Introduction to Mathematical Quantum Theory

Solution to the Exercises

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Exercise 1

Let ψ be a unit vector in $L^2(\mathbb{R})$ such that $x\psi,\ x^2\psi \in L^2(\mathbb{R})$. Prove that

$$\langle X^2\rangle_\psi \geqslant (\langle X\rangle_\psi)^2, \tag{1}$$

where as we defined in class, X is the operator given by the multliplication by x and

$$\langle A\rangle_\psi := \langle \psi, A\psi\rangle. \tag{2}$$

Hint: Use Jensen inequality.

Proof. Recall that Jensen inequality states that if μ is a probability measure on a measurable space Ω, f is a real valued function and Ξ is a convex function from $\mathbb{R}$ to itself, then we have

$$\Xi\left(\int_\Omega f(x)\,d\mu(x)\right) \leqslant \int_\Omega \Xi\circ f(x)\,d\mu(x).$$

Consider now the space $\Omega = \mathbb{R}$. The measure $|\psi(x)|^2\,dx$ is a probability measure because ψ has L^2-norm equal to 1. Now, if we consider $f(x) = x$ and $\Xi(t) = t^2$ in Jensen inequality we get

$$(\langle X\rangle_\psi)^2 = \left(\int_\mathbb{R} x\,|\psi(x)|^2\,dx\right)^2 \leqslant \int_\mathbb{R} x^2\,|\psi(x)|^2\,dx = \langle X^2\rangle_\psi.$$

□

Exercise 2

Let $\alpha := \{\alpha_n\}_{n\in\mathbb{Z}}$ be a sequence of complex numbers. Consider the Hilbert space of the square integrable functions $\mathfrak{h} := l^2(\mathbb{Z})$. Consider the operator that to the sequence $x := \{x_n\}_{n\in\mathbb{Z}}$ associate the sequence $M_\alpha x = \{\alpha_n x_n\}_{n\in\mathbb{Z}}$.

Suppose that $\|\alpha\|_\infty := \sup_{n\in\mathbb{Z}}|\alpha_n| < +\infty$. Prove that M_a is a well defined linear bounded operator from $\mathfrak{h}$ to itself and prove that $\|M_\alpha\| = \|\alpha\|_\infty$.

Proof. First notice that for any element of the sequence $M_\alpha x$ we get $|\alpha_n x_n| \leqslant \|\alpha\|_\infty |x_n|$. As a consequence we get

$$\|M_\alpha x\|_\mathfrak{h} = \left(\sum_{n\in\mathbb{Z}} |\alpha_n x_n|^2\right)^{\frac{1}{2}} \leqslant \|\alpha\|_\infty \left(\sum_{n\in\mathbb{Z}} |x_n|^2\right)^{\frac{1}{2}} = \|\alpha\|_\infty \|x\|_\mathfrak{h}.$$

Therefore M_α is well defined from $\mathfrak{h}$ to itself and it is trivially linear. From the previous inequality we also get that $\|M_\alpha\| \leqslant \|\alpha\|_\infty$.

To prove the equality, first define for any $j \in \mathbb{Z}$ the element $e_j := \{\delta_{j,n}\}_{n\in\mathbb{Z}} \in \mathfrak{h}$. We get that $\|e_j\|_{\mathfrak{h}} = 1$ and that $M_\alpha e_j = \alpha_j e_j$. Now, by definition of sup there is a sequence $\{n_j\}_{j\in\mathbb{N}}$ such that $|\alpha_{n_j}| \to \|\alpha\|_\infty$ as $j \to +\infty$, and we then get

$$\|\alpha\|_\infty = \lim_{j\to+\infty} |\alpha_{n_j}| = \lim_{j\to+\infty} \|M_\alpha e_{n_j}\|_{\mathfrak{h}} \leqslant \lim_{j\to+\infty} \|M_\alpha\| \|e_{n_j}\|_{\mathfrak{h}} = \|M_\alpha\|,$$

concluding the proof.

