Week 10 Worksheet

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Exercise 1. The matrix elements of x and p in the harmonic oscillator eigenbasis $\{|n\rangle\}$ are given by

$$\begin{aligned} x_{mn} &= \langle m|x|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\delta_{m,n+1}\sqrt{n+1} + \delta_{m,n-1}\sqrt{n}) \\ p_{mn} &= i\sqrt{\frac{m\omega\hbar}{2}}(\delta_{m,n+1}\sqrt{n+1} - \delta_{m,n-1}\sqrt{n}). \end{aligned}$$

a) For finite-dimensional matrices, show that $\mathrm{tr}([A, B]) = 0$, where for an $(n \times n)$-matrix A, the **trace** $\mathrm{tr}(A)$ is the sum of the diagonal entries of A.
Hint: Write $\mathrm{tr}(AB)$ in summation notation as $\sum_{i,j} c_{ij}$; that is, determine the scalars c_{ij} in terms of the matrix elements of A and B.

b) *Paradox.* From the result of (a), it would seem that the expressions for the matrix elements of x and p imply that $\hbar = 0$, since $[x, p] = i\hbar$. Use the matrix elements x_{mn} and p_{mn} to calculate xp and px, and explain in detail why the paradoxical conclusion $\hbar = 0$ is invalid.

c) ***Bonus.*** Derive the expressions for x_{mn} and p_{mn} given in the problem statement, using that

$$\begin{aligned} a^\dagger |n\rangle &= \sqrt{n+1}\,|n+1\rangle \\ a\,|n\rangle &= \sqrt{n}\,|n-1\rangle \end{aligned}$$

and

$$a^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega x - ip).$$

a) Given a matrix A with entries a_{ij}, $\mathrm{tr}(A) = \sum_i a_{ii}$. Since the matrix entries of AB are $a_{ik}b_{kj}$, where a_{ij} and b_{ij} are the entries of A and B, respectively, $\mathrm{tr}(AB) = \sum_{i,j} a_{ij}b_{ji}$. On the other hand, $\mathrm{tr}(BA) = \sum_{i,j} b_{ij}a_{ji} = \sum_{i,j} a_{ji}b_{ij} = \sum_{i,j} a_{ij}b_{ji} = \mathrm{tr}(AB)$, where in the second-to-last equality we swap the dummy indices $i \leftrightarrow j$.

b) We first calculate the matrix elements of xp:

$$\begin{aligned} (xp)_{ik} = x_{ij}\,p_{jk} &= \frac{i\hbar}{2}\left(\delta_{i,j+1}\sqrt{j+1} + \delta_{i,j-1}\sqrt{j}\right)\left(\delta_{j,k+1}\sqrt{k+1} - \delta_{j,k-1}\sqrt{k}\right) \\ (px)_{ik} = p_{ij}\,x_{jk} &= \frac{i\hbar}{2}\left(\delta_{i,j+1}\sqrt{j+1} - \delta_{i,j-1}\sqrt{j}\right)\left(\delta_{j,k+1}\sqrt{k+1} + \delta_{j,k-1}\sqrt{k}\right). \end{aligned}$$

Notice that the only difference in the two expressions is that in $(xp)_{ik}$, the first factor is a sum and the second factor a difference, while in $(px)_{ik}$, it's the other way around. Thus, when we take their difference, we immediately see that the only terms that survive will be the cross terms:

$$\begin{aligned}(xp)_{ik} - (px)_{ik} =& i\hbar\left(-\delta_{i,j+1}\delta_{j,k-1}\sqrt{(j+1)k} + \delta_{i,j-1}\delta_{j,k+1}\sqrt{j(k+1)}\right)\\ =& i\hbar\left(-\delta_{i,k}k + \delta_{i,k+1}(k+1)\right),\end{aligned}$$

where we use the sum over the j index to collapse Kronecker deltas of the form $\delta_{i,j+1}\delta_{j,k-1} = \delta_{i,k}$, for example. Summing this over $i = k$, we get what looks like an infinite sum of the form $\sum_n 1$, which doesn't converge! This is because the operators x, p are not of "trace class;" they're unbounded operators, which means me can't take their trace. A symptom of this is the fact that the eigenfunctions of x and p, which are δ-functions and plane waves, respectively, are not normalizable. For example, if we look at $[x, p] = i\hbar$, we see that on the RHS we have the *infinite-dimensional* identity operator, which is also unbounded! Indeed, if we took its trace, we get ∞, since $\sum_{n=0}^{\infty} 1 = \infty$. So there is no paradox: The trace of both sides is undefined and can't be computed; that's why we get what appears to be a non-converging sum for the trace of $[x, p]$.

c) We use the formulas

$$\begin{aligned}x =& \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)\\ p =& i\sqrt{\frac{\hbar m\omega}{2}}(a^\dagger - a).\end{aligned}$$

Then, we compute

$$\begin{aligned}x_{mn} =& \sqrt{\frac{\hbar}{2m\omega}}(a_{mn} + a^\dagger_{mn})\\ p_{mn} =& i\sqrt{\frac{\hbar m\omega}{2}}(a^\dagger_{mn} - a_{mn}).\end{aligned}$$

Plugging in $a_{mn} = \delta_{m,n-1}\sqrt{n}$ and $a^\dagger_{mn} = \delta_{m,n+1}\sqrt{n+1}$ gives the result.

