



## Functional Calculus

### Homework Problems

#### 30. Functional calculus for matrices revisited (30 points)

Let  $H = h_0 \text{id}_{\mathbb{C}^2} + \sum_{j=1}^3 h_j \sigma_j$  be a hermitian  $2 \times 2$  matrix written in terms of the Pauli matrices  $\sigma_1, \sigma_2$  and  $\sigma_3$ .

- (i) Compute the projection-valued measure associated to  $H$ .
- (ii) Show that the functional calculus introduced on Sheet 01 coincides with the functional calculus from Chapter 6 of the lecture notes.
- (iii) Prove that the following inequality is *false*:

$$\left| (\sigma_3 + \text{id}_{\mathbb{C}^2}) + (\sigma_1 - \text{id}_{\mathbb{C}^2}) \right| \leq |\sigma_3 + \text{id}_{\mathbb{C}^2}| + |\sigma_1 - \text{id}_{\mathbb{C}^2}|$$

- (iv) Show that the analogous inequality for the traces *does* hold true:

$$\text{Tr} \left| (\sigma_3 + \text{id}_{\mathbb{C}^2}) + (\sigma_1 - \text{id}_{\mathbb{C}^2}) \right| \leq \text{Tr} |\sigma_3 + \text{id}_{\mathbb{C}^2}| + \text{Tr} |\sigma_1 - \text{id}_{\mathbb{C}^2}|$$

#### Solution:

- (i) The spectrum is purely discrete,  $\sigma(H) = \sigma_{\text{disc}}(H) = \{E_-, E_+\}$  [1], where the eigenvalues are  $E_{\pm} = h_0 \pm \sqrt{h_1^2 + h_2^2 + h_3^2}$  [1]. That means the spectral measure is pure point since its support is the discrete set  $\{E_-, E_+\}$ . Thus, the eigenprojections

$$P_{\pm} \stackrel{[1]}{=} \frac{1}{2} \left( \text{id}_{\mathbb{C}^2} + \frac{\sum_{j=1}^3 h_j \sigma_j}{\sqrt{h_1^2 + h_2^2 + h_3^2}} \right)$$

are related to the projection-valued measure via

$$P(\Lambda) \stackrel{[1]}{=} (P_- + P_+) P(\Lambda) \stackrel{[1]}{=} 1_{\Lambda}(\{E_-\}) P_- + 1_{\Lambda}(\{E_+\}) P_+$$

as  $P_- + P_+ = \text{id}_{\mathbb{C}^2}$  [1].

- (ii) In Problem 02 of Sheet 01, we have defined

$$f(H) \stackrel{[1]}{=} f(E_+) P_+ + f(E_-) P_-$$

where  $f : \mathbb{R} \rightarrow \mathbb{C}$  was a suitable function.

Compared to the definition in Chapter 06,

$$f(H) \stackrel{[1]}{=} \int_{\mathbb{R}} dP(\lambda) f(\lambda),$$

we see with the help of (i) that the two definitions coincide:

$$\begin{aligned} f(H) &\stackrel{[1]}{=} \int_{\mathbb{R}} dP(\lambda) f(\lambda) \stackrel{[1]}{=} \int_{\mathbb{R}} d\lambda (\delta(\lambda - E_-) P_- + \delta(\lambda - E_+) P_+) \lambda \\ &\stackrel{[1]}{=} f(E_+) P_+ + f(E_-) P_- \end{aligned}$$

- (iii) We will repeatedly use the formulas from Sheet 01. Let us start with the left-hand side: the eigenvalues of the matrix on the left  $\sigma_3 + \text{id}_{\mathbb{C}^2} + \sigma_1 - \text{id}_{\mathbb{C}^2} = \sigma_1 + \sigma_3$  are  $E_{\pm}^{\text{left}} = \pm\sqrt{1^2 + 1^2} = \pm\sqrt{2}$  [1] with eigenprojections

$$P_{\pm}^{\text{left}} \stackrel{[1]}{=} \frac{1}{2} \left( \text{id}_{\mathbb{C}^2} \pm \frac{\sigma_1 + \sigma_3}{\sqrt{2}} \right).$$

