Introduction to Mathematical Quantum Theory

Solution to the Exercises

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Exercise 1

Let $\mathcal{H}$ be an Hilbert space. Let A and B linear operators on $\mathcal{H}$ such that there exists $\alpha \in \mathbb{C} \setminus \{0\}$ such that

$$[A, B] = \alpha \,\mathrm{id}\,. \tag{1}$$

Prove that A and B cannot be both bounded.

Hint: Assume both bounded; consider $\|[A, B^n]\|$ and find an absurd.

Proof. Assume that both A and B are bounded operators. Consider for any $n \in \mathbb{N}$ the commutator between A and B^n. We have

$$[A, B^n] = \left[A, BB^{n-1}\right] = [A, B]\, B^{n-1} + B\left[A, B^{n-1}\right] = \alpha B^{n-1} + B\left[A, B^{n-1}\right].$$

We can then prove by induction that $[A, B^n] = n\alpha B^{n-1}$; indeed if $n = 1$ the statement is trivially true, and if we assume the statement to be true for $n - 1$ we get

$$[A, B^n] = \alpha B^{n-1} + B\left[A, B^{n-1}\right] = \alpha B^{n-1} + B\left((n-1)\,\alpha B^{n-2}\right) = n\alpha B^{n-1}.$$

Consider now the norm of the commutator; we get

$$\begin{aligned} \|[A, B^n]\| &= \|AB^n - B^n A\| \leqslant 2\,\|A\|\,\|B^n\| \\ &\leqslant \|A\|\,\|B\|^n\,. \end{aligned}$$

Given that $[A, B] \neq 0$ we can deduce that $\|A\| \neq 0$. We then get that

$$\|B^n\| \geqslant \frac{\alpha}{2\,\|A\|} n \left\|B^{n-1}\right\| \geqslant \ldots \geqslant \left(\frac{\alpha}{2\,\|A\|}\right)^{n-1} n!\,\|B\| > 0$$

and from this we deduce that for any $n \in \mathbb{N}$ we have $B^n \neq 0$. We then get

$$n\,|\alpha|\left\|B^{n-1}\right\| \leqslant 2\,\|A\|\,\|B^n\| \leqslant 2\,\|A\|\,\|B\|\left\|B^{n-1}\right\| \quad \Longrightarrow \quad n\,|\alpha| \leqslant \|A\|\,\|B\|\,.$$

Given that the last inequality holds for any n this gives us a contradiction.

□

Exercise 2

a Prove that for any $\alpha \in \mathbb{C}$ such that $\mathrm{Re}(\alpha) > 0$,

$$\left(\int_{\mathbb{R}} e^{-\frac{x^2}{2\alpha}} dx\right)^2 = \int_{\mathbb{R}^2} e^{-\frac{x^2+y^2}{2\alpha}} dx dy \tag{2}$$

$$= 2\pi\alpha, \tag{3}$$

where the integral over $\mathbb{R}^2$ can be evaluated using polar coordinates. Deduce that

$$\int_{\mathbb{R}} e^{-\frac{x^2}{2\alpha}} dx = \sqrt{2\pi\alpha}, \tag{4}$$

where the square root is the one with positive real part.

b For all $B \geqslant A > 0$ and $\alpha \in \mathbb{C}\setminus\{0\}$ we have

$$\int_A^B e^{-\frac{x^2}{2\alpha}} dx = -\frac{\alpha}{x} e^{-\frac{x^2}{2\alpha}}\Big|_A^B - \int_A^B \frac{\alpha}{x^2} e^{-\frac{x^2}{2\alpha}} dx. \tag{5}$$

Using this, prove that the integral in (4) is convergent for all nonzero α with $\mathrm{Re}(\alpha) \geqslant 0$, provided the integral is interpreted as a principle value when not absolutely convergent, where the principal value is defined as

$$\mathrm{PV} \int_{\mathbb{R}} f(x)\, dx := \lim_{R\to\infty} \int_{-R}^{R} f(x)\, dx. \tag{6}$$

c Prove that the result of **a** is also valid for nonzero values of α with $\mathrm{Re}(\alpha) = 0$, at least in the principal value.

