Karlsruhe Institute of Technology

A Crash Course towards the Spectral Theorem

1st Problem Class on Mathematical Phyiscs · Summer Term 2013

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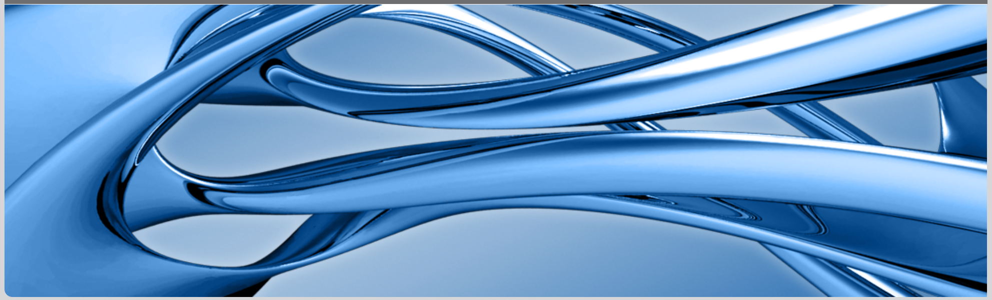

Outline

Acknowledgement

This talk is based on slides provided by my colleague

Dipl.-Math. Dominik Müller

at GRK 1294 basing on an earlier talk given by him at the University of Ulm.

I would like to thank him for his support.

Literature

Besides Dominik's talk, the following literature was also helpful:

- Peer Christian Kunstmann, *Spectral Theory*, Notes of a lecture course given in summer 2011.
- Walter Rudin, *Functional analysis*, McGraw-Hill, Princeton.
- Dirk Werner, *Funktionalanalysis*, Springer, Berlin.

Introduction

Spectral theorem for matrices

Let $A \in \mathscr{L}(\mathbb{C}^d)$ be selfadjoint, i.e., $A = A^*$. Then:

1. $\sigma(A) = \{\lambda_1, \dots, \lambda_d\}$ with $\lambda_n \in \mathbb{R}$ counted acc. to its multiplicity.
2. $\mathbb{C}^d$ has an orthonormal basis $\{e_1, \dots, e_n\}$ of eigenvectors of A.
3. A can be written as

$$A = \sum_{n=1}^{d} \lambda_n E_n$$

where $E_n x = \langle x, e_n \rangle e_n$.
$E_n \in \mathscr{L}(\mathbb{C}^d)$ is the orthogonal projection of $\mathbb{C}^d$ onto the eigenspace corresponding to λ_n.

Spectral resolution

Thus, for any $A \in \mathscr{L}(\mathbb{C}^d)$ and all $\varphi \in \mathbb{C}^d$,

$$\langle \varphi, A\varphi \rangle = \sum_{n=1}^{d} \lambda_n \langle \varphi, E_n \varphi \rangle = \int_{\sigma(A)} \lambda \langle \varphi, E(d\lambda)\varphi \rangle,$$

where $E(\Omega) := \sum_{n=1}^{d} \chi_{\{\lambda_n \in \Omega\}} E_n$ for any $\Omega \in \mathfrak{B}(\mathbb{R})$.

Spectral resolution

$$E(\Omega) := \sum_{n=1}^{d} \chi_{\{\lambda_n \in \Omega\}} E_n, \qquad \Omega \in \mathfrak{B}(\mathbb{R}).$$

E is a measure on $\mathfrak{B}(\mathbb{R})$ with values in $\mathscr{L}(\mathbb{C}^d)$. Moreover,

1. $E(\mathbb{R}) = E(\sigma(A)) = \mathbf{1}$, $E(\emptyset) = 0$,
2. $E(\Omega)$ is a selfadjoint projection,
3. $E(\Omega_1 \cap \Omega_2) = E(\Omega_1)E(\Omega_2)$,
4. $\Omega_1 \cap \Omega_2 = \emptyset \implies E(\Omega_1 \cup \Omega_2) = E(\Omega_1) + E(\Omega_2)$.

E is called the **spectral resolution** of A.

Spectral measure

If E is the spectral resolution of A and $\varphi \in \mathbb{C}^d$, then

$$\mu_\varphi(\Omega) := \langle \varphi, E(\Omega)\varphi \rangle$$

defines a complex measure $\mu_\varphi : \mathfrak{B}(\mathbb{R}) \longrightarrow \mathbb{C}$, the s.c. **spectral measure**.

