Foundations of Quantum Mechanics (APM 421 H)

University of Toronto

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Solutions 11
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Functional Calculus

Homework Problems

34. The Weyl criterion (19 points)

Prove the Weyl criterion:

Theorem 1 *Let H be a selfadjoint operator on a Hilbert space $\mathcal{H}$ with domain $\mathcal{D}(H)$.*

(i) $\lambda \in \sigma(H)$ holds if and only if there exists a sequence $\{\psi_n\}_{n \in \mathbb{N}}$ so that $\|\psi_n\| = 1$ and

$$\lim_{n \to \infty} \big\| H\psi_n - \lambda\, \psi_n \big\|_{\mathcal{H}} = 0.$$

(ii) We have $\lambda \in \sigma_{\mathrm{ess}}(H)$ if and only if we can choose the sequence $\{\psi_n\}_{n \in \mathbb{N}}$ to be orthonormal.

Solution:

(i) The weak Weyl criterion takes care of one direction, i. e. if there exists a Weyl sequence $\{\psi_n\}_{n \in \mathbb{N}}$ to $\lambda \in \mathbb{R}$, then necessarily $\lambda \in \sigma(H)$ [1].

For the converse direction, pick a $\lambda \in \sigma(H)$. We will now construct a Weyl sequence: since $\lambda \in \sigma(H)$ we know from Proposition 6.2.1 that the projection-valued measures $P\big((\lambda - 1/n, \lambda + 1/n)\big) \neq 0$, $n \in \mathbb{N}$, do not vanish [1]. Consequently, we can choose a normalized vector $\psi_n \in \mathrm{ran}\, P\big((\lambda - 1/n, \lambda + 1/n)\big)$ for each $n \in \mathbb{N}$ [1]. And thus, we can estimate the norm by

$$\begin{aligned} \big\| H\psi_n - \lambda\psi_n \big\|^2 &\overset{[1]}{=} \big\| (H - \lambda)\, 1_{(\lambda - 1/n, \lambda + 1/n)}(H) \psi_n \big\|^2 \\ &\overset{[1]}{=} \int_{\lambda - 1/n}^{\lambda + 1/n} \big\langle \psi_n, \mathrm{d}P(\lambda') \psi_n \big\rangle\, (\lambda' - \lambda)^2 \overset{[1]}{\leq} \frac{1}{n^2} \xrightarrow{n \to \infty} 0, \end{aligned}$$

which means $\{\psi_n\}_{n \in \mathbb{N}}$ is a Weyl sequence [1].

(ii) "⇒:" If we assume in addition that $\lambda \in \sigma_{\mathrm{ess}}(H)$, then $\mathcal{H}_n := \mathrm{ran}\, P\big((\lambda - 1/n, \lambda + 1/n)\big)$ is infinite-dimensional for all $n \in \mathbb{N}$ [1], and these spaces are nested, $\mathcal{H}_n \supseteq \mathcal{H}_{n+1}$ [1], meaning we can choose

$$\psi_{n+1} \overset{[1]}{\in} \mathcal{H}_{n+1} \cap \big(\mathrm{span}\{\psi_j\}_{j=1}^{n}\big)^{\perp}$$

because the intersection on the right-hand side is non-trivial [1]. Hence, the Weyl sequence constructed in this fashion is orthonormal [1].

"⇐:" Suppose the Weyl sequence $\{\psi_n\}_{n \in \mathbb{N}}$ to $\lambda \in \mathbb{R}$ is composed of orthonormal vectors. We already know from part (i) that $\lambda \in \sigma(H)$ [1], and all that remains to be shown is $\sigma_{\mathrm{ess}}(H)$.

Without loss of generality, we may assume that $\psi_n \in \operatorname{ran} 1_{(\lambda-1/n,\lambda+1/n)}(H)$ (otherwise select a subsequence which satisfies the above condition) [1].

Assume $\lambda \in \sigma_{\text{disc}}(H)$ [1]. Then λ is an eigenvalue of finite multiplicity; Moreover, λ cannot be the accumulation point of eigenvalues [1]. That means for $n \geq N$ large enough the intersection $\sigma(H) \cap (\lambda - 1/n, \lambda + 1/n) = \{\lambda\}$ consists only of the eigenvalue itself [1]. But then for all $n \geq N$ the subspace $\operatorname{ran} 1_{(\lambda-1/n,\lambda+1/n)}(H)$ is finite-dimensional [1], meaning that the Weyl sequence $\{\varphi_n\}_{n\in\mathbb{N}}$ cannot be chosen to consist of orthonormal vectors [1].

35. Functional calculus for the momentum operator (25 points)

Consider the momentum operator $P = -\mathrm{i}\partial_x$ on $L^2(\mathbb{R})$ with domain $\mathcal{D}(P) = H^1(\mathbb{R})$.

