R}^+)\,|\,g'(0) = (\tfrac{1}{2}\beta - 1)g(0)\}\,.
$$

KVB EXTENSION THEORY (cont.)

For the s.a. extension

$$
\begin{aligned}
S_T \; &:= \; S^* \restriction \mathcal{D}(S_T) \\
\mathcal{D}(S_T) \; &:= \; \left\{ f + S_{\mathsf{F}}^{-1}(Tv + w) + v \,\middle|\, \begin{array}{c} f \in \mathcal{D}(\overline{S})\,,\; v \in \mathcal{D}(T) \\ w \in \ker S^* \cap \mathcal{D}(T)^{\perp} \end{array} \right\},
\end{aligned}
$$

➠ $\mathfrak{m}(T) \geqslant \mathfrak{m}(S_T)\,,$

➠ $S_T \geqslant \mathbb{O} \quad \Leftrightarrow \quad T \geqslant \mathbb{O}\,,$

➠ $S_{T_1} \geqslant S_{T_2} \quad \Leftrightarrow \quad T_1 \geqslant T_2\,,$

➠ S_T is injective/surjective/invertible $\quad \Leftrightarrow \quad$ so is T ,

➠ if S_{F}^{-1} is compact, then S_T is lower semi-bdd $\quad \Leftrightarrow \quad$ so is T .

KVB EXTENSION THEORY (cont.) – negative spectrum:

$$\sigma_{-}(S_T) \;:=\; \sigma(S_T) \cap (-\infty, 0)\,,$$
$$\sigma_{-}(T) \;:=\; \sigma(T) \cap (-\infty, 0)\,.$$

- $\sigma_{-}(S_T)$ consists of a bounded below set of finite-rank eigenvalues of S_T whose only possible accumulation point is 0 *if and only if* $\sigma_{-}(T)$ has the same property.

- When the latter is the case, and $\lambda_1 \leqslant \lambda_2 \leqslant \cdots < 0$ and $t_1 \leqslant t_2 \leqslant \cdots < 0$ are the ordered sequences of negative eigenvalues (counted with multiplicity) of S_T and of T, then

$$\lambda_k \;\leqslant\; t_k \qquad \text{for } k = 1, 2, \ldots$$

- In particular, if $d_{\pm}(S) < +\infty$, then any s.a. extension of S has *finite* (possibly empty) negative spectrum, with finite-dim EV's. Same for all those S_T with $\dim \overline{\mathcal{D}(T)} < +\infty$.

KVB EXTENSION THEORY (cont.) – resolvents:

For any s.a. extension S_T of S such that S_T^{-1} is everywhere defined and bounded on $\mathcal{H}$,

$$S_T^{-1} = S_{\mathsf{F}}^{-1} + P_T\, T^{-1}\, P_T \qquad \text{(Kreĭn-type formula)}\,,$$

where $P_T : \mathcal{H} \to \mathcal{H}$ is the orthogonal projection onto the subspace $\overline{\mathcal{D}(T)}$.

Remarks:

• von Neumann theory historically more widespread, owing to the limited scientific exchange West/East in second half of XX century.

• KVB theory naturally extended by [Grubb, 1968] in application to closed extensions of closed operators: the structure of the extension scheme is the very same.

• Crucial results by Kreĭn beautifully revisited and reproduced by [Ando and Nishio, 1970]

• Boundary triplets theory is a modern self-adjoint extension scheme conceptually equivalent to and indirectly modelled on the old KVB scheme. $\rightarrow$ Puts emphasis on the extension mechanism induced by abstract boundary conditions expressed by certain boundary maps that implement the abstract Green identity of the considered symmetric operator, much in analogy to the role of the Birman extension parameter T.

(By Arlinskiĭ, Behrndt, Derkach, Hassi, Kurasov, Malamud, Sebestyén, de Snoo, Tsekanovskiĭ, initially introduced by Kočubeĭ and Bruk in the mid 1970's.)

VON NEUMANN vs KVB – **a comparison**:

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vN

1. Applies to any symmetric operator.

2. Provides 'absolute' and 'non-canonical' extension classification.

3. No spectral information on S_U can be a read out of U.

4. No ordering of the S_U's in terms of the corresponding U's.

5. No canonical expression of resolvent of S_U in terms of U.

6. No extension classification of quadratic forms (in terms of U).

KVB

1. Only applicable to (lower) semi-bounded S's
or, more generally, to symmetric S such that $\rho(S) \cap \mathbb{R} \neq \emptyset$.