The following analogue holds true in any Hilbert space $\mathscr{H}$.

The spectral theorem for unbounded, selfadjoint operators

If $A : D(A) \subset \mathscr{H} \longrightarrow \mathscr{H}$ is a selfadjont linear operator, there exists a unique spectral resolution $E : \mathfrak{B}(\mathbb{R}) \longrightarrow \mathscr{L}(\mathscr{H})$ such that

$$A = \int_{\sigma(A)} \lambda E(d\lambda).$$

For any $\varphi \in \mathscr{H}$,

$$\mu_\varphi(\Omega) := \langle \varphi, E(\Omega)\varphi \rangle, \qquad \Omega \in \mathfrak{B}(\mathbb{R})$$

defines a complex measure on $\mathfrak{B}(\mathbb{R})$, the s.c. spectral measure.

Unbounded operators

1. An **operator** A is a linear map $A : D(A) \subset \mathscr{H} \longrightarrow \mathscr{H}$ s. t. the **domain** $D(A)$ is a subspace of $\mathscr{H}$. A is called **densly defined** if $\overline{D(A)} = \mathscr{H}$.
2. An operator $B : D(B) \longrightarrow \mathscr{H}$ is called an **extension** of A if $D(A) \subset D(B)$ and $A\varphi = B\varphi$ for $\varphi \in D(A)$. We write $A \subset B$.
3. $A = B :\Longleftrightarrow A \subset B$ and $B \subset A$.

Example: $A := i\frac{d}{dt}, \quad D(A) = C_0^1[0,1], \quad \mathscr{H} = L^2[0,1]$

$$C_0^1[0,1] := \{\varphi \in C^1[0,1] \ : \ \varphi(0) = \varphi(1) = 0\}.$$

- A is densly defined.
- A is not continuous, i.e., unbounded.
- $B := i\frac{d}{dt}$ defined on $D(B) = C^1[0,1]$ is an extension of A.

Example: $A := i\frac{d}{dt}, \quad D(A) = C_0^1[0,1], \quad \mathscr{H} = L^2[0,1]$

Moreover for all $\varphi, \psi \in D(A)$,

$$\begin{aligned}\langle \psi, A\varphi \rangle &= \int_0^1 \overline{\psi}\, i\frac{d\varphi}{dt}\, dt = i\overline{\psi}\varphi\Big|_0^1 - i\int_0^1 \overline{\frac{d\psi}{dt}}\,\varphi\, dt \\ &= \int_0^1 \overline{i\frac{d\psi}{dt}}\,\varphi\, dt \\ &= \langle A\psi, \varphi \rangle\end{aligned}$$

Any operator with this property is called **symmetric**.

Selfadjoint operators

Let the operator $A : D(A) \longrightarrow \mathscr{H}$ be densly defined and

$$D(A^*) := \{\psi \in \mathscr{H} \mid \varphi \mapsto \ell_\psi(\varphi) := \langle \psi, A\varphi \rangle \text{ is cont. on } D(A)\}.$$

ℓ_ψ extends to a continuous linear functional $L_\psi : \mathscr{H} \longrightarrow \mathbb{C}$ and by Fréchet-Riesz, we find a unique $z_\psi \in \mathscr{H}$ s.t.

$$\langle \psi, A\varphi \rangle = L_\psi(\varphi) = \langle z_\psi, \varphi \rangle \qquad (\varphi \in \mathscr{H}).$$

- $A^* : D(A^*) \longrightarrow \mathscr{H}$, $A^*\psi := z_\psi$ is called the **adjoint** of A.
- If A is symmetric, $D(A) \subset D(A^*)$ and hence $A \subset A^*$.
- A is called **selfadjoint** if $A = A^*$.

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Warning !!!

Any selfadjoint operator is symmetric.

However, a symmetric operator is in general **not** selfadjoint!

- **Example:** $A := \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}$ on $D(A) = C_0^1[0,1] \subset L^2[0,1]$

  Homework ☺: A is not selfadjoint.

Selfadjointness of an unbounded operator A depends crucially on its domain $D(A)$!!!