(i) Show $P = P^*$ and give $\sigma(P)$.

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

(iii) Explain how to define $U(t) := \mathrm{e}^{-\mathrm{i}tP}$ and prove that $U(t)\,U(s) = U(t+s)$.

(iv) Define the selfadjoint operator $H = P^2$ via the functional calculus associated to P and prove that it coincides with $H' = -\partial_x^2$ endowed with domain $\mathcal{D}(H') = H^2(\mathbb{R})$.

Solution:

(i) We use the Fundamental Criterion of Selfadjointness [1]: we first shown essential selfadjointness of P and then, in a second step, show that the domain of selfadjointness coincides with $H^1(\mathbb{R})$. To compute the deficiency indices $N_\pm := \dim\ker\big(P^* \pm \mathrm{i}\big)$ [1], we solve the equation

$$-\mathrm{i}\partial_x\varphi_\pm = \mp\mathrm{i}\varphi_\pm \iff \partial_x\varphi_\pm = \pm\varphi_\pm \qquad [1]$$

for both signs. Obviously, the solutions are $\varphi_\pm(x) = c\mathrm{e}^{\pm x}$ [1]. However, for neither choice of sign is $\varphi_\pm \not\in L^2(\mathbb{R})$ square-integrable [1]. Consequently, $N_\pm = 0$ and P is *essentially* selfadjoint [1]. On the other hand, the domain of P,

$$\begin{aligned}\mathcal{D}(P) = H^1(\mathbb{R}) &\overset{[1]}{=} \Big\{\varphi \in L^2(\mathbb{R}^d) \;\big|\; \mathcal{F}^{-1}\sqrt{1+\xi^2}\,\mathcal{F}\varphi \in L^2(\mathbb{R}^d)\Big\} \\ &\overset{[1]}{=} \Big\{\varphi \in L^2(\mathbb{R}^d) \;\big|\; \int_{\mathbb{R}} \mathrm{d}\xi\,\big(1+\xi^2\big)\,\mathcal{F}\varphi(\xi) < \infty\Big\} \\ &\overset{[1]}{=} \Big\{\varphi \in L^2(\mathbb{R}^d) \;\big|\; \int_{\mathbb{R}} \mathrm{d}\xi\,\xi^2\,\mathcal{F}\varphi(\xi) < \infty\Big\},\end{aligned}$$

coincides with the maximal domain,

$$\mathcal{D}(P_{\mathrm{max}}) = \big\{\varphi \in L^2(\mathbb{R}) \;\big|\; \partial_x\varphi \in L^2(\mathbb{R})\big\} \overset{[1]}{=} \mathcal{D}(P).$$

And hence, $P = P^*$ is selfadjoint.

(ii) Given that $\mathcal{F}\,P\,\mathcal{F}^{-1} = \hat{\xi}$ [1] is equivalent to a multiplication operator, we can write the projection-valued measure as

$$1_\Lambda(P) \overset{[2]}{=} \mathcal{F}^{-1}\,1_\Lambda(\hat{\xi})\,\mathcal{F}.$$

(iii) As $\lambda \mapsto \mathrm{e}^{-\mathrm{i}t\lambda}$ is a bounded Borel function [1],

$$U(t) = \mathrm{e}^{-\mathrm{i}tP} \overset{[1]}{=} \int_{\mathbb{R}} 1_{\mathrm{d}\lambda}(P)\,\mathrm{e}^{-\mathrm{i}t\lambda},$$

is defined via functional calculus. Then $U(t)\,U(s) = U(t+s)$ is an immediate consequence of $f(H)\,g(H) = (f\,g)(H)$ [1] and $\mathrm{e}^{-\mathrm{i}t\lambda}\,\mathrm{e}^{-\mathrm{i}s\lambda} = \mathrm{e}^{-\mathrm{i}(t+s)\lambda}$ on the level of functions [1].

(iv) The operator

$$H \overset{[1]}{:=} \int_{\mathbb{R}} 1_{\mathrm{d}\lambda}(P)\,\lambda^2$$

defined via functional calculus is endowed with the domain

$$\mathcal{D}(H) \overset{[1]}{:=} \Big\{\psi \in L^2(\mathbb{R}) \;\big|\; \int_{\mathbb{R}} \big\langle \psi, 1_{\mathrm{d}\lambda}(P)\psi\big\rangle\,\lambda^4 < \infty\Big\}.$$

