Homework Problems

26. Boundedness of the spectrum of an operator (6 points)

Let $T \in \mathcal{B}(\mathcal{X})$ where $\mathcal{X}$ is a Banach space. Show that

$$\sigma(T) \subseteq \big\{ z \in \mathbb{C} \mid |z| \leq \|T\| \big\}.$$

Hint: Look at the *resolvent* set.

Solution:

Pick a $z \in \mathbb{C}$ with $|z| > \|T\|$. Consequently, $\big\| T/z \big\| < 1$ [1] and we can write $(T - z)^{-1}$ in terms of the Neumann series (cf. Problem 18 (iii)) [1]

$$\big(\mathrm{id} - T/z\big)^{-1} \overset{[1]}{=} \sum_{n=0}^{\infty} \frac{T^n}{z^n},$$

and thus, $T - z = -z \left(\mathrm{id} - T/z\right)$ means we can write the resolvent as

$$(T - z)^{-1} \overset{[1]}{=} -z^{-1} \left(\mathrm{id} - T/z\right)^{-1} \overset{[1]}{=} - \sum_{n=0}^{\infty} \frac{T^n}{z^{n+1}}.$$

Hence, $|z| > \|T\|$ implies $z \in \rho(T)$ [1].

27. Boundedness of multiplication operators (12 points)

Let $V(\hat{x})$ be the multiplication operator on $L^2(\mathbb{R}^d)$ associated to the function V. Show that $V(\hat{x})$ is bounded if and only if $V \in L^\infty(\mathbb{R}^d)$.

Solution:

"$\Leftarrow$:" Assume $V \in L^\infty(\mathbb{R}^d)$. Then the boundendess follows from the estimate

$$\big\lVert V(\hat{x})\varphi \big\rVert^2 \overset{[1]}{=} \int_{\mathbb{R}^d} \mathrm{d}x \, \lvert V(x) \rvert^2 \, \lvert \varphi(x) \rvert^2 \overset{[1]}{\leq} \lVert V \rVert_{L^\infty}^2 \int_{\mathbb{R}^d} \mathrm{d}x \, \lvert \varphi(x) \rvert^2 \overset{[1]}{=} \lVert V \rVert_{L^\infty}^2 \, \lVert \varphi \rVert^2 .$$

"$\Rightarrow$:" Now assume the multiplication operator $V(\hat{x}) \in \mathcal{B}\big(L^2(\mathbb{R}^d)\big)$ is bounded, but suppose the associated function is not essentially bounded, $V \not\in L^\infty(\mathbb{R}^d)$ [1]. Then for any $\varepsilon > 0$ the Lebesgue measure of the set

$$M_\varepsilon := \big\{ x \in \mathbb{R}^d \;\vert\; \lvert V(x) \rvert > \lVert V(\hat{x}) \rVert + \varepsilon \big\}$$

is positive, $\mathcal{L}(M_\varepsilon) > 0$ [2]. Then pick a subset $\Lambda \subseteq M_\varepsilon$ of finite and positive Lebesgue measure (the Lebesgue measure of M_ε could be infinite) and consider the function $\varphi(x) = 1_\Lambda(x)$ [1]. Since $0 < \lVert \varphi \rVert = \mathrm{vol}(\Lambda) < +\infty$, the vector $\varphi \neq 0 \in L^2(\mathbb{R}^d)$ is not the 0 vector [1]. On the other hand, the lower bound

$$\big\lVert V(\hat{x})\varphi \big\rVert^2 = \int_{\mathbb{R}^d} \mathrm{d}x \, \lvert V(x) \rvert^2 \, \lvert \varphi(x) \rvert^2 \overset{[1]}{\geq} \big(\lVert V(\hat{x}) \rVert + \varepsilon \big)^2 \, \lVert \varphi \rVert^2$$

contradicts that $\lvert V \rvert$ can take values which are larger than $\lVert V(\hat{x}) \rVert$ on a set of positive measure [1], because evidently $\big\lVert V(\hat{x})\varphi \big\rVert \leq \lVert V(\hat{x}) \rVert \, \lVert \varphi \rVert$ [1]. That means $V \in L^\infty(\mathbb{R}^d)$ [1]. In fact, we have just shown that $\lVert V(\hat{x}) \rVert = \lVert V \rVert_{L^\infty}$.