Thus, the absolute value of the left-hand side is

$$\left| (\sigma_3 + \text{id}_{\mathbb{C}^2}) + (\sigma_1 - \text{id}_{\mathbb{C}^2}) \right| \stackrel{[1]}{=} |+\sqrt{2}| P_+^{\text{left}} + |-\sqrt{2}| P_-^{\text{left}} \stackrel{[1]}{=} \sqrt{2} \text{id}_{\mathbb{C}^2}.$$

Now to the right-hand side: eigenvalues and eigenprojections of the first term are  $E_{\pm}^{\text{right},1} = 1 \pm 1$  [1] and

$$P_{\pm}^{\text{right},1} \stackrel{[1]}{=} \frac{1}{2} (\text{id}_{\mathbb{C}^2} \pm \sigma_3)$$

while those of the second term are  $E_{\pm}^{\text{right},2} = -1 \pm 1$  [1]

$$P_{\pm}^{\text{right},2} \stackrel{[1]}{=} \frac{1}{2} (\text{id}_{\mathbb{C}^2} \mp \sigma_1).$$

That means their absolute values are

$$\begin{aligned} |\sigma_3 + \text{id}_{\mathbb{C}^2}| &\stackrel{[1]}{=} |2| \cdot P_+^{\text{right},1} + |0| \cdot P_-^{\text{right},1} \stackrel{[1]}{=} \text{id}_{\mathbb{C}^2} + \sigma_3, \\ |\sigma_1 - \text{id}_{\mathbb{C}^2}| &\stackrel{[1]}{=} |0| \cdot P_+^{\text{right},2} + |-2| \cdot P_-^{\text{right},2} \stackrel{[1]}{=} \text{id}_{\mathbb{C}^2} + \sigma_1. \end{aligned}$$

Consequently, the eigenvalues of their sum

$$|\sigma_3 + \text{id}_{\mathbb{C}^2}| + |\sigma_1 - \text{id}_{\mathbb{C}^2}| \stackrel{[1]}{=} 2\text{id}_{\mathbb{C}^2} + \sigma_1 + \sigma_3$$

are  $E_{\pm}^{\text{sum}} = 2 \pm \sqrt{2}$  [1], and since  $E_-^{\text{sum}} = 2 - \sqrt{2} < \sqrt{2}$  [1], the inequality is necessarily false [1].

- (iv) The trace of the matrix on the left is  $2\sqrt{2}$  while that of the matrix on the right is 4, and hence, the inequality involving the traces is satisfied,

$$\text{Tr} \left| (\sigma_3 + \text{id}_{\mathbb{C}^2}) + (\sigma_1 - \text{id}_{\mathbb{C}^2}) \right| \stackrel{[1]}{=} 2\sqrt{2} \stackrel{[1]}{\leq} 4 \stackrel{[1]}{=} \text{Tr} |\sigma_3 + \text{id}_{\mathbb{C}^2}| + \text{Tr} |\sigma_1 - \text{id}_{\mathbb{C}^2}|.$$

### 31. Projections and functional calculus (15 points)

Let  $P$  be a selfadjoint operator on a Hilbert space  $\mathcal{H}$ . Show that  $P$  is an orthogonal projection if and only if  $\sigma(P) \subseteq \{0, 1\}$ .

**Solution:**

“ $\Rightarrow$ ” Suppose  $P$  is an orthogonal projection. Orthogonal projections are bounded, and the spectrum is closed and bounded by Problem 26. Let us define the bounded function

$$f(\lambda) \stackrel{[1]}{=} \begin{cases} \lambda^2 & |\lambda| \leq 2\|P\| \\ 0 & \text{else} \end{cases}.$$

Then we can use functional calculus to express  $P^2$  as  $f(P)$ ,

$$\begin{aligned} P^2 &\stackrel{[1]}{=} f(P) \stackrel{[1]}{=} \int_{\mathbb{R}} 1_{d\lambda}(P) f(\lambda) \stackrel{[1]}{=} \int_{\sigma(P)} 1_{d\lambda}(P) \lambda^2 \\ &\stackrel{[1]}{=} P \stackrel{[1]}{=} \int_{\sigma(P)} 1_{d\lambda}(P) \lambda, \end{aligned}$$

and deduce that on  $\sigma(P)$  the equation  $\lambda^2 = \lambda$  holds [1]. Evidently, the only two solutions to this equation are 0 and 1, i. e.  $\sigma(P) \subseteq \{0, 1\}$  [1].