Exercise 2. *Unitary Operators.* An operator U is called **unitary** if $UU^\dagger = U^\dagger U = 1$. This problem shows that in an infinite dimensional Hilbert space, if an operator preserves the norm of all vectors and possesses both a left and right inverse, then it is unitary.

a) Let U be some operator on a finite-dimensional vector space, and let $|\psi'\rangle = U|\psi\rangle$. Show that $\langle\psi'|\psi'\rangle = \langle\psi|\psi\rangle$ if and only if U is unitary.

b) Consider the Hilbert space for a particle moving in one dimension (which is infinite-dimensional). Let $|n\rangle$ be the usual harmonic oscillator eigenbasis, with $n = 0, 1, \ldots$ Define an operator U by

$$U|n\rangle = |n+1\rangle.$$

Show that if $|\psi'\rangle = U|\psi\rangle$, then $\langle\psi'|\psi'\rangle = \langle\psi|\psi\rangle$. Then show that

$$U^\dagger U = \mathbb{1},$$

so that U has a left inverse, and it is $U^\dagger$. Does U have a right inverse? Is U unitary?
Hint: What is the value of $UU^\dagger$ on $|0\rangle$?

a) If U is unitary, then $UU^\dagger = \mathbb{1}$, so $\langle\psi'|\psi'\rangle = \langle\psi|U^\dagger U|\psi\rangle = \langle\psi|\psi\rangle$ for all ψ. On the other hand, if U preserves the norm of all vectors, then you can use the polarization identity to win: An arbitrary inner product satisfies

$$\langle n|m\rangle = \frac{1}{4}(\langle n+m|n+m\rangle - \langle n-m|n-m\rangle),$$

so we see that inner products of the form $\langle n|UU^\dagger|m\rangle$ or $\langle n|U^\dagger U|m\rangle$ can always be expressed in terms of norms.

b) Note that the formula

$$\langle n|U^\dagger U|n\rangle = \langle n+1|n+1\rangle = 1 = \langle n|n\rangle$$

is true for any basis vector $|n\rangle$ (since they are normalized). Given an arbitrary vector $|\psi\rangle = \sum \psi_n |n\rangle$, we can use orthornormality of the $|n\rangle$ to conclude that

$$\langle\psi|U^\dagger U|\psi\rangle = \sum_{n,m} \psi_n^* \psi_m \langle n|U^\dagger U|m\rangle = \sum_{n,m} \psi_n^* \psi_m \langle n+1|m+1\rangle = \sum |\psi_n|^2 = \langle\psi|\psi\rangle .$$

Now, we want to show that $U^\dagger U = 1$. This follows from the definition of U. Indeed, the previous calculation shows that the diagonal matrix elements of $U^\dagger U$ are the same as the identity matrix, and we just need to check that the off-diagonal matrix elements vanish. Let's check:

$$\langle n|U^\dagger U|m\rangle = 0$$

if $n \neq m$ by the definition of U. Similarly, we could do the same for $UU^\dagger$: Consider

$$\langle m|U^\dagger|n\rangle .$$

By letting $U^\dagger$ act on $\langle m|$, we see that this is the same as

$$\langle m+1|n\rangle = \delta_{m+1,n},$$

so that if we write $U^\dagger|n\rangle$ in terms of the basis elements $|m\rangle$, we immediately see that

$$U^\dagger|n\rangle = |n-1\rangle .$$

In particular, that means $U^\dagger|0\rangle = 0$, so that $UU^\dagger = 1 - \langle 0|\,|0\rangle$, so U is not unitary!

Exercise 3. *Some More Unitary Operators.* Let H be a hermitian operator and $U = e^{iH}$.

a) Show that U is unitary. (Notice the analogy with scalars: If θ is real, then $e^{i\theta}$ has unit modulus.)

b) If U_1, U_2 are unitary operators, show that U_1U_2 is unitary. If U_1U_2 is unitary, does that imply that U_1 and U_2 are?

c) ***Challenge.*** Show that $\det(U) = e^{i\,\mathrm{tr}(H)}$.

a) Since H is hermitian, $(e^{iH})^\dagger = e^{-iH}$. Since H commutes with itself, this implies that $e^{iH}(e^{iH})^\dagger = (e^{iH})^\dagger e^{iH} = 1$.

b) We check

$$(U_1 U_2)^\dagger = U_2^\dagger U_1^\dagger,$$

so

$$(U_1 U_2)^\dagger U_1 U_2 = 1.$$

Similarly,

$$U_1 U_2 = (U_1 U_2)^\dagger = 1.$$

c) We diagonalize $H = VDV^\dagger$ with V unitary. Then

$$U = Ve^{iD}V^\dagger,$$

and

$$\det U = \det V \det(e^{iD}) \det(V^\dagger) = \det(e^{iD}).$$

But

$$e^{iD} = \mathrm{diag}(e^{id_1}, \ldots, e^{id_n}),$$

where $D = \mathrm{diag}(d_1, \ldots, d_n)$. This gives the result.