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The Spectrum

Let $A : D(A) \longrightarrow \mathscr{H}$ be densly defined and $\lambda - A := \lambda\mathbf{1} - A$.

Definition

- $\lambda \in \mathbb{C}$ belongs to the **resolvent set** $\varrho(A)$ of A if
  1. $\lambda - A : D(A) \longrightarrow \mathscr{H}$ is bijective and
  2. $(\lambda - A)^{-1} \in \mathscr{L}(\mathscr{H})$

  In this case, $R_\lambda(A) := (\lambda - A)^{-1}$ is called the **resolvent** of A.
- The **spectrum** of A is then given by $\sigma(A) := \mathbb{C} \setminus \varrho(A)$.

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The Spectrum

1. The spectrum of an operator is always a closed subset of $\mathbb{C}$.
2. If $A : H \longrightarrow H$ is compact, $\sigma(A)$ is discrete.
3. If $A : H \longrightarrow H$ is bounded and symmetric, $\sigma(A) \subset [-\|A\|, \|A\|]$.
4. If $A : D(A) \longrightarrow \mathscr{H}$ is unbounded neither (2) nor (3) holds.
   - E. g., consider

     $$A : H^2(\mathbb{R}) \subset L^2(\mathbb{R}) \longrightarrow L^2(\mathbb{R}), \quad \varphi \mapsto \varphi''$$

     Then $\sigma(A) = [0, \infty)$.

A roadmap to the spectral theorem

For a selfadjoint operator A, we will construct:

1. $A \rightsquigarrow$ strongly continuous unitary group $U(t) = e^{-iAt}$,
2. $\rightsquigarrow$ measureable functional calculus,
3. $\rightsquigarrow$ spectral resolution,
4. $\rightsquigarrow$ spectral measure.

Strongly continuous unitary groups

Lemma

Let $A \in \mathscr{L}(\mathscr{H})$ be symmetric and $(U(t))_{t\in\mathbb{R}}$ in $\mathscr{L}(\mathscr{H})$ be given by

$$U(t) := e^{-iAt} := \sum_{n=0}^{\infty} \frac{(-iA)^n}{n!} t^n,$$

where $A^0 := \mathbf{1}$. Then:

1. $U(t+s) = U(t)U(s)$ and $U(t)^* = U(-t) = U(t)^{-1}$,
2. $t \mapsto U(t)\varphi$ is continuous for all $\varphi \in \mathscr{H}$,
3. $i\frac{d}{dt}U(t)\varphi\Big|_{t=0} = A\varphi$ for all $\varphi \in \mathscr{H}$.

Proof: Homework ☺.

Strongly continuous unitary groups

Any family $(U(t))_{t\in\mathbb{R}}$ of operators on $\mathscr{H}$ satisfying the properties (1) and (2) of the proceeding Lemma is called a **strongly continuous unitary group (SCUG)**.

The operator $A : D(A) \longrightarrow \mathscr{H}$ with

$$D(A) := \left\{ \varphi \in \mathscr{H} \;\middle|\; \frac{d}{dt}U(t)\varphi := \lim_{t\to 0} \frac{U(t)\varphi - \varphi}{t} \text{ exists} \right\}$$

and

$$A\varphi := i\frac{d}{dt}U(t)\varphi\Big|_{t=0}$$

is called the (infinitesimal) **generator** of U.

Strongly continuous unitary groups

Theorem

Any selfadjoint operator generates a SCUG.

More precisely: if A is selfadjoint, there exists a SCUG $(U(t))_{t\in\mathbb{R}}$ s.t.

$$A\varphi := i\frac{d}{dt}U(t)\varphi\Big|_{t=0}, \qquad \varphi \in D(A).$$

We will write

$$U(t) = e^{-iAt}.$$

Strongly continuous unitary groups

Sketch of the proof:

1. $B_\mu\varphi := \mathrm{i}\mu(\mathrm{i}\mu - A)^{-1}\varphi \to \varphi$ as $\mu \to \pm\infty$ for all $\varphi \in \mathscr{H}$,
2. $A_\mu := B_\mu A B_{-\mu} = A_\mu^* \in \mathscr{L}(\mathscr{H})$ if $\mu > 0$ and $A_\mu\varphi \to A\varphi$ as $\mu \to \infty$.
3. $U(t)\varphi := \lim_{\mu\to\infty} \mathrm{e}^{-\mathrm{i}A_\mu t}\varphi$ exists for all $\varphi \in \mathscr{H}$, $t \in \mathbb{R}$.
4. $(U(t))_{t\in\mathbb{R}}$ is a SCUG generated by A.

