Introduction to Mathematical Quantum Theory

Solution to the Exercises

– 05.05.2020 –

Teacher: Prof. Chiara Saffirio

Assistent: Dr. Daniele Dimonte – daniele.dimonte@unibas.ch

Exercise 1

Let $k \in \mathbb{Z}$, $d \in \mathbb{N}$, $k + d \neq 0$. Let D be defined as

$$D := \begin{cases} C_c^\infty\left(\mathbb{R}^d\right) & \text{if } k \geqslant 0, \\ C_c^\infty\left(\mathbb{R}^d \setminus \{\mathbf{0}\}\right) & \text{if } k \leqslant -1,\ k + d \neq 0. \end{cases} \tag{1}$$

Prove that for any $\psi \in D$

$$\int_{\mathbb{R}^d} |\mathbf{x}|^k \left|\psi(\mathbf{x})\right|^2 d\mathbf{x} \leqslant \frac{4}{|k+d|^2} \int_{\mathbb{R}^d} |\mathbf{x}|^{k+2} \left|\nabla\psi(\mathbf{x})\right|^2 d\mathbf{x}. \tag{2}$$

Hint: Use the fact that

$$|\mathbf{x}|^k = \frac{1}{k+d} \sum_{j=1}^{d} \frac{\partial}{\partial x_j}\left(|\mathbf{x}|^k x_j\right) \tag{3}$$

to integrate by part on the left hand side of (2) *and then use the Cauchy-Schwartz inequality.*

Remark: Notice that in particular if $k = -2$ (and $d \neq 2$) this implies that as operators

$$\frac{1}{|\mathbf{x}|^2} \leqslant -\frac{4}{|d-2|}\Delta. \tag{4}$$

A generalisation of this formula is called in the literature the **Hardy inequality**.

Proof. We will use the shorthand notation of div for a divergence of a vector field, meaning that if $\mathbf{F}$ is a vector field on $\mathbb{R}^d$, we define

$$\operatorname{div} \mathbf{F}(\mathbf{x}) := \sum_{j=1}^{d} \frac{\partial}{\partial x_j} F_j(\mathbf{x}).$$

With this notation in mind we have that the Green theorem can be written as

$$\int_{\mathbb{R}^d} \operatorname{div} F(\mathbf{x})\, g(\mathbf{x})\, d\mathbf{x} = -\int_{\mathbb{R}^d} F \cdot \nabla g(\mathbf{x})\, d\mathbf{x},$$

and we can write $|\mathbf{x}|^k = (k+d)^{-1} \operatorname{div}\left(|\mathbf{x}|^k \mathbf{x}\right)$.

Let $\psi \in D$ and consider the left-hand side of (2); we get

$$\begin{aligned}
\int_{\mathbb{R}^d} |\mathbf{x}|^k |\psi(\mathbf{x})|^2 \, d\mathbf{x} &= \frac{1}{k+d} \int_{\mathbb{R}^d} \operatorname{div}\left(|\mathbf{x}|^k x\right) |\psi(\mathbf{x})|^2 \, d\mathbf{x} \\
&= -\frac{1}{k+d} \int_{\mathbb{R}^d} |\mathbf{x}|^k x \cdot \nabla \left(|\psi(\mathbf{x})|^2\right) d\mathbf{x} \\
&= -\frac{2}{k+d} \int_{\mathbb{R}^d} |\mathbf{x}|^k x \cdot \operatorname{Re}\left(\overline{\psi(\mathbf{x})} \nabla \psi(\mathbf{x})\right) d\mathbf{x} \\
&\leqslant \frac{2}{|k+d|} \int_{\mathbb{R}^d} |\mathbf{x}|^{k+1} |\psi(\mathbf{x})| \, |\nabla \psi(\mathbf{x})| \, d\mathbf{x} \\
&\leqslant \frac{2}{|k+d|} \left(\int_{\mathbb{R}^d} |\mathbf{x}|^{2(k+1-\eta)} |\psi(\mathbf{x})|^2 \, d\mathbf{x} \right)^{\frac{1}{2}} \left(\int_{\mathbb{R}^d} |\mathbf{x}|^{2\eta} |\nabla \psi(\mathbf{x})| \, d\mathbf{x} \right)^{\frac{1}{2}}.
\end{aligned}$$

