Homework for Bonus Points

This homework sheet is for bonus points. However, *all problems are immediately relevant for the final exam* and finishing them will be useful as part of the preparation independently of the bonus points. You need not finish all problems, anything you submit will count in your favor.

Homework Problems

37. The Banach space of trace class operators (10 points)

Let $A \in \mathcal{B}(\mathcal{H})$ be a bounded operator on an infinite-dimensional, separable Hilbert space. Then define the trace

$$\mathrm{Tr}\, A := \sum_{n=1}^{\infty} \langle \varphi_n, A\varphi_n \rangle$$

where $\{\varphi_n\}_{n\in\mathbb{N}}$ is an arbitrary orthonormal basis of $\mathcal{H}$. We have already shown that the definition of Tr does not depend on the choice of basis. The goal of this problem is to characterize elements of the Banach space of trace class operators

$$\mathcal{T}^1(\mathcal{H}) := \bigl\{ A \in \mathcal{B}(\mathcal{H}) \;\mid\; \mathrm{Tr}\, |A| < \infty \bigr\}$$

with norm $\lVert A \rVert_{\mathcal{T}^1} := \mathrm{Tr}\, |A|$. This will be done in steps:

(i) For an arbitrary $A \in \mathcal{B}(\mathcal{H})$, define $|A| := \sqrt{A^* A}$ via functional calculus. Prove that $|A| \geq 0$.

Now suppose $H \in \mathcal{B}(\mathcal{H})$ is bounded and selfadjoint so that $\sigma_{\mathrm{disc}}(H) = \{E_n\}_{n\in\mathcal{I}}$ and $\sigma_{\mathrm{ess}}(H) \subseteq \{0\}$. Here, the eigenvalues E_n are counted according to their multiplicities, and the index set $\mathcal{I}$ is $\mathbb{N}$ in case H has infinitely many eigenvalues and $\mathcal{I} = \{1, \ldots, N\}$ if the number of non-zero eigenvalues is finite.

(ii) Show that any eigenfunction of H and is an eigenfunction of $|H|$.

(iii) Prove $|\sigma(H)| = \sigma(|H|)$.

Now suppose $H \in \mathcal{B}(\mathcal{H})$ is just bounded and selfadjoint.

(iv) Use the Weyl Criterion to show that Tr $|H| < \infty$ implies $\sigma_{\mathrm{ess}}(|H|) = \sigma_{\mathrm{ess}}(H) \subseteq \{0\}$.

(v) Show that for $H \in \mathcal{T}^1(\mathcal{H})$ we have

$$\lVert H \rVert_{\mathcal{T}^1} = \sum_{n=1}^{\infty} |E_n|$$

where $\sigma_{\mathrm{p}}(H) = \{E_n\}_{n\in\mathbb{N}}$ (i. e. E_n may be 0).

(vi) Let ρ be a density operator. Prove that $\sigma_{\mathrm{ess}}(\rho) \subseteq \{0\}$ and that $\sigma_{\mathrm{disc}}(\rho) \subseteq [0, 1]$.

Solution:

(i) $H := A^*A$ is a bounded selfadjoint operator. Moreover, $A^*A \geq 0$ since

$$\big\langle \psi, A^*A\psi \big\rangle = \|A\psi\|^2 \geq 0.$$

Hence, we can take the square root of $H = A^*A$ defined via functional calculus. The fact that $\lambda \mapsto \sqrt{\lambda}$ is unbounded is immaterial because $\sigma(H)$ is a bounded subset of $[0, +\infty)$ and $f(H)$ is solely determined by the behavior of f on $\sigma(H)$. Thus, we set

$$|A| := \sqrt{A^*A} = \int_{\sigma(A^*A)} 1_{\mathrm{d}\lambda}(A^*A)\,\sqrt{\lambda}.$$

(ii) First of all, under these conditions H has a basis of eigenvalues, and we can express H just as in Problem 33. The fact that we admit the case $\sigma_{\text{ess}}(H) = \{0\}$ does not change the story, because the zero eigenvalue does not contribute to the sum

$$H = \sum_{n\in\mathbb{N}} E_n\,|\varphi_n\rangle\langle\varphi_n|.$$

Consequently, we have by functional calculus

$$|H| = \sum_{n\in\mathbb{N}} |E_n|\;|\varphi_n\rangle\langle\varphi_n|,$$

and any eigenfunction of H to E_n is an eigenfunction of $|H|$ to $|E_n|$.

