QM Homework Problems 1 – Solutions

1 This is an example of the fact that self-adjoint linear operators have orthogonal eigenvectors and real eigenvalues. The first main point is that there can be degeneracy, in which case two arbitrary eigenvectors with the same eigenvalue are not necessarily orthogonal. However, an orthogonal basis can always be chosen, though it is not unique. The second point is that in quantum mechanics we assume there is not a degenerate spectrum if we consider all compatible measurements. In this case you can easily check that $[\widehat{A}, \widehat{B}] = 0$ (at least on any linear combination of the states mentioned in the problem.) This means that we can find eigenvectors of both operators and (if the eigenvalues of $\widehat{B}$ are different) these eigenvectors will be orthogonal.

The problem is essentially to find which linear combinations of $|\alpha\rangle$ and $|\beta\rangle$ are eigenvectors of $\widehat{B}$. These will automatically also be eigenvectors of $\widehat{A}$ since any linear combination of $|\alpha\rangle$ and $|\beta\rangle$ is an eigenvector of $\widehat{A}$ with eigenvalue a. So consider an arbitrary state:

$$|\gamma\rangle = c_1|\alpha\rangle + c_2|\beta\rangle \ , \qquad c_1, c_2 \in \mathbf{C}$$

Since we know how $\widehat{B}$ acts on $|\alpha\rangle$ and $|\beta\rangle$, it is easy to show that:

$$\widehat{B}|\gamma\rangle = (2c_1 - 3c_2)|\alpha\rangle + (-3c_1 + 2c_2)|\beta\rangle$$

We want to find eigenvalues of $\widehat{B}$ so we want to find c_1 and c_2 so that:

$$\widehat{B}|\gamma\rangle = b|\gamma\rangle = bc_1|\alpha\rangle + bc_2|\beta\rangle$$

for some b. Since $|\alpha\rangle$ and $|\beta\rangle$ are independent we have an ordinary matrix eigenvalue problem:

$$\begin{pmatrix} 2 & -3 \\ -3 & 2 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = b \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

What we have really done here is to represent an arbitrary state $|\gamma\rangle$ by the column vector $\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$ and the operators $\widehat{A}$ and $\widehat{B}$ by the matrices $\begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix}$ and $\begin{pmatrix} 2 & -3 \\ -3 & 2 \end{pmatrix}$ acting on column vectors.

Simple linear algebra shows that there are two distinct eigenvalues, $b = -1$ and $b = 5$, with corresponding eigenvectors $\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = N_1 \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and

$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = N_2 \begin{pmatrix} 1 \\ -1 \end{pmatrix}$ where N_1 and N_2 are arbitrary complex normalisation constants.

This means that there are two independent simultaneous eigenstates of $\widehat{A}$ and $\widehat{B}$ which we can label by the eigenvalues as $|a, b\rangle$:

$$\begin{aligned} |a, -1\rangle &= N_1(|\alpha\rangle + |\beta\rangle) \\ |a, 5\rangle &= N_2(|\alpha\rangle - |\beta\rangle) \end{aligned}$$

It is easy to check that these eigenvectors are orthogonal (as they must be since they are eigenstates of $\widehat{B}$ with different eigenvalues)

$$\begin{aligned} \langle a, -1|a, 5\rangle &= N_1^* N_2(\langle\alpha| + \langle\beta|)(|\alpha\rangle - |\beta\rangle) \\ &= N_1^* N_2(\langle\alpha|\alpha\rangle - \langle\alpha|\beta\rangle + \langle\beta|\alpha\rangle - \langle\beta|\beta\rangle) \\ &= N_1^* N_2(1 - 0 + 0 - 1) = 0 \end{aligned}$$

Similarly we can calculate:

$$\begin{aligned} \langle a, -1|a, -1\rangle &= 2|N_1|^2 \\ \langle a, 5|a, 5\rangle &= 2|N_2|^2 \end{aligned}$$

so we can normalise the eigenvectors by choosing $N_1 = N_2 = 1/\sqrt{2}$. Note that we could multiply N_1 and N_2 by arbitrary phases $\exp(i\theta_1)$ and $\exp(i\theta_2)$ so even without degeneracy an orthonormal basis is not quite unique.