“ $\Leftarrow$ ” Suppose  $\sigma(P) \subseteq \{0, 1\}$  where  $P$  is selfadjoint [1]. As the spectrum is bounded, so is the operator  $P$  [1]. Then we can use the same reasoning as above in reverse: let  $f$  be as above: since  $\lambda^2 = \lambda$  on  $\sigma(P)$  [1], we deduce  $P^2 = P$  from

$$\begin{aligned} P^2 &\stackrel{[1]}{=} f(P) \stackrel{[1]}{=} \int_{\mathbb{R}} 1_{d\lambda}(P) f(\lambda) \stackrel{[1]}{=} \int_{\sigma(P)} 1_{d\lambda}(P) \underbrace{\lambda^2}_{=\lambda \text{ on } \sigma(P)} \\ &\stackrel{[1]}{=} \int_{\sigma(P)} 1_{d\lambda}(P) \lambda \stackrel{[1]}{=} P. \end{aligned}$$

Hence,  $P = P^* = P^2$  is an orthogonal projection [1].

### 32. The semirelativistic kinetic energy (32 points)

Consider a semirelativistic quantum particle subjected to a magnetic field  $B = \nabla_x \times A$ . (Semirelativistic here means that you are in an energy regime where one cannot yet create particle-antiparticle pairs but the energies are high enough so that one needs to take the relativistic kinetic energy.)

Assuming the vector potential  $A \in C^\infty(\mathbb{R}^3, \mathbb{R}^3)$  is smooth, the hamiltonian

$$H^A = \sqrt{m^2 + (-i\nabla_x - A(\hat{x}))^2}.$$

The purpose of this problem is to rigorously define  $H^A$ . You may use without proof that kinetic momentum  $P_j^A := -i\partial_{x_j} - A_j(\hat{x})$  and  $(P^A)^2$  (endowed with the correct domains) define selfadjoint operators.

- (i) Let  $\phi \in C^\infty(\mathbb{R}^3, \mathbb{R})$  be a phase function and  $e^{+i\phi}$  the associated unitary. Show that kinetic momentum is gauge-covariant,

$$P^{A+\nabla_x\phi} = e^{+i\phi} P^A e^{-i\phi}.$$

- (ii) Find a less laborious way to prove  $(P^{A+\nabla_x\phi})^2 = e^{+i\phi} (P^A)^2 e^{-i\phi}$ . Work smart, not hard.

- (iii) Define the semirelativistic kinetic energy  $\sqrt{m^2 + (P^A)^2}$ .

- (iv) Prove  $\sqrt{m^2 + (P^A)^2} \geq |P^A|$ .

- (v) Show  $\sqrt{m^2 + (P^{A+\nabla_x\phi})^2} = e^{+i\phi} \sqrt{m^2 + (P^A)^2} e^{-i\phi}$ .

**Solution:**

- (i) For  $\psi \in \mathcal{D}(P_j^{A+\nabla_x\phi}) := e^{+i\phi} \mathcal{D}(P_j^A)$ , we compute

$$\begin{aligned} e^{+i\phi} P_j^A e^{-i\phi} \psi &\stackrel{[1]}{=} e^{+i\phi} (-i\partial_{x_j} - A_j(\hat{x})) e^{-i\phi} \psi \\ &\stackrel{[1]}{=} e^{+i\phi} (e^{-i\phi} (-i\partial_{x_j} \psi) - i(\partial_{x_j} e^{-i\phi}) \psi - A_j(\hat{x})) \\ &\stackrel{[1]}{=} (-i\partial_{x_j} - A_j(\hat{x}) - i\partial_{x_j} \phi(\hat{x})) \psi \\ &= P_j^{A+\nabla_x\phi} \psi. \end{aligned}$$