(iii) This follows directly from (ii). Alternatively, we can argue that Theorem 6.2.4 applies to the continuous function $\lambda \mapsto |\lambda|$: Because H is bounded and $\sigma_{\text{ess}}(H) \subseteq \{0\}$ by assumption, and accumulation points of eigenvalues lie in the essential spectrum, the arguments in Problem 33 (iv) imply $\sigma_{\text{ess}}(H) = \{0\}$ is non-empty. Hence, we can omit the closure, and we have shown

$$\big|\sigma(H)\big| = \sigma(|H|).$$

(iv) To simplify the notation, we assume without loss of generality that $H \geq 0$ (meaning $H = |H|$) for otherwise replace H with $|H|$ in the following. Assume there exists a $E \in \sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(|H|)$ with $E \neq 0$, in fact $E > 0$. Thus, by the Weyl criterion, there exists an *orthonormal* sequence φ_n with

$$\lim_{n\to\infty} \big\|(H - E)\varphi_n\big\| = 0.$$

This also implies that $\langle\varphi_n, H\varphi_n\rangle \xrightarrow{n\to\infty} E$, because expressing the norm in terms of the scalar product yields

$$\begin{aligned}\big\|H\varphi_n - E\varphi_n\big\|^2 &= \big\|H\varphi_n\big\|^2 + E^2\,\|\varphi_n\|^2 - \langle E\,\varphi_n, H\varphi_n\rangle - \langle H\varphi_n, E\,\varphi_n\rangle \\ &= \big\|H\varphi_n\big\|^2 + E^2 - 2E\,\langle\varphi_n, H\varphi_n\rangle \xrightarrow{n\to\infty} 0.\end{aligned}$$

Given that $\|H\varphi_n\|$ approaches E, we deduce

$$\lim_{n\to\infty} \langle\varphi_n, H\varphi_n\rangle = E.$$

By discarding the first N elements, we can ensure that $\langle\varphi_n, H\varphi_n\rangle \geq E/2$, for instance.

Then to compute the trace we may pick an orthonormal basis $\{\psi_n\}_{n\in\mathbb{N}}$ which contains $\{\varphi_n\}_{n\in\mathbb{N}}$. With that basis and $H \geq 0$ we obtain a contradiction,

$$+\infty > \mathrm{Tr}\,|H| = \sum_{n=1}^{\infty} \langle \psi_n, |H|\, \psi_n \rangle \geq \sum_{n=1}^{\infty} \langle \varphi_n, H\varphi_n \rangle \geq \sum_{n=1}^{\infty} \frac{E}{2} = +\infty.$$

That means H cannot be trace class if $\sigma_{\mathrm{ess}}(H) \not\subseteq \{0\}$.

(v) For this computation, we merely use the eigenbasis $\{\varphi_n\}_{n\in\mathbb{N}}$ of H (which by (ii) is also an eigenbasis for $|H|$) to compute the trace:

$$\big\| H \big\|_{\mathcal{T}^1} = \mathrm{Tr}\,|H| = \sum_{n=1}^{\infty} \langle \varphi_n, |H|\, \varphi_n \rangle = \sum_{n=1}^{\infty} |E_n|$$

(vi) Density operators ρ are selfadjoint and non-negative operators with trace 1. In particular, density operators are trace class, and thus, apart from 0, their spectrum is purely discrete. This means we have $\sigma_{\mathrm{ess}}(\rho) \subseteq \{0\}$. Moreover, $\rho \geq 0$ implies that the eigenvalues $E_n \geq 0$ are non-negative and $|\rho| = \rho$. Thus, by (iv) the eigenvalues E_n of ρ have to sum up to 1,

$$1 = \mathrm{Tr}\,\rho = \sum_{n=1}^{\infty} E_n.$$

Consequently, $0 \leq E_n \leq 1$ holds and we have shown $\sigma(\rho) = \sigma_{\mathrm{disc}}(\rho) \cup \sigma_{\mathrm{disc}}(\rho) \subseteq [0, 1]$.