If we choose $\eta = \frac{k+2}{2}$ we get

$$\int_{\mathbb{R}^d} |\mathbf{x}|^k |\psi(\mathbf{x})|^2 \, d\mathbf{x} \leqslant \frac{4}{|k+d|^2} \int_{\mathbb{R}^d} |\mathbf{x}|^{k+2} |\nabla \psi(\mathbf{x})| \, d\mathbf{x}.$$

□

Exercise 2

a Let $\mathcal{H} := L^2(\mathbb{R}^3)$. Define (as in class) the operator H_0 with[1]

$$\mathcal{D}(H_0) := H^2(\mathbb{R}^3) \equiv \left\{ \psi \in \mathcal{H} \middle| \, |\mathbf{k}|^2 \widehat{\psi}(\mathbf{k}) \in L^2(\mathbb{R}^3) \right\}, \tag{5}$$

$$H_0 \psi = -\Delta \psi = \left(|\mathbf{k}|^2 \widehat{\psi}(\mathbf{k}) \right)^{\vee}, \qquad \forall \psi \in \mathcal{D}(H_0). \tag{6}$$

Prove that H_0 is closed.

b Let $\mathcal{D}(H) := \mathcal{D}(H_0)$. Define $H := H_0 + \frac{1}{|\mathbf{x}|}$. Prove that H is well-defined and closed. (Assume, if necessary, to know that there exists a positive constant C such that for any $\psi \in H^2(\mathbb{R}^3)$ it holds $\|\psi\|_{L^\infty} \leqslant C \|\psi\|_{H^2}$).

Hint: Use the fact that $H^2(\mathbb{R}^3) \subseteq L^\infty(\mathbb{R}^3)$ to prove that is well-defined. To prove the closure, use (2) from Exercise 1 to show and subsequently use that $\forall \varepsilon > 0$, $\forall \psi \in \mathcal{D}(H)$

$$\left\| \frac{1}{|\mathbf{x}|} \psi \right\|_{L^2} \leqslant \frac{2}{\varepsilon} \|\psi\|_{L^2} + \varepsilon \|H_0 \psi\|_{L^2} \tag{7}$$

to get that

$$\|H_0 \psi\|_{L^2} \leqslant \frac{2}{\varepsilon(1-\varepsilon)} \|\psi\|_{L^2} + \frac{1}{1-\varepsilon} \|H\psi\|_{L^2}. \tag{8}$$

c Prove that H is symmetric.

[1]Recall that we proved in the exercise session that if $\|\psi\|_{H^2} := \left\| \left(1 + |\mathbf{k}|^2\right) \widehat{\psi} \right\|_{L^2}$, then $H^2(\mathbb{R}^3)$ is closed with respect to $\|\cdot\|_{H^2}$.

d Prove that H is self-adjoint.

Hint: Use the fact that $\frac{1}{|x|}$ *is a self-adjoint operator and apply the Kato-Rellich theorem.*

Proof. Recall that we proved in the exercise session that $H^2\left(\mathbb{R}^3\right)$ is closed with respect to $\|\cdot\|_{H^2}$. To prove **a**, then, consider a sequence $\{\psi_n\}_{n\in\mathbb{N}} \subseteq \mathcal{D}(H_0)$ such that $\psi_n \to \psi$ and $H_0\psi_n \to \phi$ in $\mathcal{H}$. As a consequence we get that $\{\psi_n\}_{n\in\mathbb{N}}$ is a Cauchy sequence with respect to $\|\cdot\|_{H^2}$ and therefore $\psi \in H^2\left(\mathbb{R}^3\right) = \mathcal{D}(H_0)$ and $H_0\psi = \varphi$, and hence H_0 is closed.