28. Selfadjointness of Schrödinger operators (9 points)

Let $H = -\Delta_x + V$ be the Schrödinger operator on $L^2(\mathbb{R}^d)$ with potential $V \in L^\infty(\mathbb{R}^d, \mathbb{R})$ equipped with domain $\mathcal{D}(H) = H^2(\mathbb{R}^d)$. Show that H is selfadjoint.

Solution:

First of all $V \in L^\infty(\mathbb{R}^d)$ defines a bounded multiplication operator [1],

$$\left\| V(\hat{x})\varphi \right\|_{L^2} \leq \| V \|_{L^\infty} \, \| \varphi \|_{L^2} \overset{[2]}{=} 0 \cdot \| -\Delta_x \varphi \|_{L^2} + \| V \|_{L^\infty} \, \| \varphi \|_{L^2}, \tag{1}$$

and seeing as V is real-valued, V is also symmetric (even selfadjoint) on $\mathcal{D}(V) = L^2(\mathbb{R}^d)$ [1]. Clearly, we have the inclusion $\mathcal{D}(-\Delta_x) = H^2(\mathbb{R}^d) \subset \mathcal{D}(V) = L^2(\mathbb{R}^d)$ [1]. Moreover, (1) also implies V is *infinitesimally* $-\Delta_x$-bounded [1], because we can even choose $a = 0$ (and $b = \| V \|_{L^\infty}$) [1]. That means Kato-Rellich applies [1], and $H = -\Delta_x + V$ equipped with domain $\mathcal{D}(H) = H^2(\mathbb{R}^d)$ defines a selfadjoint operator [1].

29. A quantum two-body system (37 points)

Consider two identical quantum particles of mass m which are interacting with one another via Coulomb repulsion. Then the Schrödinger operator which describes the two is an extension of

$$H_0 = \frac{1}{2m}\bigl(-\mathrm{i}\nabla_{x_1}\bigr)^2 + \frac{1}{2m}\bigl(-\mathrm{i}\nabla_{x_2}\bigr)^2 + \frac{e^2}{|x_1 - x_2|}$$

endowed with domain $\mathcal{D}(H_0) = \mathcal{C}^\infty_{\mathrm{c}}(\mathbb{R}^6) \subset L^2(\mathbb{R}^6)$. Here, $x_1, x_2 \in \mathbb{R}^3$ are the positions of particles 1 and 2, respectively. We will denote the selfadjoint extension of H_0 with H (establishing the existence of H will be done in part (ii) below).

(i) Write H_0 in terms of center-of-mass coordinate $x_c = \frac{1}{2}(x_1 + x_2)$ and relative coordinate $r = x_1 - x_2$.

(ii) Show that H_0 is essentially selfadjoint. What is the domain of the selfadjoint extension H?

(iii) Does the selfadjoint extension H have eigenvalues below 0? Justify your answer.

(iv) What do low-energy states look like?

Define the fermionic subspace as

$$\mathcal{H}_{\mathrm{f}} := \Bigl\{\varphi \in L^2(\mathbb{R}^6) \;\bigm|\; \varphi(x_2, x_1) = -\varphi(x_1, x_2) \text{ almost everywhere}\Bigr\},$$

and denote the restriction of H to $\mathcal{D}(H) \cap \mathcal{H}_{\mathrm{f}}$ with H_{f}.

(v) Show that H_{f} maps $\mathcal{D}(H) \cap \mathcal{H}_{\mathrm{f}}$ to $\mathcal{H}_{\mathrm{f}}$. How do you interpret this fact physically?

(vi) Explain in what sense H_{f} defines a selfadjoint operator.

(vii) Show that $\inf \sigma(H) \leq \inf \sigma(H_{\mathrm{f}})$. How do you interpret this fact physically?