38. Holomorphic functional calculus (10 points)

Let $H = H^*$ be a *bounded* selfadjoint operator and f a function which is holomorphic in a neighborhood of $\sigma(H)$. Then we define $f(H)$ via *holomorphic functional calculus* via

$$f_\Gamma(H) := \frac{\mathrm{i}}{2\pi} \int_\Gamma \mathrm{d}z \, f(z) \, (H - z)^{-1}$$

where Γ is a contour which is contained in the region of holomorphy of f which encloses $\sigma(H)$.

(i) Prove that $f_\Gamma(H)$ coincides with $f(H)$ defined via functional calculus from Chapter 6.

(ii) Use functional calculus to prove that $f_\Gamma(H)$ does not depend on the choice of contour, i. e. if Γ' is another contour enclosing $\sigma(H)$, then $f_\Gamma(H) = f_{\Gamma'}(H)$.

(iii) Use one of the resolvent identities and results from complex analysis to prove

$$f_\Gamma(H) \, g_\Gamma(H) = (f \, g)_\Gamma(H).$$

Hint: Do *not* use functional calculus here (because then, the exercise is trivial).

Solution:

(i) As H is bounded, its spectrum $\sigma(H)$ is a compact subset of $\mathbb{R}$ and $\mathbb{C}$. And because holomorphic functions are smooth, they are bounded on the compact subset $\sigma(H)$. Hence, functional calculus from Chapter 6 applies, and we can write the resolvent in terms of the projection-valued measure $P(\Lambda) = 1_\Lambda(H)$,

$$(H - z)^{-1} = \int_{\sigma(H)} \mathrm{d}P(\lambda) \, (\lambda - z)^{-1}.$$

Thus, if we combine this with Cauchy's integral theorem

$$f(\lambda) = \frac{1}{\mathrm{i}2\pi} \int_\Gamma \mathrm{d}z \, f(z) \, (z - \lambda)^{-1},$$

we obtain $f_\Gamma(H) = f(H)$,

$$\begin{aligned} f_\Gamma(H) &= \frac{\mathrm{i}}{2\pi} \int_\Gamma \mathrm{d}z \, f(z) \int_{\sigma(H)} \mathrm{d}P(\lambda) \, (\lambda - z)^{-1} \\ &= \int_{\sigma(H)} \mathrm{d}\lambda \, \mathrm{d}P(\lambda) \left(\frac{1}{\mathrm{i}2\pi} \int_\Gamma \mathrm{d}z \, f(z) \, (z - \lambda)^{-1} \right) \\ &= \int_{\sigma(H)} \mathrm{d}\lambda \, \mathrm{d}P(\lambda) \, f(\lambda). \end{aligned}$$

(ii) Since $f(H)$ (defined via functional calculus) does not make reference to any particular contour and the arguments from (i) go through as long as the contour encloses $\sigma(H)$, this follows directly from (i).

(iii) We merely need to make a slight modification to the arguments in Chapter 6.4, pages 97–99: choose two contours Γ and Γ' which both enclose $\sigma(H)$ and Γ' is assumed to be contained in the interior of Γ. Then using the (first) resolvent identity

$$-(z - w) \, (H - z)^{-1} \, (H - w)^{-1} = (H - z)^{-1} - (H - w)^{-1}$$

to write the product of resolvents as a difference of resolvents, we obtain

$$\begin{aligned} f_\Gamma(H)\,g_{\Gamma'}(H) &= \left(\frac{\mathrm{i}}{2\pi}\right)^2 \int_\Gamma \mathrm{d}z \int_{\Gamma'} \mathrm{d}w\, f(z)\, g(w)\, (H-z)^{-1}\, (H-w)^{-1} \\ &= -\left(\frac{\mathrm{i}}{2\pi}\right)^2 \int_\Gamma \mathrm{d}z \int_{\Gamma'} \mathrm{d}w\, f(z)\, g(w)\, (z-w)^{-1}\, (H-z)^{-1} \\ &\qquad + \left(\frac{\mathrm{i}}{2\pi}\right)^2 \int_\Gamma \mathrm{d}z \int_{\Gamma'} \mathrm{d}w\, f(z)\, g(w)\, (z-w)^{-1}\, (H-w)^{-1}. \end{aligned}$$