Hint: Given $\eta \neq 0$, show that the principal value from A to $+\infty$ of $\exp\left[-\frac{x^2}{2(\gamma+i\eta)}\right]$ *is small for large A, uniformly in $\gamma \in [0,1]$.*

d Prove that

$$\frac{1}{2\pi} \mathrm{PV} \int_{\mathbb{R}} e^{ikx} e^{-i\frac{\hbar t}{2m}k^2} dk = \sqrt{\frac{m}{2\pi i\hbar t}} e^{i\frac{m}{2\hbar t}x^2}, \tag{7}$$

where the square root is the one with real positive part.

Proof. We start by proving point **a**. Using polar coordinates we get

$$\left(\int_{\mathbb{R}} e^{-\frac{x^2}{2\alpha}} dx\right)^2 = \int_{\mathbb{R}^2} e^{-\frac{x^2+y^2}{2\alpha}} dx dy = 2\pi \int_0^{+\infty} e^{-\frac{\rho^2}{2\alpha}} \rho d\rho = -2\pi\alpha e^{-\frac{\rho^2}{2\alpha}}\Big|_0^{+\infty} = 2\pi\alpha.$$

To recover the integral we want is enough to apply the square root, and given that for real values of α the integral we get is positive, we choose the positive determination of the square root to get

$$\int_{\mathbb{R}} e^{-\frac{x^2}{2\alpha}} dx = \sqrt{2\pi\alpha}.$$

To prove **b** we first use (5) to estimate the principal value. Fix $A > 0$; then we get

$$\begin{aligned}
\mathrm{PV}\int_{\mathbb{R}} e^{-\frac{x^2}{2\alpha}}\,dx &= \lim_{R\to+\infty}\int_{-R}^{R} e^{-\frac{x^2}{2\alpha}}\,dx = \int_{-A}^{A} e^{-\frac{x^2}{2\alpha}}\,dx + 2\lim_{R\to+\infty}\int_{A}^{R} e^{-\frac{x^2}{2\alpha}}\,dx \\
&= \int_{-A}^{A} e^{-\frac{x^2}{2\alpha}}\,dx + 2\lim_{R\to+\infty}\left[-\frac{\alpha}{x}e^{-\frac{x^2}{2\alpha}}\Big|_{A}^{R} - \int_{A}^{R}\frac{\alpha}{x^2}e^{-\frac{x^2}{2\alpha}}\,dx\right] \\
&= \int_{-A}^{A} e^{-\frac{x^2}{2\alpha}}\,dx + 2\lim_{R\to+\infty}\left[-\frac{\alpha}{R}e^{-\frac{R^2}{2\alpha}} + \frac{\alpha}{A}e^{-\frac{A^2}{2\alpha}} - \int_{A}^{R}\frac{\alpha}{x^2}e^{-\frac{x^2}{2\alpha}}\,dx\right].
\end{aligned}$$

Now using that $\mathrm{Re}\,(\alpha) \geqslant 0$ we have that

$$\left|e^{-\frac{R^2}{2\alpha}}\right| \leqslant e^{-\mathrm{Re}\left(\frac{R^2}{2\alpha}\right)} \leqslant 1, \qquad \left|\frac{1}{x^2}e^{-\frac{R^2}{2\alpha}}\right| \in L^1\,(A,+\infty)$$

and applying this to the limit we get that

$$\mathrm{PV}\int_{\mathbb{R}} e^{-\frac{x^2}{2\alpha}}\,dx = \int_{-A}^{A} e^{-\frac{x^2}{2\alpha}}\,dx + \frac{2\alpha}{A}e^{-\frac{A^2}{2\alpha}} - \int_{A}^{+\infty}\frac{2\alpha}{x^2}e^{-\frac{x^2}{2\alpha}}\,dx,$$

and therefore the integral is convergent for any α with $\mathrm{Re}\,(\alpha) \geqslant 0$.