Solution:

(i) Evidently, the potential written in center-of-mass coordinates is $e^2/|r|$ [1], so now we only need to rewrite the kinetic energy. The x_1- and x_2-derivatives of a function of $x_c = \frac{1}{2}(x_1 + x_2)$ and $r = x_1 - x_2$,

$$\begin{aligned}
\nabla_{x_1}\psi(x_c, r) &\overset{[1]}{=} \nabla_{x_c}\psi(x_c, r) \cdot \nabla_{x_1}\bigl(\tfrac{1}{2}(x_1 + x_2)\bigr) + \nabla_r\psi(x_c, r) \cdot \nabla_{x_1}(x_1 - x_2) \\
&\overset{[1]}{=} \bigl(\tfrac{1}{2}\nabla_{x_c} + \nabla_r\bigr)\psi(x_c, r), \\
\nabla_{x_2}\psi(x_c, r) &\overset{[1]}{=} \nabla_{x_c}\psi(x_c, r) \cdot \nabla_{x_2}\bigl(\tfrac{1}{2}(x_1 + x_2)\bigr) + \nabla_r\psi(x_c, r) \cdot \nabla_{x_2}(x_1 - x_2) \\
&\overset{[1]}{=} \bigl(\tfrac{1}{2}\nabla_{x_c} - \nabla_r\bigr)\psi(x_c, r),
\end{aligned}$$

then lead to expressions for the kinetic energy:

$$\begin{aligned}
-\Delta_{x_1} - \Delta_{x_2} &= -\nabla_{x_1}^2 - \nabla_{x_2}^2 \overset{[1]}{=} \bigl(\tfrac{1}{2}\nabla_{x_c} + \nabla_r\bigr)^2 - \bigl(\tfrac{1}{2}\nabla_{x_c} - \nabla_r\bigr)^2 \\
&\overset{[1]}{=} -\tfrac{1}{2}\Delta_{x_c} - 2\Delta_r
\end{aligned}$$

Note that the cross terms have cancelled. Hence, if we rewrite H_0 in center-of-mass coordinates, we obtain

$$H_0 \overset{[1]}{=} -\frac{1}{4m}\Delta_{x_c} - \frac{1}{m}\Delta_r + \frac{e^2}{|r|}.$$

(ii) The Hilbert space $L^2(\mathbb{R}^6) \cong L^2(\mathbb{R}^3_{x_c}) \otimes L^2(\mathbb{R}^3_r)$ decomposes as the direct sum of a center-of-mass contribution and a relative coordinate contribution.

$$H_0 \overset{[1]}{=} H_{\mathrm{c}} \otimes \mathrm{id} + \mathrm{id} \otimes H_{\mathrm{rel}}$$

where $H_{\mathrm{c}} = -\frac{1}{4m}\Delta_{x_c}$ [1] and $H_{\mathrm{rel}} = -\frac{1}{m}\Delta_r + \frac{e^2}{|r|}$ [1] are both endowed with the domains $\mathcal{C}^\infty_{\mathrm{c}}(\mathbb{R}^3)$ [1]. That is because if a function $\varphi \in L^2(\mathbb{R}^3_{x_1} \times \mathbb{R}^3_{x_2})$ is smooth and compact support, then the reparametrization in terms of x_c and r,

$$\psi(x_c, r) = \varphi\big(x_c + \tfrac{r}{2}, x_c - \tfrac{r}{2}\big),$$

is also smooth and has compact support. Now, H_0 is essentially selfadjoint if and only if H_{c} and H_{rel} are [1]: the essential selfadjointness of H_{c} and $-\frac{1}{m}\Delta_r$ (with domain $\mathcal{C}^\infty_{\mathrm{c}}(\mathbb{R}^3)$) is immediate (cf. the discussion on pp. 75–76 of the lecture notes) [2], and in both cases the domain of selfadjointness is $H^2(\mathbb{R}^3)$. (Alternatively, one may check by hand that the deficiency indices of $-\Delta_x$ with domain $\mathcal{C}^\infty_{\mathrm{c}}(\mathbb{R}^3)$ are 0 since none of the non-trivial solutions to $-\Delta_x \varphi_\pm = \mp \mathrm{i} \varphi_\pm$ are in $L^2(\mathbb{R}^3)$.)

Now given that the repulsive Coulomb potential satisfies the conditions of Theorem 5.2.25 (the sign of the potential does not enter, so the proof is a trivial modification of that of Corollary 5.2.27) [1], H_{rel} has a selfadjoint extension with domain $H^2(\mathbb{R}^3)$ [1]. Hence, H_0 is essentially selfadjoint [1], and the domain of its unique selfadjoint extension is $H^2(\mathbb{R}^6)$ [1].