Measureable functional calculus

Let $f \in B(\mathbb{R}) := \{f : \mathbb{R} \longrightarrow \mathbb{C} \mid f \text{ is measureable \& bounded}\}$ and A be a selfadjoint operator.

We want to **insert** A in f, i.e., we are looking for a map

$$\Phi_A : B(\mathbb{R}) \longrightarrow \mathscr{L}(\mathscr{H}), \quad f \mapsto \Phi_A(f) =: f(A),$$

a s.c. **functional calculus**.

We will first define this map on the space of Schwartz functions

$$\mathcal{S}(\mathbb{R}) := \left\{ f \in C^\infty(\mathbb{R}) \;\middle|\; \sup_{t\in\mathbb{R}} |t^m f^{(n)}(t)| < \infty \; (n, m \in \mathbb{N}) \right\}.$$

Measureable functional calculus

Using the Fourier transform, we have for any $f \in \mathcal{S}(\mathbb{R})$:

$$f(x) = \int \mathrm{e}^{\mathrm{i}xt}\, \hat{f}(t)\,\mathrm{d}t \qquad \text{and} \qquad \hat{f}(t) = \frac{1}{2\pi}\int \mathrm{e}^{-\mathrm{i}tx} f(x)\,\mathrm{d}x.$$

So, we aim to define

$$\begin{aligned}\Phi_A(f) = f(A) &= \int \mathrm{e}^{-\mathrm{i}A(-t)}\,\hat{f}(t)\,\mathrm{d}t \\ &= \int U(-t)\,\hat{f}(t)\,\mathrm{d}t.\end{aligned}$$

Measureable functional calculus

For $f \in \mathcal{S}(\mathbb{R})$, consider the bounded & coercive sesquilinearform

$$b_f(\psi, \varphi) = \int \hat{f}(t)\,\langle \psi, U(-t)\varphi\rangle\,\mathrm{d}t \qquad (\varphi, \psi \in \mathscr{H}).$$

By the Lax-Milgram theorem, we may then define $\Phi_A(f)$ to be the uniquely determined operator in $\mathscr{L}(\mathscr{H})$ s. t.

$$b_f(\psi, \varphi) = \langle \psi, \Phi_A(f)\varphi\rangle.$$

Measureable functional calculus

The so obtained mapping $\Phi_A : \mathcal{S}(\mathbb{R}) \longrightarrow \mathcal{L}(\mathcal{H})$ satisfies

1. $\Phi_A(\alpha f + \beta g) = \alpha\Phi_A(f) + \beta\Phi_A(g)$,
2. $\Phi_A(fg) = \Phi_A(f)\Phi_A(g)$,
3. $\Phi_A(\bar{f}) = \Phi_A(f)^*$.

Extension Theorem

- Any map $\Phi : \mathcal{S}(\mathbb{R}) \longrightarrow \mathcal{L}(\mathcal{H})$ satisfying the properties (1) to (3) admits a unique extension $\widehat{\Phi} : B(\mathbb{R}) \longrightarrow \mathcal{L}(\mathcal{H})$.
- If $f_n, f \in B(\mathbb{R})$ s.t. $f_n \overset{\text{b.p.}}{\rightarrow} f$, then $\Phi(f_n) \overset{\sigma}{\rightarrow} \Phi(f)$.

Uniqueness

Since $\mathcal{S}(\mathbb{R})$ is dense in $C_0(\mathbb{R}) := \{f \in C(\mathbb{R}) : \lim_{|t|\to\infty} f(t) = 0\}$, it is sufficient to extend

$$\Phi : C_0(\mathbb{R}) \longrightarrow \mathcal{L}(\mathcal{H}).$$

Lemma

$B(\mathbb{R})$ is the smallest superset of $C_0(\mathbb{R})$ being closed under bounded pointwise convergence.