Because Γ' is contained in the interior of Γ, the function $w \mapsto g(w)\,(z-w)^{-1}$ is holomorphic on a region which contains Γ'; in particular, it has no residuals in the interior of Γ', and thus

$$\int_{\Gamma'} \mathrm{d}w\, g(w)\, (z-w)^{-1} = 0$$

which means the first term in the sum vanishes. On the other hand, $z \mapsto f(z)\,(z-w)^{-1}$ *does* have a single residual in the interior of Γ, and consequently, we obtain

$$\int_\Gamma f(z)\,(z-w)^{-1} = -\mathrm{i}2\pi\, f(w).$$

That means we have shown

$$\begin{aligned} \ldots &= -\left(\frac{\mathrm{i}}{2\pi}\right)^2 \int_\Gamma \mathrm{d}z\, \underbrace{\left(\int_{\Gamma'} \mathrm{d}w\, g(w)\,(z-w)^{-1}\right)}_{=0} f(z)\,(H-z)^{-1} \\ &\qquad + \left(\frac{\mathrm{i}}{2\pi}\right)^2 \underbrace{\left(\int_{\Gamma'} \mathrm{d}w \int_\Gamma \mathrm{d}z\, f(z)\,(z-w)^{-1}\right)}_{=-\mathrm{i}2\pi\, f(w)} g(w)\,(H-w)^{-1} \\ &= \frac{\mathrm{i}}{2\pi} \int_{\Gamma'} \mathrm{d}w\, f(w)\, g(w)\,(H-w)^{-1} = (f\,g)_{\Gamma'}(H). \end{aligned}$$

By (ii) we can replace Γ' by Γ on the left- and right-hand side, meaning we have shown

$$f_\Gamma(H)\, g_\Gamma(H) = (f\,g)_\Gamma(H).$$

39. Selfadjointness (10 points)

Consider the Hamilton operator

$$H = -\Delta_x - \frac{1 - \cos|x|}{|x|^3}$$

endowed with domain $\mathcal{D}(H) = H^2(\mathbb{R}^3)$.

(i) Prove that H is selfadjoint.

(ii) How many eigenvalues does H have below 0? Justify your answer.

Solution:

(i) The domain $\mathcal{D}(H) = H^2(\mathbb{R}^3)$ coincides with the domain of selfadjointness of $-\Delta_x$, and we need to check whether we can apply Theorem 5.2.25, i. e. whether the potential is of class $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Clearly, away from $x = 0$, the potential is bounded, and all we need to check is whether the singularity at $x = 0$ is square integrable. Taylor expanding $1 - \cos r$ around $r = |x| = 0$ yields

$$\begin{aligned} \frac{1 - \cos r}{r^3} &= -\frac{\sum_{n=1}^\infty \frac{(-1)^n}{(2n)!} r^{2n}}{r^3} \\ &= \frac{1}{r} \sum_{n=0}^\infty \frac{(-1)^n}{(2n+2)!} r^{2n}, \end{aligned} \tag{1}$$

and the potential has a Coulombic $1/|x|$ singularity at $x = 0$. That means the potential is in $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, and consequently, Theorem 5.2.25 applies – H is selfadjoint.

(ii) The sum on the right-hand side of equation (1) is non-negative for all $r \geq 0$, and thus

$$H = -\Delta_x - \frac{1 - \cos|x|}{|x|^3} \leq -\Delta - \frac{1}{2\,|x|} = H_{\mathrm{C}}$$

holds on $\mathcal{D}(H) = H^2(\mathbb{R}^3) = \mathcal{D}(H_{\mathrm{C}})$. That means we also deduce

$$E_n(H) \leq E_n(H_{\mathrm{C}})$$

where the E_n are defined as on p. 71 of the lecture notes. Since H_{C} has infinitely many eigenvalues below 0, so does H.

40. Hamilton operators for spin systems

Define the operator

$$H_0 = -\mathrm{i}\partial_{x_1} \otimes \sigma_1 - \mathrm{i}\partial_{x_2} \otimes \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i}\partial_{x_1} - \partial_{x_2} \\ -\mathrm{i}\partial_{x_1} + \partial_{x_2} & 0 \end{pmatrix}$$

equipped with domain $\mathcal{D}(H_0) = \mathcal{C}^\infty_{\mathrm{c}}(\mathbb{R}^2, \mathbb{C}^2)$ where σ_1 and σ_2 are the first two Pauli matrices.