- (ii) Writing  $(P^A)^2 = P^A \cdot P^A$  and using the result from (i), we obtain

$$\begin{aligned} e^{+i\phi} (P^A)^2 e^{-i\phi} &\stackrel{[1]}{=} e^{+i\phi} P^A e^{-i\phi} \cdot e^{+i\phi} P^A e^{-i\phi} \\ &\stackrel{[1]}{=} P^{A+\nabla_x\phi} \cdot P^{A+\nabla_x\phi} \stackrel{[1]}{=} (P^{A+\nabla_x\phi})^2. \end{aligned}$$

Note that the unitary  $e^{+i\phi}$  relates the domains  $\mathcal{D}((P^A)^2)$  and  $\mathcal{D}((P^{A+\nabla_x\phi})^2) \stackrel{[1]}{=} e^{+i\phi} \mathcal{D}((P^A)^2)$ .

- (iii) The semirelativistic kinetic energy is defined via functional calculus:  $(P^A)^2 \geq 0$  is non-negative [1] and selfadjoint [1] with domain  $\mathcal{D}((P^A)^2)$ , and consequently, the semirelativistic kinetic energy is the operator

$$\sqrt{m^2 + (P^A)^2} \stackrel{[2]}{:=} \int_0^{+\infty} 1_{d\lambda}((P^A)^2) \sqrt{m^2 + \lambda}$$

endowed with domain

$$\mathcal{D}\left(\sqrt{m^2 + (P^A)^2}\right) \stackrel{[2]}{:=} \left\{ \psi \in L^2(\mathbb{R}^3) \mid \int_0^{+\infty} \langle \psi, 1_{d\lambda}((P^A)^2) \psi \rangle (m^2 + \lambda) < \infty \right\}.$$

(Since the spectrum  $\sigma((P^A)^2) \subseteq [0, +\infty)$  is non-negative, we can omit the absolute value sign.)

(iv) We define

$$|P^A| \stackrel{[2]}{=} \sqrt{(P^A)^2} \stackrel{[1]}{=} \int_0^{+\infty} 1_{d\lambda}((P^A)^2) |\lambda|$$

analogously to the semirelativistic kinetic energy endowed with domain

$$\begin{aligned} \mathcal{D}(|P^A|) &\stackrel{[1]}{=} \left\{ \psi \in L^2(\mathbb{R}^3) \mid \int_0^{+\infty} \langle \psi, 1_{d\lambda}((P^A)^2) \psi \rangle \lambda < \infty \right\} \\ &\stackrel{[1]}{=} \left\{ \psi \in L^2(\mathbb{R}^3) \mid \int_0^{+\infty} \langle \psi, 1_{d\lambda}((P^A)^2) \psi \rangle (m^2 + \lambda) < \infty \right\} \\ &\stackrel{[1]}{=} \mathcal{D}\left(\sqrt{m^2 + (P^A)^2}\right). \end{aligned}$$

The domain of  $|P^A|$  coincides with the domain of  $\sqrt{m^2 + (P^A)^2}$  [1], and consequently, the gauge-covariance of  $\sqrt{m^2 + (P^A)^2} \geq |P^A|$  follows from  $\sqrt{m^2 + \lambda} \geq \sqrt{\lambda}$  on the level of functions [1] and functional calculus [1].

(v) The covariance of  $(P^A)^2$  proven in (ii) also implies that the projection-valued measure of this operator is also gauge-covariant,

$$1_{\Lambda}\left((P^{A+\nabla_x\phi})^2\right) = e^{+i\phi} 1_{\Lambda}\left((P^A)^2\right) e^{-i\phi}. \quad (1)$$

