UNIVERSITY OF TORONTO

Foundations of Quantum Mechanics
(APM 421 H)

Winter 2014
Solutions 4
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Operators

Homework Problems

12. Projections (19 points)

Consider the multiplication operator $P = p(\hat{x})$ on $L^2(\mathbb{R}^d)$ associated to the function

$$p(x) = \begin{cases} 1 & x \geq 0 \\ 0 & x < 0 \end{cases}.$$

(i) Find 2 eigenfunctions.

(ii) Compute $\sigma(P)$.

(iii) Determine the nature of the spectrum, i. e. determine $\sigma_{\mathrm{p}}(P)$, $\sigma_{\mathrm{cont}}(P)$, and $\sigma_{\mathrm{r}}(P)$.

(iv) Prove that P is an orthogonal projection.

Solution:

(i) For instance, consider the functions

$$\psi_0(x) \overset{[1]}{=} \begin{cases} 1 & x \in [-1, 0] \\ 0 & \text{else} \end{cases}, \qquad \psi_1(x) \overset{[1]}{=} \begin{cases} 1 & x \in [0, 1] \\ 0 & \text{else} \end{cases}.$$

(All that is important is that one of them is zero on $[0, +\infty)$ and the other is zero on $(-\infty, 0]$.) Then clearly, ψ_0 is an eigenfunction to the eigenvalue 0, $(P\psi_0)(x) = p(x)\,\psi_0(x) = 0$ [1], while ψ_1 is an eigenfunction to the eigenvalue 1, $(P\psi_1)(x) = p(x)\,\psi_1(x) = \psi_1(x)$ [1].

(ii) First of all, P has two eigenvalues, namely 0 and 1 [2]: the eigenvectors to the eigenvalue 1 are functions which vanish almost everywhere on $(-\infty, 0)$. Similarly, eigenvectors to the eigenvalue 0 are functions which vanish almost everywhere on $[0, +\infty)$.

Since $(P - z)\varphi = 0$ means that $\big((P - z)\varphi\big)(x) = 0$ for almost all $x \in \mathbb{R}$ [1]. Thus, for all $z \neq 0, 1$ we have $(P - z)\varphi \neq 0$ for all $\varphi \neq 0$ [1], i. e. $P - z$ is invertible as long as $z \neq 0, 1$ [1], and we have shown $\sigma(P) = \{0, 1\}$ [1].

(iii) Since all vectors are eigenvectors, the spectrum consists just of point spectrum,

$$\sigma_{\mathrm{p}}(P) \overset{[1]}{=} \sigma(P) = \{0, 1\}, \qquad \sigma_{\mathrm{cont}}(P) \overset{[1]}{=} \emptyset, \qquad \sigma_{\mathrm{r}}(P) \overset{[1]}{=} \emptyset.$$

(iv) p is a real-valued, bounded function, and hence, by problem 11 (ii) $P^* = P$ [2]. (Otherwise, one needs to show this by hand for this special case.)

To see $P^2 = P$, we note $p^2 = p$ in the sense of functions and conclude

$$(P^2\varphi)(x) \overset{[1]}{=} p(x)^2\,\varphi(x) \overset{[1]}{=} p(x)\,\varphi(x) \overset{[1]}{=} (P\varphi)(x).$$

Thus, $P = P^* = P^2$ is an orthogonal projection [1].

13. The discrete Laplacian (24 points)

Consider the Hilbert space $\ell^2(\mathbb{Z})$ with the usual scalar product $\langle \cdot\,, \cdot \rangle_{\ell^2(\mathbb{Z})}$. Define the shift operator

$$\mathfrak{s} : \ell^2(\mathbb{Z}) \longrightarrow \ell^2(\mathbb{Z}),\ (\mathfrak{s}\psi)(n) := \psi(n-1)$$

as well as the shift by $a \in \mathbb{Z}$ lattice units, $\mathfrak{s}_a := \mathfrak{s}^a$. Consider the *discrete Laplacian*

$$\Delta : \ell^2(\mathbb{Z}) \longrightarrow \ell^2(\mathbb{Z}),\ (\Delta\psi)(n) := \psi(n+1) + \psi(n-1) - 2\psi(n).$$

(i) Compute $\mathfrak{s}_a^*$ and prove that $\mathfrak{s}_a$ is unitary.

(ii) Show that Δ is a bounded operator on $\ell^2(\mathbb{Z})$.

(iii) Show that $\mathfrak{s}_a$ and Δ commute, i. e. $[\mathfrak{s}_a, \Delta] := \mathfrak{s}_a\Delta - \Delta\mathfrak{s}_a = 0$.