2. 'Relative', and 'canonical': parametrises each extension S_T
in terms of the reference extension S_{F} (which has "$T = \infty$").

3. Lower semi-boundedness and features of $\sigma(S_T)$ below $\mathfrak{m}(S)$
can be read out from the (*simpler!*) T.

4. $S_{T_1} \geqslant S_{T_2} \;\Leftrightarrow\; T_1 \geqslant T_2$.

5. Kreĭn-type formulas for resolvent of S_T in terms of T.

6. Has a natural counterpart extension scheme for quadratic forms.

Clearly, *both* are powerful tools.

In certain physical contexts a clever synergy of both **vN** and **KVB** is needed: A. Michelangeli, *Models of zero-range interaction for the bosonic trimer at unitarity*, Rev. Math. Phys. 33 2150010 (2021)

Both are classical and well established schemes:

- Dunford and Schwartz, *Linear operators* (1958)
- Reed and Simon, *Methods of modern mathematical physics. II* (1975)
- Weidmann, *Linear operators in Hilbert space* (1980)
- Schmüdgen, *Unbounded self-adjoint operators on Hilbert space* (2012)

A recent thorough discussion from the original sources:
M. Gallone, A. Michelangeli, A. Ottolini *Kren-Viik-Birman self-adjoint extension theory revisited*, INdAM-Springer series, vol. 42, 239-304 (2020)

Springer Monographs in Mathematics

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Self-Adjoint Extension Schemes and Modern Applications to Quantum Mechanics

Springer

Application to Hydrogenoid atoms with 'central perturbations'

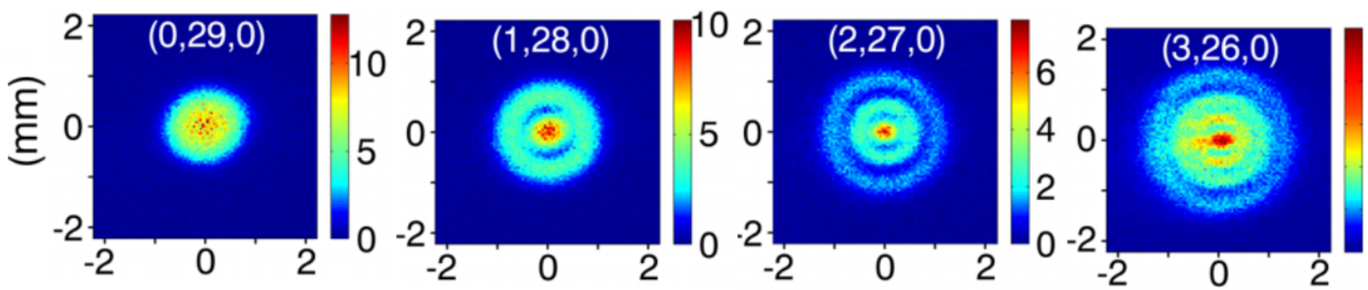
Models for valence electron of hydrogenoid atoms

$$H_{\mathrm{Hydr}} = -\frac{\hbar^2}{2m_{\mathrm{e}}}\Delta - \frac{Ze^2}{|x|} \qquad (\text{on } L^2(\mathbb{R}^3))$$

further subject to a point-like perturbation supported at $x = 0$.

Long lasting mathematical investigation: [Zorbas, 1980], [Albeverio, Gesztesy, Høegh-Krohn, Streit, 1983], [Bulla and Gesztesy, 1985].

Renewed physical interest in photoionisation microscopy with excitation of a quasi-bound Stark state in Hydrogen atoms [Stodolna et al, Phys. Rev. Lett. 2013]:



The point-like perturbation is supported at $x = 0$,
$\Rightarrow$ search for self-adjoint realisations of

$$\Big(-\frac{\hbar^2}{2m_{\mathrm{e}}}\Delta - \frac{Ze^2}{|x|}\Big)\Big|_{C^\infty_c(\mathbb{R}^3\setminus\{0\})}$$

Upon exploiting spherical symmetry, and in suitable units, problem boils down to the search of self-adjoint extensions in $L^2(\mathbb{R}^+)$ of

$$S := -\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\nu}{r} + \boxed{\frac{\nu^2}{4\kappa^2}\mathbb{1}}\,, \qquad \mathcal{D}(S) := C^\infty_0(\mathbb{R}^+)$$

$\rightarrow$ observe the <u>shift</u> by $\frac{\nu^2}{4\kappa^2}$ so as to make $\mathfrak{m}(S) > 0$ $(0 < \kappa < \frac{1}{2})$
and to make it suited for the KVB extension scheme.