Uniqueness

Suppose $\widehat{\Phi}, \widehat{\Psi} : B(\mathbb{R}) \longrightarrow \mathcal{L}(\mathcal{H})$ are both extensions of Φ. Then,

$$M := \{f \in B(\mathbb{R}) : \widehat{\Phi}(f) = \widehat{\Psi}(f)\}$$

is a superset of $C_0(\mathbb{R})$ and closed under bounded pointwise convergence.

Hence, $M = B(\mathbb{R})$.

Existence

A linear functional $L : C_0(\mathbb{R}) \longrightarrow \mathbb{C}$ is said to be **positive** if $L(f) \geq 0$ whenever $f \geq 0$.

Riesz representation theorem

If $L : C_0(\mathbb{R}) \longrightarrow \mathbb{C}$ is a positive linear funtional, there exists a unique measure $\mu : \mathfrak{B}(\mathbb{R}) \longrightarrow \mathbb{C}$ s. t. $\mu(\mathbb{R}) \leq \|L\| < \infty$ and

$$L(f) = \int f \, d\mu \qquad (f \in C_0(\mathbb{R})).$$

Existence

For any $\varphi \in \mathscr{H}$, the linear functional

$$L_\varphi : C_0(\mathbb{R}) \longrightarrow \mathbb{C}, \quad f \mapsto \langle \varphi, \Phi(f)\varphi \rangle$$

is positive since $f \geq 0$ implies that also

$$L_\varphi(f) = \|\Phi(\sqrt{f})\varphi\|^2 \geq 0.$$

By the Riesz representation theorem, we thus find a measure μ_φ s.t.

$$\langle \varphi, \Phi(f)\varphi \rangle = \int f \, d\mu_\varphi$$

Existence

Since $\mu_\varphi(\mathbb{R}) \leq \|\varphi\| < \infty$,

$$\int f d\mu_\varphi = \langle \varphi, \Phi(f)\varphi \rangle$$

is defined for any $f \in B(\mathbb{R})$. Moreover,

$$B(\psi, \varphi) := \langle \psi, \Phi(f)\varphi \rangle$$

defines a bounded, coercive sesquilinearform on $\mathscr{H}$. Lax-Milgram now implies the existence of an operator $\hat{\Phi}(f) \in \mathscr{L}(\mathscr{H})$ s.t.

$$\langle \psi, \hat{\Phi}(f)\varphi \rangle = B(\psi, \varphi) \qquad (\varphi, \psi \in \mathscr{H}).$$

Measurable functional calculus

Theorem

If A is selfadjoint, there exists a unique linear mapping

$$\Phi_A : B(\mathbb{R}) \longrightarrow \mathscr{L}(\mathscr{H})$$

satisfying

1. $\Phi_A(fg) = \Phi_A(f)\Phi_A(g)$ and $\Phi_A(\bar{f}) = \Phi_A(f)^*$,
2. $f_n, f \in B(\mathbb{R})$ s.t. $f_n \overset{\text{b.p.}}{\to} f, \implies \Phi_A(f_n) \overset{\sigma}{\to} \Phi_A(f)$,
3. $\Phi_A(e_t) = e^{-iAt}$, where $e_t(x) := e^{-itx}$.

Spectral resolution

Corollary

If A is selfadjoint, there exists a uniquely determined measure $E : \mathfrak{B}(\mathbb{R}) \longrightarrow \mathscr{L}(\mathscr{H})$ satisfying

1. $E(\mathbb{R}) = E(\sigma(A)) = \mathbf{1}$, $E(\emptyset) = 0$,
2. $E(\Omega)$ is a self-adjoint projection,
3. $E(\Omega_1 \cap \Omega_2) = E(\Omega_1)E(\Omega_2)$,
4. $\Omega_1 \cap \Omega_2 = \emptyset \implies E(\Omega_1 \cup \Omega_2) = E(\Omega_1) + E(\Omega_2)$.

E is called the **spectral resolution** of A.

Proof: Define $E(\Omega) := \Phi_A(\chi_\Omega)$ for any $\Omega \in \mathfrak{B}(\mathbb{R})$. ∎

Spectral measure

Let A be selfadjoint and E be the spectral resolution of A.

Corollary

For $\varphi \in H$, let $\mu_\varphi : \mathfrak{B}(\mathbb{R}) \longrightarrow \mathbb{C}$ given by

$$\mu_\varphi(\Omega) := \langle \varphi, E(\Omega)\varphi \rangle$$

defines a complex measure on $\mathfrak{B}(\mathbb{R})$, the s.c. **spectral measure**.