(iv) Compute Δ^*.

(v) Determine E_k so that

$$\psi_k(n) := \mathrm{e}^{+\mathrm{i}nk}, \qquad\qquad n \in \mathbb{Z}, k \in [-\pi, +\pi],$$

is an eigenvalue to the discrete Laplacian,

$$(\Delta\psi_k)(n) = E_k\psi_k(n).$$

Is ψ_k an element of $\ell^2(\mathbb{Z})$?

Remark: The Hilbert space $\ell^2(\mathbb{Z})$ is often used in solid state physics where the shift operator $(\mathfrak{s}\widehat{\psi})(n) := \widehat{\psi}(n-1)$ is interpreted as translating the particle by one lattice unit.

Solution:

(i) Let $\varphi, \psi \in \ell^2(\mathbb{Z})$ and $a \in \mathbb{Z}$. The adjoint operator $\mathfrak{s}_a^*$ is then $\mathfrak{s}_{-a}$,

$$\begin{aligned}\langle\varphi, \mathfrak{s}_a\psi\rangle &\overset{[1]}{=} \sum_{n\in\mathbb{Z}} \overline{\varphi(n)}\,(\mathfrak{s}_a\psi)(n) \overset{[1]}{=} \sum_{n\in\mathbb{Z}} \overline{\varphi(n)}\,\psi(n-a) \overset{[1]}{=} \sum_{k\in\mathbb{Z}} \overline{\varphi(k+a)}\,\psi(k)\\ &\overset{[1]}{=} \sum_{k\in\mathbb{Z}} \overline{(\mathfrak{s}_{-a}\varphi)(k)}\,\psi(k) \overset{[1]}{=} \langle\mathfrak{s}_{-a}\varphi, \psi\rangle.\end{aligned}$$

$\mathfrak{s}_{-a}$ is also the inverse to $\mathfrak{s}_a$ [1], since

$$\big(\mathfrak{s}_{-a}\mathfrak{s}_a\varphi\big)(n) = (\mathfrak{s}_a\varphi)(n+a) = \varphi(n+a-a) = \varphi(n)$$

holds for all $\varphi \in \ell^2(\mathbb{Z})$ and $n \in \mathbb{Z}$. This means $\mathfrak{s}_a$ is unitary [1].

(ii) We recognize that actually $\Delta = \mathfrak{s} + \mathfrak{s}^* - 2$ [1], so we deduce Δ is bounded

$$\lVert\Delta\rVert \overset{[1]}{\leq} \lVert\mathfrak{s}\rVert + \lVert\mathfrak{s}^*\rVert + \lVert 2\rVert \overset{[1]}{=} 4.$$

(iii) Translations commute amongst one another, $\mathfrak{s}_a\,\mathfrak{s}_b = \mathfrak{s}_{a+b} = \mathfrak{s}_b\,\mathfrak{s}_a$ [1], and hence,

$$\begin{aligned}\mathfrak{s}_a\,\Delta &\overset{[1]}{=} \mathfrak{s}_a\,\mathfrak{s} + \mathfrak{s}_a\,\mathfrak{s}^* - 2\mathfrak{s}_a\\ &\overset{[1]}{=} \mathfrak{s}\,\mathfrak{s}_a + \mathfrak{s}^*\,\mathfrak{s}_a - 2\mathfrak{s}_a \overset{[1]}{=} \Delta\,\mathfrak{s}_a\end{aligned}$$

Hence, $[\mathfrak{s}_a, \Delta]\psi = 0$ and $\mathfrak{s}_a$ commutes with Δ [1].

(iv) We will see that the discrete Laplacian Δ is selfadjoint: for all $\varphi, \psi \in \ell^2(\mathbb{Z})$ we have

$$\begin{aligned}
\big\langle \varphi, \Delta\psi \big\rangle &\overset{[1]}{=} \langle \varphi, \mathfrak{s}\psi \rangle + \langle \varphi, \mathfrak{s}^*\psi \rangle - 2\,\langle \varphi, \psi \rangle \\
&\overset{[1]}{=} \langle \mathfrak{s}^*\varphi, \psi \rangle + \langle \mathfrak{s}\varphi, \psi \rangle - 2\,\langle \varphi, \psi \rangle \\
&\overset{[1]}{=} \big\langle \Delta\varphi, \psi \big\rangle,
\end{aligned}$$

i. e. $\Delta^* = \Delta$ is selfadjoint [1].