Self-adjoint extension problem for S within the KVB scheme solved by M. Gallone, A. Michelangeli, *Hydrogenoid spectra with central perturbations*, Rep. Math. Phys. 84, 215-243 (2019).

Run the KVB machinery:

$\cdot\ \mathcal{D}(S^*) = \left\{ g \in L^2(\mathbb{R}^+) \,\middle|\, -g'' - \frac{\nu}{r} g + \frac{\nu^2}{4\kappa^2} \in L^2(\mathbb{R}^+) \right\},$

$S^* g = 0 \quad \Rightarrow$ a Wittaker equation for g ,

$\ker S^* = \mathrm{span}\{\Phi_\kappa\}, \quad \Phi_\kappa(r) := \mathscr{W}_{\kappa,\frac{1}{2}}(\frac{\nu}{\kappa} r)$ (a Tricomi function),

$\mathcal{D}(\overline{S}) = H_0^2(\mathbb{R}^+),$

$S_{\mathrm{F}}^{-1} \Phi_\kappa =: \Psi_\kappa,$

$\mathcal{D}(S_{\mathrm{F}}) = \mathcal{D}(\overline{S}) \dotplus S_{\mathrm{F}}^{-1} \ker S^* = H_0^2(\mathbb{R}^+) + \mathrm{span}\{\Psi_\kappa\} = H^2(\mathbb{R}^+) \cap H_0^1(\mathbb{R}^+).$

Thus, the family $(S_\beta)_{\beta \in \mathbb{R} \cup \{\infty\}}$ of self-adjoint extensions of S:

$\mathcal{D}(S_\beta) := \left\{ f + \beta c_0 \Psi_\kappa + c_0 \Phi_\kappa \,\middle|\, f \in H_0^2(\mathbb{R}^+),\, c_0 \in \mathbb{C} \right\}, \quad S_\beta := S^* \upharpoonright \mathcal{D}(S_\beta).$

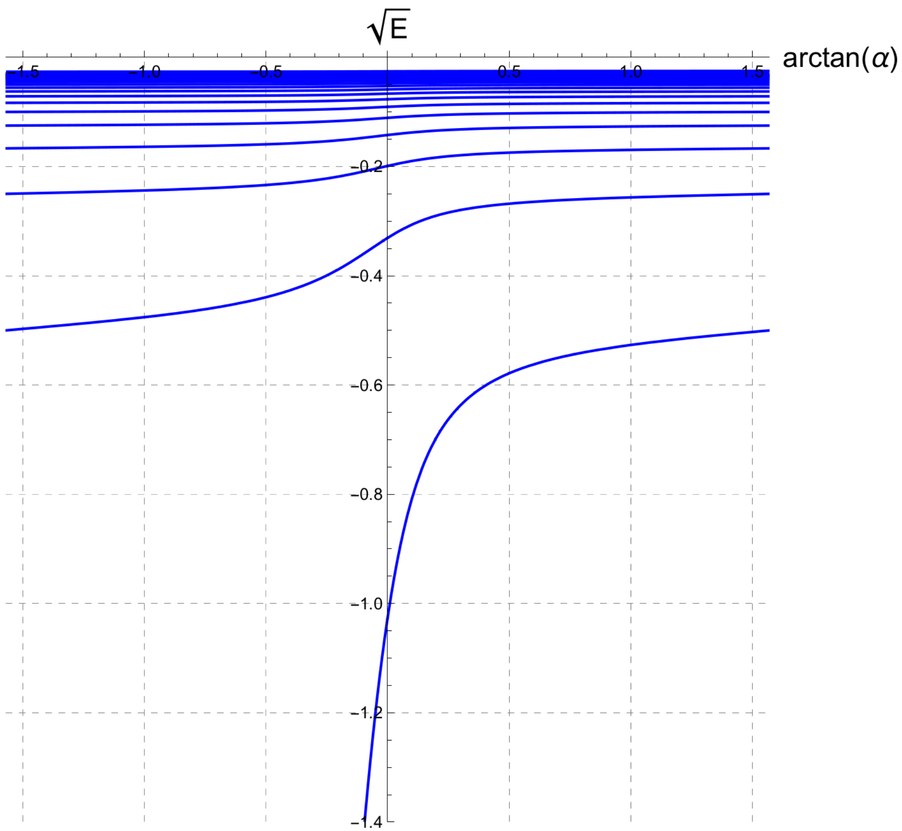
Exploiting asymptotics of Ψ_κ and Φ_κ as $r \downarrow 0$ and setting for $g \in \mathcal{D}(S_\beta)$