To see why this procedure is referred to as diagonalising the states with respect to these operators, consider how $\widehat{A}$ and $\widehat{B}$ act on an arbitrary state

$$|\psi\rangle = u|a, -1\rangle + v|a, 5\rangle\ , \qquad u, v \in \mathbf{C}$$

It is clear that:

$$\begin{aligned} \widehat{A}|\psi\rangle &= au|a, -1\rangle + av|a, 5\rangle \\ \widehat{B}|\psi\rangle &= -u|a, -1\rangle + 5v|a, 5\rangle \end{aligned}$$

Now, in this basis, we can represent $|\psi\rangle$ by the two-component column vector $\begin{pmatrix} u \\ v \end{pmatrix}$. Then we see that $\widehat{A}$ and $\widehat{B}$ are represented by two-by-two matrices M_A and M_B where:

$$M_A \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} au \\ av \end{pmatrix} = \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}$$

$$M_B \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} -u \\ 5v \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & 5 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}$$

So we see that in this basis the operators $\widehat{A}$ and $\widehat{B}$ can be represented by diagonal matrices. Note that operators can be represented by different matrices depending on how we choose to represent the states.

2(a) Recall that the adjoint of an operator is defined in terms of the inner product by:

$$\langle\alpha|\widehat{A}^\dagger|\beta\rangle = \langle\beta|\widehat{A}|\alpha\rangle^*$$

for all state vectors $|\alpha\rangle$ and $|\beta\rangle$.

In this case we represent $|\alpha\rangle$ and $|\beta\rangle$ by two-component column vectors $\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}$ and $\begin{pmatrix}\beta_1\\ \beta_2\end{pmatrix}$ where α_1, α_2, β_1 and β_2 are complex numbers. Then $\widehat{A}$ is represented by a two-by-two matrix M_A so that:

$$\begin{aligned}\langle\beta|\widehat{A}|\alpha\rangle^* &= \left(\begin{pmatrix}\beta_1^* & \beta_2^*\end{pmatrix} M_A \begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}\right)^* \\ &= \begin{pmatrix}\alpha_1^* & \alpha_2^*\end{pmatrix} M_A^\dagger \begin{pmatrix}\beta_1\\ \beta_2\end{pmatrix}\end{aligned}$$

So we see that the adjoint operator is represented by the Hermitian conjugate of the matrix M_A.

The definition of a self-adjoint operator is one which satisfies $\widehat{A}^\dagger = \widehat{A}$. So we just have to check which of the matrices is Hermitian.

$$\begin{aligned}\begin{pmatrix}1 & 3\\ 3 & 4\end{pmatrix}^\dagger &= \begin{pmatrix}1 & 3\\ 3 & 4\end{pmatrix} \\ \left(i\begin{pmatrix}1 & -1\\ 1 & 0\end{pmatrix}\right)^\dagger &= i^*\begin{pmatrix}1 & 1\\ -1 & 0\end{pmatrix} = i\begin{pmatrix}-1 & -1\\ 1 & 0\end{pmatrix} \\ \left(i\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\right)^\dagger &= i^*\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = i\begin{pmatrix}0 & -1\\ -1 & 0\end{pmatrix} \\ \begin{pmatrix}1 & -i\\ i & 1\end{pmatrix}^\dagger &= \begin{pmatrix}1 & i^*\\ (-i)^* & 1\end{pmatrix} = \begin{pmatrix}1 & -i\\ i & 1\end{pmatrix}\end{aligned}$$

So the first and last correspond to self-adjoint operators while the second and third do not.