And if we assume for a moment that we have shown the gauge-covariance of the projection-valued measure, then also the semirelativistic kinetic energy inherits the gauge-covariance,

$$\begin{aligned} \sqrt{m^2 + (P^{A+\nabla_x\phi})^2} &\stackrel{[1]}{=} \int_{\mathbb{R}} 1_{d\lambda}\left((P^{A+\nabla_x\phi})^2\right) \sqrt{m^2 + \lambda} \\ &\stackrel{[1]}{=} \int_{\mathbb{R}} e^{+i\phi} 1_{\Lambda}\left((P^A)^2\right) e^{-i\phi} \sqrt{m^2 + \lambda} \\ &\stackrel{[1]}{=} e^{+i\phi} \sqrt{m^2 + (P^A)^2} e^{-i\phi}. \end{aligned}$$

Hence, it remains to show equation (1). From the gauge-covariance of the resolvent,

$$\left((P^{A+\nabla_x\phi})^2 - z\right)^{-1} \stackrel{[1]}{=} e^{+i\phi} \left((P^A)^2 - z\right)^{-1} e^{-i\phi},$$

and the Herglotz representation theorem,

$$\begin{aligned} \left\langle e^{-i\phi} \psi, \left((P^A)^2 - z\right)^{-1} e^{-i\phi} \psi \right\rangle &\stackrel{[1]}{=} \int_{\mathbb{R}} d\mu_{e^{-i\phi}\psi}^A(\lambda) (\lambda - z)^{-1} \\ &\stackrel{[1]}{=} \left\langle \psi, \left((P^{A+\nabla_x\phi})^2 - z\right)^{-1} \psi \right\rangle \\ &\stackrel{[1]}{=} \int_{\mathbb{R}} d\mu_{\psi}^{A+\nabla_x\phi}(\lambda) (\lambda - z)^{-1}, \end{aligned}$$

we can relate the measures of  $(P^A)^2$  and vector  $e^{-i\phi}\psi$  to that of  $(P^{A+\nabla_x\phi})^2$  and vector  $\psi$  (as indicated by the superscripts on the measures) [1]. Thus, we deduce the gauge-covariance for the projection-valued measure,

$$\begin{aligned} \left\langle \psi, e^{-i\phi} 1_{\Lambda}\left((P^A)^2\right) e^{-i\phi} \psi \right\rangle &\stackrel{[1]}{=} \int_{\Lambda} d\mu_{e^{-i\phi}\psi}^A(\lambda) \stackrel{[1]}{=} \int_{\Lambda} d\mu_{\psi}^{A+\nabla_x\phi}(\lambda) \\ &\stackrel{[1]}{=} \left\langle \psi, 1_{\Lambda}\left((P^{A+\nabla_x\phi})^2\right) \psi \right\rangle. \end{aligned}$$

### 33. Resolution of the identity (30 points)

Suppose  $H$  be a selfadjoint operator on a Hilbert space  $\mathcal{H}$  whose spectrum is purely discrete, i. e.  $\sigma(H) = \sigma_{\text{disc}}(H) = \{E_n\}_{n \in \mathbb{N}}$ . Here, the eigenvalues  $E_n$  are repeated according to their multiplicity.

- (i) Express the projection-valued measure in terms of the eigenfunctions of  $\varphi_n$ .
- (ii) Write out  $H = \int_{\mathbb{R}} dP(\lambda) \lambda$  explicitly.
- (iii) Prove that there exists a resolution of the identity with respect to the eigenfunctions  $\varphi_n$ ,

$$\text{id}_{\mathcal{H}} = \sum_{n \in \mathbb{N}} |\varphi_n\rangle\langle\varphi_n|.$$

Put another way, show that  $\text{span}\{\varphi_n\}_{n \in \mathbb{N}} = \mathcal{H}$ .

- (iv) Show that  $H$  is necessarily unbounded.