(i) Show that H_0 is equivalent to a *hermitian*-matrix-valued multiplication operator.

(ii) Prove that H_0 is essentially selfadjoint.

(iii) Is the the selfadjoint extension $H := \overline{H_0}$ bounded from below? Justify your answer.

(iv) Show that $K := C\big(\mathrm{id}_{L^2(\mathbb{R}^2)} \otimes \sigma_2\big)$ commutes with H on $\mathcal{D}(H)$.

Solution:

(i) By Fourier transform we obtain

$$H_0^{\mathcal{F}} := \mathcal{F}\, H_0\, \mathcal{F}^{-1} = \hat{\xi}_1 \otimes \sigma_1 + \hat{\xi}_2 \otimes \sigma_2 = \begin{pmatrix} 0 & \hat{\xi}_1 - \mathrm{i}\hat{\xi}_2 \\ \hat{\xi}_1 + \mathrm{i}\hat{\xi}_2 & 0 \end{pmatrix} =: T(\hat{\xi})$$

where $H_0^{\mathcal{F}}$ is endowed with the domain $\mathcal{D}(H_0^{\mathcal{F}}) = \mathcal{F}\mathcal{C}^\infty_{\mathrm{c}}(\mathbb{R}^3, \mathbb{C}^2)$. Put another way, H_0 is unitarily equivalent to the matrix-valued multiplication operator associated to T.

(ii) The essential selfadjointness of H_0 is equivalent to that of $H_0^{\mathcal{F}}$. Since $T(\xi)$ is a hermitian matrix, the operator $H_0^{\mathcal{F}}$ (and consequently also H_0) is symmetric: for $\varphi, \psi \in \mathcal{C}^\infty_{\mathrm{c}}(\mathbb{R}^3, \mathbb{C}^2)$ we thus obtain

$$\begin{aligned} \big\langle \varphi, H_0 \psi \big\rangle &= \big\langle \mathcal{F}\varphi, H_0^{\mathcal{F}}\, \mathcal{F}\psi \big\rangle = \big\langle \mathcal{F}\varphi, T(\hat{\xi})\, \mathcal{F}\psi \big\rangle \\ &= \big\langle T(\hat{\xi})\, \mathcal{F}\varphi, \mathcal{F}\psi \big\rangle = \big\langle H_0 \varphi, \psi \big\rangle. \end{aligned}$$

H_0 and $H_0^{\mathcal{F}}$ are also densely defined, and thus, we may use the Fundamental Criterion, i. e. we need to check whether $\ker(H_0^* \pm \mathrm{i}) = \{0\}$. Again, we may phrase that in terms of $T(\hat{\xi})$: the eigenvalues of $T(\xi)$ are real, namely $\pm\,|\xi|$, which implies that the equation

$$T(\hat{\xi})\hat{\varphi}_\pm = \mp \mathrm{i}\hat{\varphi}_\pm$$

has no non-trivial solution. Thus, $H_0^{\mathcal{F}}$ and H_0 are essentially selfadjoiint.

(iii) H is *not* bounded from below, because we can write T as

$$H^{\mathcal{F}} = T(\hat{\xi}) = |\xi|\; P_+(\hat{\xi}) - |\xi|\; P_-(\hat{\xi})$$

and evidently, the spectrum of $H^{\mathcal{F}}$ is all of $\mathbb{R}$, $\sigma(H) = \sigma(H^{\mathcal{F}}) = \mathbb{R}$.

(iv) First of all, we note that K leaves the domain invariant. Then using $\sigma_j^2 = \mathrm{id}_{\mathbb{C}^2}$, $\sigma_1\,\sigma_2 = -\sigma_2\,\sigma_1$, $C\,\sigma_1 = \sigma_1\,C$ and $C\,\sigma_2 = -\sigma_2\,C$, we deduce

$$K\,\big(-\mathrm{i}\partial_{x_j} \otimes \sigma_j\big) = \big(-\mathrm{i}\partial_{x_j} \otimes \sigma_j\big)\,K$$

for $j = 1, 2$, meaning that also the sum commutes with K on the domain of selfadjointness $\mathcal{D}(H)$,

$$[H, K] = 0.$$

41. The discrete position operator

Let us define the position operator Q on $\ell^2(\mathbb{Z})$ via

$$(Q\psi)(n) := n\,\psi(n)$$

where the domain $\mathcal{D}(Q) \subseteq \ell^2(\mathbb{Z})$ has yet to be determined.