To prove **c** is enough to consider $\alpha = i\eta$ with $\eta \in \mathbb{R}\setminus\{0\}$. In this case we get

$$\begin{aligned}
\mathrm{PV}\int_{\mathbb{R}} e^{i\frac{x^2}{2\eta}}\,dx &= \lim_{R\to+\infty}\int_{-R}^{R} e^{i\frac{x^2}{2\eta}}\,dx = \lim_{R\to+\infty}\int_{-R}^{R}\lim_{\gamma\to0^+} e^{-\frac{x^2}{2(\gamma+i\eta)}}\,dx \\
&= \lim_{R\to+\infty}\lim_{\gamma\to0^+}\int_{-R}^{R} e^{-\frac{x^2}{2(\gamma+i\eta)}}\,dx,
\end{aligned}$$

where in the last equality we could bring the limit outside of the integral because the integrand is uniformly bounded in modulus by 1 which is integrable in $[-R,R]$. From the formula above and from the fact that now $\mathrm{Re}\,(\gamma+i\eta) > 0$ we now have that

$$\int_{-R}^{R} e^{-\frac{x^2}{2(\gamma+i\eta)}}\,dx = \sqrt{2\pi\,(\gamma+i\eta)} - 2\int_{R}^{+\infty} e^{-\frac{x^2}{2(\gamma+i\eta)}}\,dx.$$

Moreover we can assume that $\gamma \in [0,1]$ and use **b** to get that

$$\begin{aligned}
\left|\int_{R}^{+\infty} e^{-\frac{x^2}{2(\gamma+i\eta)}}\,dx\right| &= \lim_{L\to+\infty}\left|\int_{R}^{L} e^{-\frac{x^2}{2(\gamma+i\eta)}}\,dx\right| \\
&= \lim_{L\to+\infty}\left|-\frac{\gamma+i\eta}{L}e^{-\frac{L^2}{2(\gamma+i\eta)}} + \frac{\gamma+i\eta}{R}e^{-\frac{R^2}{2(\gamma+i\eta)}} - \int_{R}^{L}\frac{\gamma+i\eta}{x^2}e^{-\frac{x^2}{2(\gamma+i\eta)}}\,dx\right| \\
&= \left|\frac{\gamma+i\eta}{R}e^{-\frac{R^2}{2(\gamma+i\eta)}} - \int_{R}^{+\infty}\frac{\gamma+i\eta}{x^2}e^{-\frac{x^2}{2(\gamma+i\eta)}}\,dx\right| \\
&\leqslant \frac{4}{R}\,|\gamma+i\eta|\,e^{-\frac{R^2}{2}\mathrm{Re}\left(\frac{1}{\gamma+i\eta}\right)} \leqslant \frac{4\sqrt{1+\eta^2}}{R},
\end{aligned}$$

and therefore, passing to the limit we get

$$\left|\lim_{R\to+\infty}\lim_{\gamma\to0^+}\int_{R}^{+\infty} e^{-\frac{x^2}{2(\gamma+i\eta)}}\,dx\right| \leqslant \lim_{R\to+\infty}\lim_{\gamma\to0^+}\frac{4\sqrt{1+\eta^2}}{R} = 0.$$

As a consequence we get that

$$\text{PV} \int_{\mathbb{R}} e^{i\frac{x^2}{2\eta}} dx = \lim_{R\to+\infty} \lim_{\gamma\to 0^+} \sqrt{2\pi(\gamma + i\eta)} = \sqrt{2\pi i\eta},$$

which concludes the proof of **c**.

To prove **d** we first notice that

$$\frac{\hbar t}{2m}k^2 - kx = \frac{\hbar t}{2m}\left(k - \frac{mx}{\hbar t}\right)^2 - \frac{mx^2}{2\hbar t}.$$

Using **c** we then get

$$\begin{aligned}\frac{1}{2\pi}\text{PV}\int_{\mathbb{R}} e^{ikx} e^{-i\frac{\hbar t}{2m}k^2} dk &= \frac{e^{i\frac{m}{2\hbar t}x^2}}{2\pi}\text{PV}\int_{\mathbb{R}} e^{-i\frac{\hbar t}{2m}k^2} dk \\ &= \sqrt{\frac{m}{2\pi i\hbar t}} e^{i\frac{m}{2\hbar t}x^2},\end{aligned}$$

which concludes our proof.