□

Exercise 3

Consider the Hilbert space $\mathfrak{h} := L^2(\mathbb{R})$. And the operator H define

$$\mathcal{D}(H) := H^2(\mathbb{R}) = \left\{\psi \in L^2(\mathbb{R}) \mid k^2\widehat{\psi} \in L^2(\mathbb{R})\right\}$$
$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(X),$$

where the operator $(V(X)\psi)(x) = V(x)\psi(x)$, with

$$V(x) := \begin{cases} -C & \text{if } |x| \leqslant A, \\ 0 & \text{if } |x| > A, \end{cases} \tag{3}$$

and with A and C positive constants. Consider $E \in (-\infty, -C]$ and prove that there is no nonzero $\psi_E \in \mathcal{D}(H)$ such that

$$H\psi_E = E\psi_E. \tag{4}$$

Proof. Suppose there exists E such in the text of the exercise. Given that $\psi_E \neq 0$ we can assume that $\|\psi_E\|_{\mathfrak{h}} = 1$ As a consequence we get

$$E = \langle\psi_E, E\psi_E\rangle = \langle\psi_E, H\psi_E\rangle = \langle\psi_E, -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_E\rangle + \langle\psi_E, V(X)\psi_E\rangle.$$

Given that $\psi_E \in \mathcal{D}(H)$ we can integrate by part the first term and obtain

$$\langle\psi_E, -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_E\rangle = \frac{\hbar^2}{2m}\langle\frac{\partial}{\partial x}\psi_E, \frac{\partial}{\partial x}\psi_E\rangle = \frac{\hbar^2}{2m}\left\|\frac{\partial}{\partial x}\psi_E\right\| \geqslant 0.$$

On the other hand we have

$$\langle\psi_E, V(X)\psi_E\rangle \geqslant -|\langle\psi_E, V(X)\psi_E\rangle| \geqslant -\|V\|_\infty \|\psi_E\|_{\mathfrak{h}}^2 = -C.$$

Given that $E \in (-\infty, -C]$ we get

$$-C \geqslant E \geqslant \langle\psi_E, -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_E\rangle + \langle\psi_E, V(X)\psi_E\rangle \geqslant \langle\psi_E, V(X)\psi_E\rangle \geqslant -C,$$

and therefore $E = -C$.

Now as we saw in class the function ψ_E needs to satisfy the following equation

$$\begin{cases} -\dfrac{\hbar^2}{2m}\psi_E'' = -C\psi_E & \text{if } |x| \leqslant A, \\ -\dfrac{\hbar^2}{2m}\psi_E'' = (C+E)\,\psi_E = 0 & \text{if } |x| > A, \\ \lim\limits_{x\to\pm A^-} \psi_E(x) = \lim\limits_{x\to\pm A^+} \psi_E(x), \\ \lim\limits_{x\to\pm A^-} \psi_E'(x) = \lim\limits_{x\to\pm A^+} \psi_E'(x). \end{cases}$$

Suppose now $x \in (-\infty, -A)$. Then we get $\psi_E = c_0 + c_1 x$. Given that $\psi_E \in \mathfrak{h} = L^2(\mathbb{R})$, we then get that $c_0 = c_1 = 0$. Proceeding similarly for $x \in (A, +\infty)$ we get that $\psi_E(x) = 0$ for any $|x| > A$.

So ψ_E solves

$$\begin{cases} \psi_E'' = \dfrac{2mC}{\hbar^2}\psi_E & \text{if } |x| \leqslant A, \\ \psi_E(\pm A) = \psi_E'(\pm A) = 0. \end{cases} \tag{5}$$

Now the solution to the differential equation is $\psi_E(x) = c_+ e^{\left(\sqrt{2mC}/\hbar\right)x} + c_- e^{-\left(\sqrt{2mC}/\hbar\right)x}$. From the fact that $\psi_E(-A) = \psi_E(A)$ we get

$$(c_+ - c_-)\sinh\left(\frac{\sqrt{2mC}}{\hbar}A\right) = 0,$$

which in particular implies $c_+ = c_-$. As a consequence we get

$$\psi_E(x) = 2c_+ \cosh\left(\frac{\sqrt{2mC}}{\hbar}x\right).$$

Using the fact that $\psi_E(A) = 0$ we get $c_+ = 0$, implying that the unique eigenfunction corresponding to E is the zero vector, which is absurd and concludes our proof.

□

Exercise 4

Let $\mathfrak{h}$, H and $\mathcal{D}(H)$ as in Exercise 3. In class we saw that for any $E \in (-C, 0)$ there is always at least one nonzero even solution ψ_E to the problem $H\psi_E = E\psi_E$.

Prove that if $A\sqrt{2mC}\hbar \leqslant \frac{\pi}{2}$ there are no nonzero odd solutions, and for larger values of C there is always at least one.