To prove **b** we first prove that H is well defined. Given that $\psi \in H^2\left(\mathbb{R}^3\right) \subseteq L^\infty\left(\mathbb{R}^3\right)$, we get that

$$\begin{aligned}\left\|\frac{1}{|\mathbf{x}|}\psi\right\|_{L^2}^2 &= \int_{\mathbb{R}^3} \frac{1}{|\mathbf{x}|^2} |\psi(\mathbf{x})|^2 \, dx \leqslant \|\psi\|_{L^\infty} \int_{B_1(\mathbf{0})} \frac{1}{|\mathbf{x}|^2} d\mathbf{x} + \int_{\mathbb{R}^3 \setminus B_1(\mathbf{0})} |\psi(\mathbf{x})|^2 \, d\mathbf{x} \\ &\leqslant 4\pi \|\psi\|_{L^\infty} + \|\psi\|_{L^2} \leqslant (4\pi C + 1) \|\psi\|_{H^2}.\end{aligned}$$

We then use Hardy inequality and the fact that for any $\eta > 0$ we have $|\mathbf{k}|^2 \leqslant 1/\eta + \eta/4\,|\mathbf{k}|^4$, to obtain for any $\psi \in C_c^\infty\left(\mathbb{R}^3 \setminus \{\mathbf{0}\}\right)$ that

$$\begin{aligned}\left\|\frac{1}{|\mathbf{x}|}\psi\right\|_{L^2}^2 &\leqslant 4\|\nabla\psi\|_{L^2}^2 = 4\int_{\mathbb{R}^3} |\mathbf{k}|^2 \left|\widehat{\psi}(\mathbf{k})\right|^2 d\mathbf{x} \leqslant \frac{4}{\eta}\|\psi\|_{L^2}^2 + \eta\|H_0\psi\|_{L^2}^2 \\ &\leqslant \left(\frac{2}{\sqrt{\eta}}\|\psi\|_{L^2} + \sqrt{\eta}\|H_0\psi\|_{L^2}\right)^2.\end{aligned}$$

Calling $\eta = \varepsilon^2$ we obtain (7). As a consequence we get for any $\psi \in C_c^\infty\left(\mathbb{R}^3 \setminus \{\mathbf{0}\}\right)$

$$\|H_0\psi\|_{L^2} \leqslant \|H\psi\|_{L^2} + \left\|\frac{1}{|\mathbf{x}|}\psi\right\|_{L^2} \leqslant \|H\psi\|_{L^2} + \frac{2}{\varepsilon}\|\psi\|_{L^2} + \varepsilon\|H_0\|_{L^2}.$$

Choosing $\varepsilon < 1$ and collecting the identical terms on the left we obtain (8).

Suppose $\{\psi_n\}_{n\in\mathbb{N}} \subseteq \mathcal{D}(H)$ and that $\psi_n \to \psi$ and $H\psi_n \to \varphi$ in $\mathcal{H}$; then the sequences $\{\psi_n\}_{n\in\mathbb{N}}$ and $\{H\psi_N\}_{n\in\mathbb{N}}$ are Cauchy sequences and using (8) we get that also $\{H_0\psi_n\}_{n\in\mathbb{N}}$ is. From **a** we then get that $\psi \in \mathcal{D}(H_0) = \mathcal{D}(H)$ and that $H_0\psi_n \to H_0\psi$. Moreover we get that

$$\begin{aligned}\lim_{n\to+\infty}\left\|\frac{1}{|\mathbf{x}|}(\psi_n - \psi)\right\|_{L^2} &\leqslant \lim_{n\to+\infty}(4\pi C + 1)\|\psi_n - \psi\|_{H^2} \\ &= \lim_{n\to+\infty}(4\pi C + 1)\sqrt{\|\psi_n - \psi\|_{L^2}^2 + \|H_0(\psi_n - \psi)\|_{L^2}^2} = 0,\end{aligned}$$

and as a consequence $H\psi_n \to H\psi$, so H is closed.

To prove **c**, consider $\psi,\ \varphi \in \mathcal{D}(H) = H^2\left(\mathbb{R}^3\right)$; then we get

$$\langle\psi, H^*\varphi\rangle = \langle H\psi, \varphi\rangle = \langle -\Delta\psi, \varphi\rangle + \langle\frac{1}{|\mathbf{x}|}\psi, \varphi\rangle.$$

We already showed in class that $-\Delta$ is symmetric, so we get that

$$\langle\psi, H^*\varphi\rangle = \langle\psi, -\Delta\varphi\rangle + \langle\psi, \frac{1}{|\mathbf{x}|}\varphi\rangle = \langle\psi, H\varphi\rangle,$$

and therefore H is symmetric.