Since it is clear that H acts on $\varphi \in \mathcal{D}(H)$ as $\varphi \mapsto -\partial_x^2 \varphi$ [1], it remains to show $\mathcal{D}(H) = \mathcal{D}(H') = H^2(\mathbb{R})$. As we can express the projection-valued measure as a multiplication operator after Fourier transform, we can rewrite the imposed condition from $\mathcal{D}(H)$ as

$$\begin{aligned} \int_{\mathbb{R}} \langle \psi, 1_{\mathrm{d}\lambda}(P)\psi \rangle \, \lambda^4 &\overset{[1]}{=} \int_{\mathbb{R}} \langle \mathcal{F}\psi, 1_{\mathrm{d}\lambda}(\hat{\xi}) \, \mathcal{F}\psi \rangle \, \lambda^4 \\ &\overset{[1]}{=} \int_{\mathbb{R}} \mathrm{d}\lambda \, \left| \lambda^2 \, \mathcal{F}\psi(\lambda) \right|^2 \\ &\overset{[1]}{=} \left\| \hat{\xi}^2 \, \mathcal{F}\psi \right\|^2 < \infty. \end{aligned}$$

That, however, is equivalent to saying $\varphi \in H^2(\mathbb{R})$ [1], and we have shown $\mathcal{D}(H) = H^2(\mathbb{R}) = \mathcal{D}(H')$ [1].

36. Functional calculus for the position operator (31 points)

Suppose $H = -\partial_x^2 + V = H^*$ is a selfadjoint operator on $L^2(\mathbb{R})$ with domain $\mathcal{D}(H)$, and consider the position operator $Q = \hat{x}$ equipped with domain

$$\mathcal{D}(Q) = \bigl\{ \varphi \in L^2(\mathbb{R}) \;\mid\; \hat{x}\varphi \in L^2(\mathbb{R}) \bigr\}.$$

You may use without proof that Q is selfadjoint.

(i) Show that $Q(t) := \mathrm{e}^{+\mathrm{i}tH}\, Q\, \mathrm{e}^{-\mathrm{i}tH}$ satisfies the Heisenberg equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}t} Q(t) = \mathrm{i}\, \bigl[H, Q(t) \bigr].$$

A formal computation suffices (i. e. you may ignore questions of domains).

(ii) Prove that also $Q(t) = Q(t)^*$ is selfadjoint.

(iii) Let $\bigl(V(\hat{x})\psi\bigr)(x) := V(x)\, \psi(x)$ be the multiplication operator associated to a bounded Borel function $V : \mathbb{R} \longrightarrow \mathbb{C}$. Prove that $V(\hat{x})$ coincides with $V(Q)$ (defined through functional calculus associated to Q).

(iv) Prove $\bigl(V(Q)\bigr)(t) := \mathrm{e}^{+\mathrm{i}tH}\, V(Q)\, \mathrm{e}^{-\mathrm{i}tH}$ coincides with $V\bigl(Q(t)\bigr)$.

Solution:

(i) Using that H and $\mathrm{e}^{\pm \mathrm{i}tH}$ commute (Theorem 4.3.5) [1], we compute the time-derivative and collect the terms accordingly:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} Q(t) &\overset{[1]}{=} \bigl(\tfrac{\mathrm{d}}{\mathrm{d}t} \mathrm{e}^{+\mathrm{i}tH} \bigr)\, Q\, \mathrm{e}^{-\mathrm{i}tH} + \mathrm{e}^{+\mathrm{i}tH}\, Q\, \bigl(\tfrac{\mathrm{d}}{\mathrm{d}t} \mathrm{e}^{-\mathrm{i}tH} \bigr) \\
&\overset{[1]}{=} +\mathrm{i}H\, \mathrm{e}^{+\mathrm{i}tH}\, Q\, \mathrm{e}^{-\mathrm{i}tH} + \mathrm{e}^{+\mathrm{i}tH}\, Q\, \bigl(-\mathrm{i}H \mathrm{e}^{-\mathrm{i}tH} \bigr) \\
&\overset{[1]}{=} \mathrm{i}\, \bigl[H, Q(t) \bigr]
\end{aligned}$$

(ii) $(A\,B)^* \overset{[1]}{=} B^*\, A^*$ and $\bigl(\mathrm{e}^{-\mathrm{i}tH}\bigr)^* \overset{[1]}{=} \mathrm{e}^{+\mathrm{i}tH}$ implies immediately

$$\begin{aligned}
\bigl(Q(t)\bigr)^* &\overset{[1]}{=} \Bigl(\mathrm{e}^{+\mathrm{i}tH}\, Q\, \mathrm{e}^{-\mathrm{i}tH} \Bigr)^* \overset{[1]}{=} \bigl(\mathrm{e}^{-\mathrm{i}tH} \bigr)^*\, Q^*\, \bigl(\mathrm{e}^{+\mathrm{i}tH} \bigr)^* \\
&\overset{[1]}{=} \mathrm{e}^{+\mathrm{i}tH}\, Q\, \mathrm{e}^{-\mathrm{i}tH} \overset{[1]}{=} Q(t).
\end{aligned}$$