□

Exercise 3

Consider a separable Hilbert space $\mathcal{H}$ and a complete orthonormal system for it $\{\varphi_n\}_{n\in\mathbb{N}}$. Assume that φ_∞ cannot be written as a finite linear combination of elements of $\{\varphi_n\}_{n\in\mathbb{N}}$. Let D denote the dense linear subspace of $\mathcal{H}$ consisting of all finite linear combinations of elements of $\{\varphi_n\}_{n\in\mathbb{N}}$ and of φ_∞. On D define the operator $T : D \to \mathcal{H}$ defined as

$$T\left(\alpha_\infty\varphi_\infty + \sum_{n\in\mathbb{N}} \alpha_n\varphi_n\right) := \alpha_\infty\varphi_\infty. \tag{8}$$

Prove that T is not bounded.

Hint: Use the closed graph theorem.

Proof. Suppose that T is bounded. Given that D is dense in $\mathcal{H}$, we can define $\widetilde{T}$ an extension of T to $\mathcal{H}$. Consider now the graph of $\widetilde{T}$; given that $\{\varphi_n\}_{n\in\mathbb{N}}$ is a complete orthonormal system there exists a sequence $\{\beta_n\}_{n\in\mathbb{N}}$ such that

$$\lim_{N\to+\infty} \sum_{n=0}^{N} \beta_n\varphi_n = \varphi_\infty.$$

Recall the definition of $G\left(\widetilde{T}\right) := \left\{\left(\psi, \widetilde{T}\psi\right) \mid \psi \in \mathcal{H}\right\} \subseteq \mathcal{H} \times \mathcal{H}$. Given that we have that

$$T\left(\sum_{n=0}^{N} \beta_n\varphi_n\right) = 0,$$

we get that $\left(\sum_{n=0}^{N}\beta_n\varphi_n, 0\right) \in G\left(\widetilde{T}\right)$, and as a consequence $(\varphi_\infty, 0) \in \overline{G\left(\widetilde{T}\right)}$. On the other hand, by definition of T we get that $T\varphi_\infty = \varphi_\infty$, and therefore that $(\varphi_\infty, 0) \notin G\left(\widetilde{T}\right)$. For this reason we get that $G\left(\widetilde{T}\right) \neq \overline{G\left(\widetilde{T}\right)}$. On the other hand $\widetilde{T}$ is trivially linear on $\mathcal{H}$, so we can apply the closed graph theorem to imply that T cannot be bounded.

□

Exercise 4

Recall the definition of $H^2(\mathbb{R})$ as

$$H^2(\mathbb{R}) := \left\{\psi \in L^2(\mathbb{R}) \mid k^2\widehat{\psi} \in L^2(\mathbb{R})\right\}$$

Recall that in class we defined the map that to any initial datum $\psi_0 \in L^2(\mathbb{R})$ would associate $\psi_t := \widetilde{U}_0(t)\psi_0$, defined via the Hamiltonian $H_0 := -\frac{\partial^2}{\partial x^2}$ with domain $\mathcal{D}(H_0) = H^2(\mathbb{R})$. Indeed if $U_0(t)\psi_0$ is defined for any $\psi_0 \in \mathcal{S}(\mathbb{R})$ as the unique solution to

$$\begin{cases} i\hbar\partial_t\left(U_0(t)\psi_0\right) = H_0U_0(t)\psi_0 \\ U_0(t)\psi_0|_{t=0} = \psi_0, \end{cases} \tag{9}$$

then $\widetilde{U}_0(t)$ is defined by density on the whole space $L^2(\mathbb{R})$, and coincides with $U_0(t)$ on $\mathcal{S}(\mathbb{R})$.

Prove that if $\psi_0 \in D(H_0)$ then $\psi_t \in \mathcal{D}(H_0)$.

Proof. We saw in class that $\widetilde{U}_0(t)$ has an explicit form; indeed for any $\psi_0 \in L^2(\mathbb{R})$ we get thet

$$\mathcal{F}\left(\widetilde{U}_0(t)\psi_0\right)(k) = e^{-i\frac{\hbar t}{2m}k^2}\widehat{\psi}_0(x),$$

where $\mathcal{F}$ indicates the Fourier transform operator

Now, if $\psi_0 \in H^2(\mathbb{R})$, we get by definition that $k^2\psi_0 \in L^2(\mathbb{R})$. As a consequence we also get $k^2\mathcal{F}\left(\widetilde{U}_0(t)\psi_0\right) \in L^2(\mathbb{R})$, and therefore $\widetilde{U}_0(t)\psi_0 \in H^2(\mathbb{R})$.

□