$g_0 := \lim_{r \downarrow 0} g(r), \quad g_1 := \lim_{r \downarrow 0} r^{-1} \Big(g(r) - g_0(1 - \nu r \ln r) \Big), \quad \alpha_\beta \equiv \alpha(\beta)$

(in fact, $g(r) = g_0(1 - \nu r \ln r) + g_1 r + o(r^{3/2})$), one re-writes

$$\mathcal{D}(S_\beta) := \left\{ g \in \mathcal{D}(S^*) \,\middle|\, g_1 = (4\pi \alpha_\beta)\, g_0 \right\}.$$

Spectral analysis (consistent with KVB general results):



Negative spectrum of $S_\alpha - \frac{\nu^2}{4\kappa^2}\mathbb{1}$ consists of *simple* eigenvalues

$$E_n^{(\nu,\alpha)}\,, \quad n \in \mathbb{N}$$

($E_n^{(\nu,\alpha)}$ and eigenfunctions explicit!).

The choice $\alpha = \infty$ (i.e. $\beta = \infty$) selects the Friedrichs extension $\to$ the ordinary Hydrogenoid Hamiltonian

$$E_n^{(\nu,\alpha=\infty)} = -\frac{\nu^2}{4n^2}$$

Details in [Gallone, Michelangeli (2019)].

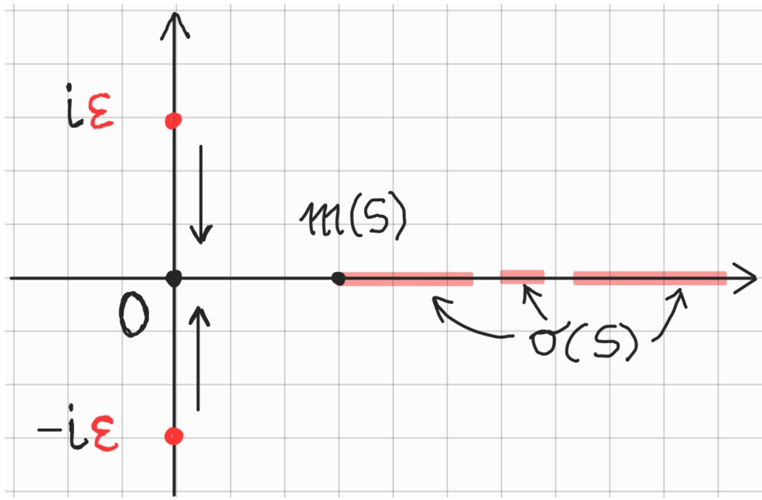
A glance on recent activity [Caruso, Michelangeli, Ottolini (2022)]:
links between the **vN** and the **KVB** extension parametrisations

For a densely defined and symmetric S with, say, $\mathfrak{m}(S) > 0$
each one s.a. extension $\widetilde{S}$ of S is both $\widetilde{S} = S_U$ and $\widetilde{S} = S_T$:
what correspondence $U^{(\widetilde{S})} \leftrightarrow T^{(\widetilde{S})}$?

Key idea: the **vN** deficiency spaces converge to the **KVB** one when they are taken at a spectral point on $\mathbb{C}$ that converges to a point in $\mathbb{R}$:

$$\ker(S^* \mp \mathrm{i}\,\varepsilon\,\mathbb{1}) \xrightarrow{\varepsilon\downarrow 0} \ker S^*$$

in the gap metric for closed subspaces of $\mathcal{H}$ (projection→projection).



Theorem. [Caruso, Michelangeli, Ottolini (2022)]
Let S be densely defined and symmetric on $\mathcal{H}$ with $\mathfrak{m}(S) > 0$.
Assume further the non-trivial case $d_-(S) = d_+(S) \geqslant 1$
($\Rightarrow$ S admits non-trivial self-adjoint extensions).

Let $\widetilde{S}$ be any such extension,
and w.r.t. the deficiency spaces $\ker(S^* \mp \mathrm{i}\,\varepsilon\,\mathbb{1})$, resp., $\ker S^*$
let U_ε, resp., T be the **vN** and the **KVB** extension parameters.