(iii) Since $V \in L^{\infty}(\mathbb{R})$, both, $V(\hat{x})$ and $V(Q)$ define bounded operators by Problem 27 [1] and Lemma 6.1.7 [1], respectively. We have to show $\bigl(V(Q)\psi\bigr)(x) = V(x)\, \psi(x)$ [1]: the projection-valued measure

$$1_{\Lambda}(Q) = 1_{\Lambda}(\hat{x})$$

is simply the multiplication operator associated to the characteristic function 1_{Λ} [1]. Consequently, the two operators agree,

$$\begin{aligned}
\bigl(V(Q)\psi\bigr)(x) &\overset{[1]}{=} \int_{\mathbb{R}} \bigl(1_{\mathrm{d}\lambda}(\hat{x})\psi \bigr)(x)\, V(\lambda) \\
&\overset{[1]}{=} \int_{\mathbb{R}} \mathrm{d}\lambda\, \delta(\lambda - x)\, \psi(x)\, V(\lambda) \\
&\overset{[1]}{=} V(x)\, \psi(x) \overset{[1]}{=} \bigl(V(\hat{x})\psi \bigr)(x).
\end{aligned}$$

(iv) Once we show

$$1_\Lambda\big(Q(t)\big) = \mathrm{e}^{+\mathrm{i}tH}\, 1_\Lambda(Q)\, \mathrm{e}^{-\mathrm{i}tH}, \tag{1}$$

we immediately deduce

$$\begin{aligned}
\big(V(Q)\big)(t) &\overset{[1]}{=} \mathrm{e}^{+\mathrm{i}tH} \left(\int_{\mathbb{R}} 1_{\mathrm{d}\lambda}(Q)\, V(\lambda)\right) \mathrm{e}^{-\mathrm{i}tH} \\
&\overset{[1]}{=} \int_{\mathbb{R}} \mathrm{e}^{+\mathrm{i}tH}\, 1_{\mathrm{d}\lambda}(Q)\, \mathrm{e}^{-\mathrm{i}tH}\, V(\lambda) \\
&\overset{[1]}{=} \int_{\mathbb{R}} 1_{\mathrm{d}\lambda}\big(Q(t)\big)\, V(\lambda) \\
&\overset{[1]}{=} V\big(Q(t)\big).
\end{aligned}$$

The only thing left to show is equation (1), and this is done akin to showing covariance in Problem 32: using the "covariance" of the resolvent

$$\big(Q(t) - z\big)^{-1} \overset{[1]}{=} \mathrm{e}^{+\mathrm{i}tH}\, (Q - z)^{-1}\, \mathrm{e}^{-\mathrm{i}tH},$$

we obtain with the help of the Herglotz representation theorem a connection between the measure for $Q(t)$ and vector ψ, and Q for the vector $\mathrm{e}^{-\mathrm{i}tH}\psi$ [1],

$$\begin{aligned}
\big\langle \psi, \big(Q(t) - z\big)^{-1}\psi \big\rangle &\overset{[1]}{=} \int_{\mathbb{R}} \mathrm{d}\mu_\psi^{Q(t)}(\lambda)\, (\lambda - z)^{-1} \\
&\overset{[1]}{=} \Big\langle \mathrm{e}^{-\mathrm{i}tH}\psi, (Q - z)^{-1}\, \mathrm{e}^{-\mathrm{i}tH}\psi \Big\rangle \\
&\overset{[1]}{=} \int_{\mathbb{R}} \mathrm{d}\mu^Q_{\mathrm{e}^{-\mathrm{i}tH}\psi}(\lambda)\, (\lambda - z)^{-1}.
\end{aligned}$$

Consequently, also the projection-valued measure satisfies the same covariance relation, because

$$\begin{aligned}
\big\langle \psi, 1_\Lambda\big(Q(t)\big)\psi \big\rangle &\overset{[1]}{=} \int_\Lambda \mathrm{d}\mu_\psi^{Q(t)}(\lambda) \overset{[1]}{=} \int_\Lambda \mathrm{d}\mu^Q_{\mathrm{e}^{-\mathrm{i}tH}\psi}(\lambda) \\
&\overset{[1]}{=} \Big\langle \psi, \mathrm{e}^{+\mathrm{i}tH}\, 1_\Lambda(Q)\, \mathrm{e}^{-\mathrm{i}tH}\psi \Big\rangle.
\end{aligned}$$

This proves equation (1), and thus also $\big(V(Q)\big)(t) = V\big(Q(t)\big)$ [1].