(v) We apply Δ to the sequence ψ_k with entries $\psi_k(n) = \mathrm{e}^{+\mathrm{i}nk}$, $k \in [-\pi, +\pi]$ and obtain

$$\begin{aligned}
(\Delta\psi_k)(n) = \psi_k(n+1) + \psi_k(n-1) - 2\psi_k(n) &\overset{[1]}{=} \mathrm{e}^{+\mathrm{i}(n+1)k} + \mathrm{e}^{+\mathrm{i}(n-1)k} - 2\mathrm{e}^{+\mathrm{i}nk} \\
&\overset{[1]}{=} \big(\mathrm{e}^{+\mathrm{i}k} + \mathrm{e}^{-\mathrm{i}k} - 2\big)\,\mathrm{e}^{+\mathrm{i}nk} \overset{[1]}{=} \big(2\cos k - 2\big)\,\mathrm{e}^{+\mathrm{i}nk} \overset{[1]}{=}: E_k\,\psi_k(n).
\end{aligned}$$

Since $|\psi_k(n)| = \big|\mathrm{e}^{+\mathrm{i}nk}\big| = 1$ is independent of $n \in \mathbb{Z}$, the sequence ψ_k cannot be square summable, because $\psi_k \in \ell^2(\mathbb{Z})$ necessarily implies $\lim_{|n|\to\infty} \psi_k(n) = 0$ [1].

14. Position and momentum representation (15 points)

Consider $\ell^2(\mathbb{Z})$ with the usual scalar $\langle \cdot\,, \cdot \rangle_{\ell^2(\mathbb{Z})}$ product and $L^2([0, 2\pi])$ endowed with the scalar product

$$\big\langle \widehat{\varphi}, \widehat{\psi} \big\rangle_{L^2([0,2\pi])} := \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}k \, \overline{\widehat{\varphi}(k)} \, \widehat{\psi}(k).$$

Define the Fourier transform

$$\begin{aligned} \mathcal{F} : L^2([0, 2\pi]) &\longrightarrow \ell^2(\mathbb{Z}), \\ \psi(n) = \big(\mathcal{F}\widehat{\psi}\big)(n) &:= \big\langle \mathrm{e}^{+\mathrm{i}nk}, \widehat{\psi} \big\rangle_{L^2([0,2\pi])} \end{aligned}$$

and its inverse

$$\ell^2(\mathbb{Z}) \ni \psi \mapsto \big(\mathcal{F}^{-1}\psi\big)(k) = \sum_{n \in \mathbb{Z}} \psi(n) \, \mathrm{e}^{+\mathrm{i}nk}.$$

You may use without proof that $\mathcal{F}$ is unitary.

(i) For the shift operator $(\mathfrak{s}\widehat{\psi})(n) := \widehat{\psi}(n-1)$, compute $\mathcal{F}^{-1} \, \mathfrak{s} \, \mathcal{F}$.

(ii) For the discrete Laplacian from problem 13, compute the momentum representation $\mathcal{F}^{-1} \, \Delta \, \mathcal{F}$.

(iii) What is the connection between ψ_k from problem 13 (v) in the position representation and $\mathcal{F}^{-1} \, \Delta \, \mathcal{F}$ in the momentum representation? Heuristically, what is the inverse Fourier transform of ψ_k?

(iv) Is $\Delta \geq 0$? Justify your answer.

Solution:

(i) Pick $\widehat{\psi} \in L^2([0, 2\pi])$. Then a straightforward computation yields

$$\begin{aligned} \big(\mathcal{F}^{-1} \, \mathfrak{s} \, \mathcal{F}\widehat{\psi}\big)(k) &\overset{[1]}{=} \sum_{n \in \mathbb{Z}} \big(\mathfrak{s} \, \mathcal{F}\widehat{\psi}\big)(n) \, \mathrm{e}^{+\mathrm{i}nk} \overset{[1]}{=} \sum_{n \in \mathbb{Z}} (\mathcal{F}\widehat{\psi})(n-1) \, \mathrm{e}^{+\mathrm{i}k} \, \mathrm{e}^{+\mathrm{i}(n-1)k} \\ &= \mathrm{e}^{+\mathrm{i}k} \sum_{n' \in \mathbb{Z}} (\mathcal{F}\widehat{\psi})(n') \, \mathrm{e}^{+\mathrm{i}n'k} \overset{[1]}{=} \mathrm{e}^{+\mathrm{i}k} \, \widehat{\psi}(k). \end{aligned}$$

Hence, the discrete Laplacian in momentum representation is the multiplication operator $\mathcal{F}^{-1} \, \mathfrak{s} \, \mathcal{F} = \mathrm{e}^{+\mathrm{i}\hat{k}}$ [1].