Proof. Proceeding as in class it is easy to see that any odd solution ψ_E to $H\psi_E = E\psi_E$ is such that

$$\psi_E(x) = \begin{cases} ce^{-\frac{\sqrt{2m|E|}}{\hbar}(x-A)} & \text{if } x > A, \\ -ce^{\frac{\sqrt{2m|E|}}{\hbar}(x+A)} & \text{if } x > A. \end{cases}$$

This explicit form of the solution outside the ball $|x| \leqslant A$ gives us boundary conditions for the problem that the solution needs to solve inside the ball:

$$\begin{cases} -\dfrac{\hbar^2}{2m}\psi_E'' = (C+E)\,\psi_E, \\ \psi_E(\pm A) = \pm c, \\ \psi_E'(\pm A) = -\dfrac{\sqrt{2m\,|E|}}{\hbar}c. \end{cases} \tag{6}$$

Out of convenience, we define, similarly as in class, the constants $\kappa := (2mC)/\hbar^2$ and $\varepsilon := -(2mE)/\hbar^2$. We then have that $E \in (-C, 0)$ if and only if $\varepsilon \in (0, \kappa)$.

We are then looking for the odd solution to the problem

$$\begin{cases} -\psi_E'' = (\kappa - \varepsilon)\,\psi_E, \\ \psi_E(\pm A) = \pm c, \\ \psi_E'(\pm A) = -\sqrt{\varepsilon}c. \end{cases}$$

A generic solution for this problem is of the form $\psi_E(x) = \alpha \sin\left(\sqrt{\kappa - \varepsilon}x\right) + \beta \cos\left(\sqrt{\kappa-\varepsilon}x\right)$, with α and β to be determined. Given that our function is odd, we have that $\beta = 0$. The boudnary conditions then gives us the following relations:

$$\begin{cases} \alpha \sin\left(\sqrt{\kappa-\varepsilon}A\right) = c, \\ \alpha\sqrt{\kappa-\varepsilon}\cos\left(\sqrt{\kappa-\varepsilon}A\right) = -\sqrt{\varepsilon}c. \end{cases}$$

If $c = 0$, the first equation tells us that if we do not want the trivial solution, $\sqrt{\kappa-\varepsilon}A = \eta\pi$, with $\eta \in \mathbb{Z}$. This implies that $\cos\left(\sqrt{\kappa-\varepsilon}A\right) = \pm 1$, and applying this to the second equation we would deduce that $\kappa = \varepsilon$, which is not possible. So $c \neq 0$ if and only if $\alpha \neq 0$. Suppose then $c \neq 0$ (and therefore $\alpha \neq 0$). Dividing the second equation by the first one we then get the following matching condition

$$\sqrt{\kappa-\varepsilon}\cot\left(\sqrt{\kappa-\varepsilon}A\right) = -\sqrt{\varepsilon}.$$

Now, if $\sqrt{\kappa}A \leqslant \frac{\pi}{2}$ we get that $\sqrt{\kappa-\varepsilon}A \in \left(0, \frac{\pi}{2}\right)$, and as a consequence the term on the left of the matching condition is strictly positive. On the other hand the term on the right is strictly negative, therefore the matching condition cannot be satisfied and there is no odd solution to the problem.

Consider now $\sqrt{\kappa}A > \frac{\pi}{2}$; define the interval $I := \left(\max\left\{0, k - \pi^2/A^2\right\}, k - \pi^2/4A^2\right)$ and the following mapping:

$$\begin{array}{cccl} \xi: & I & \to & \mathbb{R} \\ & \varepsilon & \mapsto & \sqrt{\varepsilon} + \sqrt{\kappa-\varepsilon}\cot\left(\sqrt{\kappa-\varepsilon}A\right). \end{array}$$

If $\max\left\{0, k - \pi^2/A^2\right\} = 0$ then we have that $\sqrt{\kappa}A \leqslant \pi$ and $\cot\left(\sqrt{\kappa-\varepsilon}A\right) \in (-\infty, 0)$; in particular

$$\xi(I) = \left(-\sqrt{\kappa}\left|\cot\left(\sqrt{\kappa}A\right)\right|, \sqrt{\kappa - \frac{\pi^2}{A^2}}\right).$$

If $\max\left\{0, k - \pi^2/A^2\right\} = k - \pi^2/A^2$ then we have that

$$\xi\left(I\right) = \left(-\infty, \sqrt{\kappa - \frac{\pi^2}{A^2}}\right).$$

In both cases $0 \in \xi\left(I\right)$ and we have that there is a solution to the matching conditions, which implies the existence of a nontrivial odd solution. $\square$