To prove **d** notice that if we define the operator V as the operator given by

$$\mathcal{D}(V) := \left\{ \psi \in \mathcal{H} \middle| \frac{1}{|x|}\psi(x) \in \mathcal{H} \right\}$$
$$V\psi(x) := \frac{1}{|x|}\psi(x),$$

this is a well defined self-adjoint operator. Indeed it is trivially symmetric, and therefore V^* is an extension of V. Furthermore, let ψ in $\mathcal{D}(V^*)$ and consider $\phi \in \mathcal{S}(\mathbb{R}^3)$ the space of Schwartz functions. In particular $\phi \in \mathcal{D}(V)$, and we get

$$|\langle \psi, V\phi \rangle| \leqslant C_\psi \|\phi\|_{L^2}.$$

As a consequence, using Riesz theorem, there exists an element $\xi \in L^2(\mathbb{R}^3)$ such that $\langle \xi, \phi \rangle = \langle \psi, V\phi \rangle$ for any $\phi \in \mathcal{S}(\mathbb{R}^3)$. This in particular implies that $V\psi = \xi$ almost everywhere, and therefore $V\psi \in L^2(\mathbb{R}^3)$. By the definition of the domain of V we get $\psi \in \mathcal{D}(V)$ and V is self-adjoint.

Now, choosing $\varepsilon < 1$ we can use (7) to first get that $\mathcal{D}(H_0) \subseteq \mathcal{D}(V)$. We are then in the hypothesis of the Kato-Rellich theorem, and we can conclude that $H = H_0 + V$ is self-adjoint.

$\square$

Exercise 3

Let $\mathcal{H}$ an Hilbert space and let $A,\ B \in \mathcal{B}(\mathcal{H})$, $A^* = A$, $B^* = B$

a Suppose[2] $A \geqslant \mathrm{id}$; prove that A is invertible with $A^{-1} \in \mathcal{B}(\mathcal{H})$ and that $0 \leqslant A^{-1} \leqslant \mathrm{id}$.

b Suppose $0 \leqslant A \leqslant B$; prove that for any $\lambda > 0$, $A+\lambda\,\mathrm{id}$ and $B+\lambda\,\mathrm{id}$ are invertible with $(A+\lambda\,\mathrm{id})^{-1}$, $(B+\lambda\,\mathrm{id})^{-1} \in \mathcal{B}(\mathcal{H})$ and that we have $(B+\lambda\,\mathrm{id})^{-1} \leqslant (A+\lambda\,\mathrm{id})^{-1}$.

c Suppose $0 \leqslant A \leqslant B$; prove that $\sqrt{A} \leqslant \sqrt{B}$.

Hint: Prove and use the fact that

$$\sqrt{x} = \frac{1}{\pi}\int_0^{+\infty} \frac{1}{\sqrt{\lambda}}\left(1 - \frac{\lambda}{x+\lambda}\right) d\lambda, \qquad \forall x \geqslant 0. \tag{9}$$

Proof. To prove **a** we first notice that $A \geqslant \mathrm{id}$ implies that $\sigma(A) \subseteq [1, +\infty)$, and therefore $0 \notin \sigma(A)$. By definition of spectrum this implies that $A^{-1} \in \mathcal{B}(\mathcal{H})$. Using functional calculus, if μ is the spectral measure associated to A, for any $\psi \in \mathcal{H}$ we get

$$\langle \psi, A^{-1}\psi \rangle = \langle \psi, \int_{\sigma(A)} \frac{1}{\lambda} d\mu(\lambda)\,\psi \rangle \leqslant \sup_{\lambda \in \sigma(A)} \frac{1}{\lambda} \langle \psi, \int_{\sigma(A)} d\mu(\lambda)\,\psi \rangle \leqslant \|\psi\|^2.$$

[2]Recall that $A \geqslant 0$ if for any $\psi \in \mathcal{D}(A)$, $\langle \psi, A\psi \rangle \geqslant 0$ and that $A \geqslant B$ if $A - B \geqslant 0$.