(ii) Given that $\Delta = \mathfrak{s} + \mathfrak{s}^* - 2$ [1], we can reuse the result from (i) to conclude that in momentum representation, the discrete Laplacian is multiplication by $2\cos k - 2$,

$$\begin{aligned} \mathcal{F}^{-1} \, \Delta \, \mathcal{F} &\overset{[1]}{=} \mathcal{F}^{-1} \, \big(\mathfrak{s} + \mathfrak{s}^* - 2\big) \, \mathcal{F} \overset{[1]}{=} \mathrm{e}^{+\mathrm{i}\hat{k}} + \mathrm{e}^{-\mathrm{i}\hat{k}} - 2 \\ &\overset{[1]}{=} 2\cos \hat{k} - 2. \end{aligned}$$

(iii) The ψ_k were pseudoeigenvectors to Δ [1], meaning that while they satisfy the eigenvalue equation, they are not square-summable [1]. Heuristically, their inverse Fourier transform is the delta function $\delta(\cdot - k)$ [1], because $\mathcal{F}^{-1} \, \Delta \, \mathcal{F}$ is a multiplication operator and the eigenvectors of multiplication operators are delta distributions.

(iv) No, $\Delta \leq 0$: One can check that in Fourier representation, with $\widehat{\psi} = \mathcal{F}^{-1}\psi$

$$\begin{aligned}
\langle \psi, \Delta\psi \rangle_{\ell^2(\mathbb{Z})} &\overset{[1]}{=} \left\langle \mathcal{F}^{-1}\psi, \mathcal{F}^{-1}\Delta\mathcal{F}\mathcal{F}^{-1}\psi \right\rangle_{L^2([0,2\pi])} \\
&\overset{[1]}{=} \langle \widehat{\psi}, \big(2\cos\hat{k} - 2\big)\widehat{\psi} \rangle_{L^2([0,2\pi])} \\
&\overset{[1]}{=} \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}k \, \underbrace{\big(2\cos k - 2\big)}_{\leq 0} \big|\widehat{\psi}(k)\big|^2 \overset{[1]}{\leq} 0
\end{aligned}$$

15. Rank-1 operators (14 points)

Suppose $\varphi, \psi \neq 0$ are elements of a Hilbert space $\mathcal{H}$, and define the rank-1 operator $T = |\varphi\rangle\langle\psi|$ via

$$T\phi = \langle\psi, \phi\rangle \; \varphi.$$

(i) Find all eigenvectors and eigenvalues of T.

(ii) Compute $\sigma(T)$.

(iii) Determine the nature of the spectrum, i. e. determine $\sigma_{\mathrm{p}}(T)$, $\sigma_{\mathrm{cont}}(T)$ and $\sigma_{\mathrm{r}}(T)$.

Solution:

(i) We can read off the eigenvalues from the form of the operator: the first eigenvector is φ [1] with eigenvalue $\lambda := \langle\psi, \varphi\rangle$ [1].

The other eigenvalue is 0 [1], because for any vector ϕ perpendicular to ψ, we have $T\phi = 0$ [1], and thus the eigenspace is

$$\ker T \overset{[1]}{=} \{\psi\}^{\perp}.$$

Now there are two cases: $\psi \perp \varphi$, and then also $\lambda = 0$ and the only eigenvalue is 0 [1]. Or $\langle\psi, \varphi\rangle \neq 0$ and T has two different eigenvalues [1].

(ii) Clearly, $\{0, \lambda\} \subseteq \sigma(T)$ where $\lambda = \langle\psi, \varphi\rangle$ [1].

Since $\mathrm{ran}\, T = \mathrm{span}\{\varphi\}$ is a one-dimensional subspace, the operator $T - z$ is always invertible on $\big(\mathrm{ran}\, T\big)^{\perp}$ [1]. On the one-dimensional subspace $\mathrm{ran}\, T$, the operator is invertible if and only if $z \neq \lambda$ [1]. Hence, we have shown $\sigma(T) = \{0, \lambda\}$ [1].

(iii) By the classification introduced in Chapter 4.1, we know that

$$\sigma_{\mathrm{p}}(T) = \sigma(P) \overset{[1]}{=} \{0, \lambda\}, \qquad \sigma_{\mathrm{cont}}(T) \overset{[1]}{=} \emptyset, \qquad \sigma_{\mathrm{r}}(T) \overset{[1]}{=} \emptyset.$$