Moreover,

$$\mu_\varphi(\mathbb{R}) = \mu_\varphi(\sigma(A)) = \|\varphi\|^2.$$

Theorem

Let A be selfadjoint with functional calculus Φ_A. Then

$$\langle \varphi, f(A)\varphi \rangle = \langle \varphi, \Phi_A(f)\varphi \rangle = \int_{\sigma(A)} f \, d\mu_\varphi$$

for all $f \in B(\mathbb{R})$ and all $\varphi \in H$.

Proof: Let $f = \sum_{k=1}^{n} z_k \chi_{\Omega_k}$ be an elementary function. Then

$$(\star) \qquad \langle \varphi, \Phi_A(f)\varphi \rangle = \sum_{k=1}^{n} z_k \langle \varphi, E(\Omega_k)\varphi \rangle = \sum_{k=1}^{n} z_k \mu_\varphi(\Omega_k) = \int_{\sigma(A)} f \, d\mu_\varphi.$$

Now decomposing $f = f^+ - f^-$ and approximating $f^\pm \geq 0$ by elementary functions, the theorem follows. ∎

By means of $(\star)$, we now write

$$f(A) = \Phi_A(f) = \int_{\sigma(A)} f \, dE = \int_{\sigma(A)} f(\lambda) E(d\lambda), \qquad f \in B(\mathbb{R}).$$

The Spectral theorem

Now let $f : \mathbb{R} \longrightarrow \mathbb{C}$ be **any** measureable function.

We define $\Phi(f)$ on

$$D(\Phi(f)) := \operatorname{Ran} \Phi_A\left(\frac{1}{1+|f|}\right)$$

by

$$\Phi(f)\left[\Phi_A\left(\frac{1}{1+|f|}\right)\varphi\right] := \Phi_A\left(\frac{f}{1+|f|}\right)\varphi.$$

The Spectral theorem

Theorem (Functional calculus)

Let $f : \mathbb{R} \longrightarrow \mathbb{C}$ be measureable and A be selfadjoint. Then:

1. $D(\Phi(f)) = \left\{ \varphi \in \mathscr{H} \ : \ \int |f|^2 \, \mathrm{d}\mu_\varphi < \infty \right\}$,
2. $f(A) := \Phi(f) = \int_{\sigma(A)} f \, \mathrm{d}E = \int_{\sigma(A)} f(\lambda) \, E(\mathrm{d}\lambda)$,
3. For any $\varphi \in D(\Phi(f))$, we have

$$\langle \varphi, \Phi(f)\varphi \rangle = \int_{\sigma(A)} f \, \mathrm{d}\mu_\varphi.$$

The Spectral theorem

Short Version

$$A = \Phi(\mathrm{id}_\mathbb{R}).$$

Long Version

Any selfadjoint operator A has a unique spectral resolution $E : \mathfrak{B}(\mathbb{R}) \longrightarrow \mathscr{L}(\mathscr{H})$ s.t.

$$A = \int_{\sigma(A)} \lambda E(\mathrm{d}\lambda).$$

Quantum mechanical interpretation

- The **states** of a quantum system are modelled as normed vectors φ of a Hilbert space $\mathscr{H}$.
- The **observable quantities**, e.g. position, momentum, spin, etc., are modelled as (in general unbounded) selfadjoint operators.
  - **Examples:**
    the momentum operator $p = -i\hbar\nabla$,
    the position operator $(x\varphi)(x) := x\varphi(x)$.

Quantum mechanical interpretation

If we now **measure** a quantity A at the state φ, the **probability** to find a value within $\Omega \subset \mathbb{R}$ is given by

$$\mu_\varphi(\Omega) = \langle \varphi, E(\Omega)\varphi \rangle.$$

μ_φ is the **probability distribution** of the quantity A at the state φ. Since $\mu_\varphi(\mathbb{R} \setminus \sigma(A)) = 0$, only values in $\sigma(A)$ can be found.

However, the **expectation**

$$\int \lambda \, \mu_\varphi(\mathrm{d}\lambda) = \langle \varphi, A\varphi \rangle$$

can attain any value in $[\inf \sigma(A), \sup \sigma(A)]$.