Decompose an arbitrary $g \in \mathcal{D}(\widetilde{S})$ accordingly:

$$f^{(g)} + S_{\mathsf{F}}^{-1}(Tv^{(g)} + w^{(g)}) + v^{(g)} \;=\; g \;=\; f_\varepsilon^{(g)} + v_\varepsilon^{(g)} - U_\varepsilon v_\varepsilon^{(g)}\,.$$

Explicitly:

$$\begin{aligned}
v_\varepsilon^{(g)} &= (2\,\mathrm{i}\,\varepsilon)^{-1} P_{\ker(S^*-\mathrm{i}\varepsilon\mathbb{1})}(\widetilde{S} + \mathrm{i}\varepsilon\mathbb{1})\boldsymbol{g}\,, \\
U_\varepsilon v_\varepsilon^{(g)} &= (2\,\mathrm{i}\,\varepsilon)^{-1} P_{\ker(S^*+\mathrm{i}\varepsilon\mathbb{1})}(\widetilde{S} - \mathrm{i}\varepsilon\mathbb{1})\boldsymbol{g}\,, \\
v^{(g)} &= (\mathbb{1} - S_{\mathsf{F}}^{-1}\widetilde{S})\boldsymbol{g}\,, \\
f^{(g)} &= S_{\mathsf{F}}^{-1}(\mathbb{1} - P_{\ker S^*})\widetilde{S}\boldsymbol{g}\,, \\
Tv^{(g)} + w^{(g)} &= P_{\ker S^*}\widetilde{S}\boldsymbol{g}\,.
\end{aligned}$$

Theorem (cont.)

Then, for each $g \in \mathcal{D}(\widetilde{S})$,

$$\boxed{f^{(g)} + S_{\mathsf{F}}^{-1}(Tv^{(g)} + w^{(g)}) + v^{(g)}} \;=\; g \;=\; \boxed{f_\varepsilon^{(g)} + v_\varepsilon^{(g)} - U_\varepsilon v_\varepsilon^{(g)}}\,,$$

one has

$$\begin{aligned} v_\varepsilon^{(g)} - U_\varepsilon v_\varepsilon^{(g)} &\overset{\varepsilon\downarrow 0}{=} S_{\mathsf{F}}^{-1}(Tv^{(g)} + w^{(g)}) + v^{(g)} + O(\varepsilon)\,, \\ f_\varepsilon^{(g)} &\overset{\varepsilon\downarrow 0}{=} f^{(g)} + O(\varepsilon) \end{aligned}$$

in the *graph norm* of S^*. Thus, in the $\mathcal{H}$-norm,

$$\begin{aligned} f_\varepsilon &\xrightarrow{\varepsilon\downarrow 0} f\,, \\ \overline{S} f_\varepsilon &\xrightarrow{\varepsilon\downarrow 0} \overline{S} f\,, \\ v_\varepsilon^{(g)} - U_\varepsilon v_\varepsilon^{(g)} &\xrightarrow{\varepsilon\downarrow 0} S_{\mathsf{F}}^{-1}(Tv^{(g)} + w^{(g)}) + v^{(g)}\,, \\ \mathrm{i}\,\varepsilon\, v_\varepsilon^{(g)} + \mathrm{i}\,\varepsilon\, U_\varepsilon v_\varepsilon^{(g)} &\xrightarrow{\varepsilon\downarrow 0} Tv^{(g)} + w^{(g)}\,. \end{aligned}$$

Allows to recover T from U_ε:

Corollary. [Caruso, Michelangeli, Ottolini (2022)]

$$\mathcal{D}(T) \;=\; \left\{ v^{(g)} \in \ker S^* \;\middle|\; \begin{array}{c} v^{(g)} := \lim_{\varepsilon\downarrow 0} (\mathbb{1} - S_{\mathsf{F}}^{-1}\widetilde{S})(v_\varepsilon^{(g)} - U_\varepsilon v_\varepsilon^{(g)})\, g \\ \text{for some } g \in \mathcal{D}(\widetilde{S}) \end{array} \right\},$$

(provides the domain of T)

$$\langle v^{(g)}, T v^{(g)} \rangle_{\mathcal{H}} \;=\; \lim_{\varepsilon\downarrow 0}\, \mathrm{i}\,\varepsilon \Big\langle (\mathbb{1} - S_{\mathsf{F}}^{-1}\widetilde{S})(v_\varepsilon^{(g)} - U_\varepsilon v_\varepsilon^{(g)})\,,\, (v_\varepsilon^{(g)} + U_\varepsilon v_\varepsilon^{(g)}) \Big\rangle_{\mathcal{H}}\,.$$

(provides the matrix elements of T, hence its action)