(iii) We will use the min-max principle: let us consider the free two-particle hamiltonian $H_{\mathrm{free}} = -\frac{1}{2m}\Delta_{x_1} - \frac{1}{2m}\Delta_{x_2}$ endowed with domain $H^2(\mathbb{R}^6)$ [1]. Then $e^2/|r| > 0$ and the fact that the domains of H and H_{free} coincide imply

$$H = -\frac{1}{2m}\Delta_{x_1} - \frac{1}{2m}\Delta_{x_2} + \frac{e^2}{|r|} \overset{[1]}{\geq} -\frac{1}{2m}\Delta_{x_1} - \frac{1}{2m}\Delta_{x_2} = H_{\mathrm{free}}.$$

Consequently, $E_n(H) \geq E_n(H_{\mathrm{free}}) = 0$ holds for all $n \in \mathbb{N}_0$ (the spectrum of H_{free} is $[0, +\infty)$, and the bottom is purely essential) [1], and thus, there can be no eigenvalues below 0. One may also see that on physical grounds: the potential is purely repulsive.

(iv) Low energy states can be best visualized in center-of-mass coordinates: the two particles are very delocalized but situated far apart. Visually, that means the probability density has two small, broad humps which are far away from one another. Hence, such a low energy state can be written as a product

$$\psi(x_c, r) \overset{[1]}{=} \phi(x_c)\, \eta(r)$$

where $\phi(x_c)$ is broad and flat (meaning $-\Delta_{x_c}\phi \approx 0$) [1] and $\eta(r) \approx 0$ for $|r|$ small [1].

(v) Let us introduce the operator $(P\psi)(x_1, x_2) := \psi(x_2, x_1)$ [1]. Clearly, P is idempotent ($P^2 = \mathrm{id}$). A quick computation yields $\Delta_{x_1} P = P\,\Delta_{x_2}$ [1], and we deduce that P commutes with H, i. e. $[H, P] = 0$ [1]. Elements of $\mathcal{H}_{\mathrm{f}}$ are those for which $P\psi = -\psi$ [1], and if we use the fact that P commutes with H, we see that H maps elements of $\mathcal{H}_{\mathrm{f}}$ onto $\mathcal{H}_{\mathrm{f}}$,

$$-H\psi = H\,P\psi = P\,H\psi. \qquad [1]$$

Consequently, $H_{\mathrm{f}} := H|_{\mathcal{H}_{\mathrm{f}}}$ defines a map $\mathcal{D}(H) \cap \mathcal{H}_{\mathrm{f}} \longrightarrow \mathcal{H}_{\mathrm{f}}$ [1].

(vi) First of all, $\mathcal{H}_{\mathrm{f}}$ is a Hilbert space, because limits of antisymmetric L^2-functions are again antisymmetric, and the Hilbert space $L^2(\mathbb{R}^6) \cong \mathcal{H}_{\mathrm{f}} \oplus \mathcal{H}_{\mathrm{f}}^\perp$ [1] (the second term consists of L^2-functions with $\varphi(x_1, x_2) = +\varphi(x_2, x_1)$).

Secondly, the above arguments show that $H = H_{\mathrm{f}} \oplus H_{\mathrm{b}}$ [1] where H_{b} is the restriction of H to the bosonic subspace $\mathcal{H}_{\mathrm{f}}^\perp$. Now $H^* = H$ implies that $H_{\mathrm{f}} = H_{\mathrm{f}}^*$ and $H_{\mathrm{b}} = H_{\mathrm{b}}^*$ are also selfadjoint [1].

(vii) The operator prescription of H and H_f are identical, the only difference are the domains – and H_f is a *restriction* of H. Thus, the inequality is an immediate consequence of the Rayleigh-Ritz principle [1] and the fact that the second infimum is taken over a strictly smaller set,

$$\inf \sigma(H) \overset{[1]}{=} \inf_{\substack{\psi \in \mathcal{D}(H) \\ \|\psi\|=1}} \langle \psi, H\psi \rangle \overset{[1]}{\leq} \inf_{\substack{\psi \in \mathcal{D}(H) \cap \mathcal{H}_\mathrm{f} \\ \|\psi\|=1}} \langle \psi, H\psi \rangle \overset{[1]}{=} \sigma(H_\mathrm{f}).$$