Proceeding analogously we also get

$$\langle\psi, A^{-1}\psi\rangle = \langle\psi, \int_{\sigma(A)} \frac{1}{\lambda} d\mu(\lambda)\,\psi\rangle \geqslant \inf_{\lambda\in\sigma(A)} \frac{1}{\lambda}\langle\psi, \int_{\sigma(A)} d\mu(\lambda)\,\psi\rangle \geqslant 0.$$

Those chains of inequalities imply that $0 \leqslant A^{-1} \leqslant \mathrm{id}$.

To prove **b** consider $\lambda > 0$; given that $\lambda > 0$, we have

$$B + \lambda\,\mathrm{id} \geqslant A + \lambda\,\mathrm{id} \Rightarrow (A + \lambda\,\mathrm{id})^{-\frac{1}{2}} (B + \lambda\,\mathrm{id}) (A + \lambda\,\mathrm{id})^{-\frac{1}{2}} \geqslant \mathrm{id},$$

where we used the fact that $A + \lambda\,\mathrm{id} \geqslant \lambda\,\mathrm{id}$ and that $(\cdot)^{-\frac{1}{2}}$ is continuous and bounded on $[\lambda, +\infty)$ to define $(A + \lambda\,\mathrm{id})^{-\frac{1}{2}}$.

Using **a** we then get that

$$\begin{aligned} \mathrm{id} &\geqslant \left[(A + \lambda\,\mathrm{id})^{-\frac{1}{2}} (B + \lambda\,\mathrm{id}) (A + \lambda\,\mathrm{id})^{-\frac{1}{2}}\right]^{-1} \\ &= (A + \lambda\,\mathrm{id})^{\frac{1}{2}} (B + \lambda\,\mathrm{id})^{-1} (A + \lambda\,\mathrm{id})^{\frac{1}{2}}. \end{aligned}$$

Multiplying both sides from left and right by $(A + \lambda\,\mathrm{id})^{-\frac{1}{2}}$ we can conclude.

To prove **c**, we first prove (9); we get

$$\begin{aligned} \int_0^{+\infty} \frac{1}{\sqrt{\lambda}} \left(1 - \frac{\lambda}{x+\lambda}\right) d\lambda &= \int_0^{+\infty} \frac{x}{\sqrt{\lambda}\,(x+\lambda)} d\lambda = \sqrt{x} \int_0^{+\infty} \frac{1}{\sqrt{\lambda}\,(1+\lambda)} d\lambda \\ &= \sqrt{x}\left[2 \arctan \sqrt{\lambda}\right]_0^{+\infty} = \pi\sqrt{x}. \end{aligned}$$

As a consequence we can write for any $\psi \in \mathcal{H}$

$$\langle\psi, \sqrt{A}\psi\rangle = \langle\psi, \int_{\sigma(A)} \sqrt{\lambda} d\mu(\lambda)\,\psi\rangle = \langle\psi, \int_{\sigma(A)} \frac{1}{\pi} \int_0^{+\infty} \frac{1}{\sqrt{t}} \left(1 - \frac{t}{t+\lambda}\right) dt d\mu(\lambda)\,\psi\rangle.$$

Now, given that $\frac{1}{\sqrt{t}}\left(1 - \frac{t}{t+\lambda}\right) \leqslant \frac{1}{\sqrt{t}}\left(1 - \frac{t}{t+\|A\|}\right) = \frac{\|A\|}{\sqrt{t}(t+\|A\|)}$ is integrable in $\sigma(A) \times [0, +\infty)$ with the measure given by the product of the spectral measure of A and the Lebesgue measure, we can exchange the order of the two integrals to get

$$\begin{aligned} \langle\psi, \sqrt{A}\psi\rangle &= \langle\psi, \frac{1}{\pi} \int_0^{+\infty} \int_{\sigma(A)} \frac{1}{\sqrt{t}} \left(1 - \frac{t}{t+\lambda}\right) d\mu(\lambda)\, dt\psi\rangle \\ &= \langle\psi, \frac{1}{\pi} \int_0^{+\infty} \frac{1}{\sqrt{t}} \left(1 - t\,(A + t\,\mathrm{id})^{-1}\right) dt\psi\rangle. \end{aligned}$$