(i) Find the domain of selfadjointness for Q and verify that Q is then indeed selfadjoint.

(ii) Compute $\sigma(Q)$ and find all spectral decompositions $\sigma_\sharp(Q)$ where $\sharp$ stands for p, c, r, disc, ess, pp, sc and ac.

(iii) Compute the projection-valued measure $1_\Lambda(Q)$ explicitly where $\Lambda \subseteq \mathbb{R}$ is a Borel set.

Solution:

(i) We propose to use

$$\begin{aligned}\mathcal{D}(Q) &= \big\{\psi \in \ell^2(\mathbb{Z}) \;\mid\; \hat{n}\psi \in \ell^2(\mathbb{Z})\big\} \\ &= \Big\{\psi \in \ell^2(\mathbb{Z}) \;\mid\; \sum_{n\in\mathbb{Z}} n^2 \left|\psi(n)\right|^2 < \infty\Big\}\end{aligned}$$

which is clearly the maximal domain. Clearly, the maximal domain is dense.

A direct computation shows that Q is symmetric on $\mathcal{D}(Q)$:

$$\begin{aligned}\langle\varphi, Q\psi\rangle &= \sum_{n\in\mathbb{Z}} \overline{\varphi(n)}\,(Q\psi)(n) = \sum_{n\in\mathbb{Z}} \overline{\varphi(n)}\,n\,\psi(n) \\ &= \sum_{n\in\mathbb{Z}} \overline{n\,\varphi(n)}\,\psi(n) = \sum_{n\in\mathbb{Z}} \overline{(Q\varphi)(n)}\,\psi(n) = \langle Q\varphi, \psi\rangle\end{aligned}$$

We use the Fundamental Criterion to show *essential* selfadjointness first: to see that $\ker(Q^* \pm \mathrm{i}) = \{0\}$, we note that

$$\hat{n}\varphi_\pm = \mp\mathrm{i}\varphi_\pm$$

cannot have a non-trivial solution, because eigenvalues of real-valued multiplication operators are necessarily real. Hence, Q is essentially selfadjoint.

To show $\mathcal{D}(Q^*) = \mathcal{D}(Q)$ (i. e. $Q^* = Q$), we note that for symmetric operators $\mathcal{D}(Q) \subseteq \mathcal{D}(Q^*)$, and because $\mathcal{D}(Q)$ is the maximal domain, the domain of Q^* has to coincide with that of Q. Hence, $Q = Q^*$ is selfadjoint.

(ii) The $\psi_k(n) = \delta_{kn}$ are the eigenfunctions of Q to the eigenvalue $k \in \mathbb{Z}$,

$$\big(Q\psi_k\big)(n) = n\,\psi_k(n) = k\,\delta_{kn} = k\,\psi_k(n).$$

Clearly, every eigenvalue is non-degenerate. Also, $\{\psi_k\}_{k\in\mathbb{Z}}$ form an orthonormal basis of $\ell^2(\mathbb{Z})$. Consequently, we have the following decompositions of the spectrum:

$$\begin{aligned}\sigma(Q) = \mathbb{Z} = \sigma_{\mathrm{p}}(Q) = \sigma_{\mathrm{pp}}(Q) = \sigma_{\mathrm{disc}}(Q) \\ \sigma_{\mathrm{ess}}(Q) = \emptyset = \sigma_{\mathrm{r}}(Q) = \sigma_{\mathrm{c}}(Q) = \sigma_{\mathrm{sc}}(Q) = \sigma(Q)\end{aligned}$$

(iii) For any Borel set $\Lambda \subseteq \mathbb{R}$ the projection-valued measure is

$$1_\Lambda(Q) = \sum_{k\in\mathbb{Z}} 1_\Lambda(k)\,|\psi_k\rangle\langle\psi_k|$$

where the $\psi_k(n) = \delta_{kn}$ are the eigenfunctions to the eigenvalue k.