**Hint:** Review the definitions of discrete and essential spectrum.

#### Solution:

- (i) Let  $\{\varphi_n\}_{n \in \mathbb{N}}$  be an orthonormal set composed of eigenfunctions (in case of degeneracies, choose an orthonormal basis for each of the eigenspace). Then the projection-valued measure is defined through

$$\langle\psi, 1_{\Lambda}(H)\psi\rangle \stackrel{[1]}{=} \int_{\mathbb{R}} d\mu_{\psi}(\lambda) 1_{\Lambda}(\lambda) \stackrel{[1]}{=} \int_{\Lambda} d\mu_{\psi}(\lambda) \quad (2)$$

We will now show that for  $\psi \in \overline{\text{span}\{\varphi_n\}_{E_n \in \Lambda}} =: \mathcal{H}_{\Lambda}$ , the right-hand side is  $\|\psi\|^2$  [1] while for  $\psi \in \mathcal{H}_{\Lambda}^{\perp}$  we get 0 [1]: if  $\varphi_n$  is an eigenfunction to  $E_n$ , we compute

$$\langle\varphi_n, (H - z)^{-1}\varphi_n\rangle \stackrel{[1]}{=} (E_n - z)^{-1} \|\varphi_n\|^2 \stackrel{[1]}{=} (E_n - z)^{-1}.$$

On the other hand, the representation theorem for Herglotz functions relates the left-hand side to the measure  $\mu_{\varphi_n}(\lambda)$

$$\langle\varphi_n, (H - z)^{-1}\varphi_n\rangle \stackrel{[1]}{=} \int_{\mathbb{R}} d\mu_{\varphi_n}(\lambda) (\lambda - z)^{-1} \stackrel{!, [1]}{=} (E_n - z)^{-1},$$

meaning that  $d\mu_{\varphi_n}(\lambda) = \delta(\lambda - E_n) \|\varphi_n\|^2 = \delta(\lambda - E_n)$  [1]. Hence, if  $\psi \in \mathcal{H}_{\Lambda}$  then the right-hand side of (2) is necessarily  $\|\psi\|^2$  [1] while if it is in the orthogonal complement, we get 0 [1]. Thus, we have shown

$$P(\Lambda) \stackrel{[1]}{=} 1_{\Lambda}(H) \stackrel{[1]}{=} \sum_{\{n \in \mathbb{N} \mid E_n \in \Lambda\}} |\varphi_n\rangle\langle\varphi_n| \stackrel{[1]}{=} \sum_{n \in \mathbb{N}} 1_{\Lambda}(E_n) |\varphi_n\rangle\langle\varphi_n|.$$

- (ii) The projection-valued measure is the infinite sum of point measures, and hence, we obtain

$$H \stackrel{[1]}{=} \int_{\mathbb{R}} dP(\lambda) \lambda \stackrel{[1]}{=} \sum_{n \in \mathbb{N}} E_n |\varphi_n\rangle\langle\varphi_n|.$$

(iii) Lemma 6.1.10 tells us that

$$P(\Lambda) \stackrel{[1]}{=} 1_\Lambda(H) \stackrel{[1]}{=} \sum_{n \in \mathbb{N}} 1_\Lambda(E_n) |\varphi_n\rangle\langle\varphi_n|$$

is a projection-valued measure, and all projection valued measures satisfy

$$\text{id}_{\mathcal{H}} \stackrel{[1]}{=} P(\mathbb{R}) \stackrel{[1]}{=} \sum_{n \in \mathbb{N}} 1_{\mathbb{R}}(E_n) |\varphi_n\rangle\langle\varphi_n| \stackrel{[1]}{=} \sum_{n \in \mathbb{N}} |\varphi_n\rangle\langle\varphi_n|.$$

This is equivalent to saying that  $\{\varphi_n\}_{n \in \mathbb{N}}$  forms an orthonormal basis of  $\mathcal{H}$ .

(iv) Assume  $H$  were bounded [1]. Then by Problem 26, we have  $\sigma(H) \subseteq \{z \in \mathbb{C} \mid |z| \leq \|H\|\}$  [1] and the spectrum is bounded [1]. Hence, the sequence  $\{E_n\}_{n \in \mathbb{N}} \subset \mathbb{R}$  is bounded [1] and consequently must have an accumulation point [1]. Such an accumulation point is part of the essential spectrum by Theorem 5.2.8 [1], and thus,  $\sigma_{\text{ess}}(H) \neq \emptyset$  [1] which contradicts our assumption that the spectrum is purely discrete [1]. Hence,  $H$  has to be unbounded [1].