Using now **b** we get that for any $\psi \in \mathcal{H}$

$$\begin{aligned} \langle\psi, \sqrt{A}\psi\rangle &= \langle\psi, \frac{1}{\pi} \int_0^{+\infty} \frac{1}{\sqrt{t}} \left(1 - t\,(A + t\,\mathrm{id})^{-1}\right) dt\psi\rangle \\ &\leqslant \langle\psi, \frac{1}{\pi} \int_0^{+\infty} \frac{1}{\sqrt{t}} \left(1 - t\,(B + t\,\mathrm{id})^{-1}\right) dt\psi\rangle = \langle\psi, \sqrt{B}\psi\rangle, \end{aligned}$$

which allows us to conclude.

□

Exercise 4

Let $\mathcal{H}$ be an Hilbert space. Let A be a linear self-adjoint operator on $\mathcal{H}$ with $A \geqslant 0$ and $\lambda > 0$. Denote with $\|\cdot\|$ the operator norm and with $\|\cdot\|_{\mathcal{H}}$ the norm induced by the inner product in the Hilbert space $\mathcal{H}$.

a Prove that $\left\|(A + \lambda \,\mathrm{id})^{-1}\right\| \leqslant 1/\lambda$.

b Prove that for all $\psi \in \mathcal{H}$,

$$\|\psi\|_{\mathcal{H}}^2 \geqslant \left\|A\,(A + \lambda \,\mathrm{id})^{-1}\,\psi\right\|_{\mathcal{H}}^2 + \lambda^2 \left\|(A + \lambda \,\mathrm{id})^{-1}\,\psi\right\|_{\mathcal{H}}^2. \tag{10}$$

Conclude that $\left\|A\,(A + \lambda \,\mathrm{id})^{-1}\right\| \leqslant 1$.

Proof. To prove **a** recall that we proved in class that if T is a self-adjoint operator and f is a continuous and bounded function we have $\|f\,(T)\| \leqslant \sup_{\zeta \in \sigma(T)} |f\,(\zeta)|$. Moreover, we also saw that if $A \geqslant 0$ then $\sigma\,(A) \subseteq [0, +\infty)$. As a consequence we get

$$\left\|(A + \lambda \,\mathrm{id})^{-1}\right\| \leqslant \sup_{\zeta \in \sigma(A)} \frac{1}{|\zeta + \lambda|} \leqslant \sup_{\zeta \in [0,+\infty)} \frac{1}{\zeta + \lambda} \leqslant \frac{1}{\lambda}.$$

To prove **b** we get that for any $\psi \in \mathcal{H}$

$$\langle \psi, (A + \lambda \,\mathrm{id})^{-1}\,A\,(A + \lambda \,\mathrm{id})^{-1}\,\psi\rangle = \langle (A + \lambda \,\mathrm{id})^{-1}\,\psi, A\,(A + \lambda \,\mathrm{id})^{-1}\,\psi\rangle \geqslant 0.$$

As a consequence we get that

$$\begin{aligned}
&\left\|A\,(A + \lambda \,\mathrm{id})^{-1}\,\psi\right\|_{\mathcal{H}}^2 + \lambda^2 \left\|(A + \lambda \,\mathrm{id})^{-1}\,\psi\right\|_{\mathcal{H}}^2 = \\
&\quad = \langle \psi, (A + \lambda \,\mathrm{id})^{-1}\left(A^2 + \lambda^2\right)(A + \lambda \,\mathrm{id})^{-1}\,\psi\rangle \\
&\quad \leqslant \langle \psi, (A + \lambda \,\mathrm{id})^{-1}\left(A^2 + 2\lambda A + \lambda^2\right)(A + \lambda \,\mathrm{id})^{-1}\,\psi\rangle = \|\psi\|_{\mathcal{H}}^2.
\end{aligned}$$

As a consequence we then get $\left\|A\,(A + \lambda \,\mathrm{id})^{-1}\,\psi\right\|_{\mathcal{H}} \leqslant \|\psi\|_{\mathcal{H}}$ which allows us to conclude that $\left\|A\,(A + \lambda \,\mathrm{id})^{-1}\right\| \leqslant 1$.

□