(b) Consider two arbitrary states $|\psi_1\rangle$ and $|\psi_2\rangle$ represented by the functions $\psi_1(x)$ and $\psi_2(x)$. Now consider the operator $\widehat{A}$ represented by the differential operator acting on the functions. Then

$$\langle\psi_2|\widehat{A}|\psi_1\rangle = \int_{-\infty}^{\infty} \mathrm{d}x\psi_2^*(x)\frac{\mathrm{d}}{\mathrm{d}x}\psi_1(x)$$

Now we can integrate by parts so that the derivative acts on ψ_2. So the expression can be written as:

$$[\psi_2^*\psi_1]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \mathrm{d}x\psi_1(x)\frac{\mathrm{d}}{\mathrm{d}x}\psi_2^*(x) = -\int_{-\infty}^{\infty} \mathrm{d}x\psi_1(x)\frac{\mathrm{d}}{\mathrm{d}x}\psi_2^*(x)$$

where we have used the boundary conditions that all allowed functions must vanish as $|x| \to \infty$[1]. Taking the complex conjugate gives us the definition of the adjoint operator:

$$\langle\psi_1|\widehat{A}^\dagger|\psi_2\rangle \;= -\int_{-\infty}^{\infty} \mathrm{d}x\psi_1^*(x)\frac{\mathrm{d}}{\mathrm{d}x}\psi_2(x)$$

So we have the result that:

$$\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^\dagger = -\frac{\mathrm{d}}{\mathrm{d}x}$$

So $\frac{\mathrm{d}}{\mathrm{d}x}$ is not a self-adjoint operator (in fact we may call it anti-self-adjoint because of the minus sign.)

We just follow the same procedure for the other operators. In the case of $\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ we have to integrate by parts twice so we get two minus signs and so this operator is self-adjoint.

In the case of $ix\frac{\mathrm{d}}{\mathrm{d}x}$ when we integrate by parts the derivative also acts on the x and so this is not a self-adjoint operator.

The operator x is self-adjoint since it is real and we can equally consider it multiplying ψ_1 or ψ_2 (we don't need to integrate by parts!)

Finally the operator $i\frac{\mathrm{d}}{\mathrm{d}x}$ is self-adjoint because we get a minus sign from integrating by parts but another minus sign from complex conjugating i.

Note that once we know the adjoint of the operators x and $\frac{\mathrm{d}}{\mathrm{d}x}$ we can calculate the adjoint of any combination of these operators. For example:

$$\left(ix\frac{\mathrm{d}}{\mathrm{d}x}\right)^\dagger = \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^\dagger x^\dagger i^* = i\frac{\mathrm{d}}{\mathrm{d}x}x$$

There are two important points to note here. The first is that this is not a self-adjoint operator because $x\frac{\mathrm{d}}{\mathrm{d}x}$ is not the same as $\frac{\mathrm{d}}{\mathrm{d}x}x$. The second more subtle point is that we must be very careful when writing something like $\frac{\mathrm{d}}{\mathrm{d}x}x$. The point is that we must remember that this is an operator and so it must be considered to act on something, in this case a complex function of x. In particular $\frac{\mathrm{d}}{\mathrm{d}x}x$ *is not* 1! In fact it is $1 + x\frac{\mathrm{d}}{\mathrm{d}x}$ as we can see by carefully considering the meaning of the operator by its action on an arbitrary function $\psi(x)$:

$$\frac{\mathrm{d}}{\mathrm{d}x}x\psi(x) = \frac{\mathrm{d}}{\mathrm{d}x}\left(x\psi(x)\right) = \psi(x) + x\frac{\mathrm{d}}{\mathrm{d}x}\psi(x) = \left(1 + x\frac{\mathrm{d}}{\mathrm{d}x}\right)\psi(x)$$

[1] Note that these boundary conditions are actually a consequence of requiring the integrals to be well-defined (not divergent.) In particular normalisable wavefunctions must vanish as $|x| \to \infty$ faster than $1/|x|^{1/2}$ so that $\int_{-\infty}^{\infty} \mathrm{d}x\psi^*(x)\psi(x)$ is finite. As we will see in specific examples later in the course the wavefunctions typically vanish exponentially and so $x^m\psi(x)$ vanishes at infinity for any m.

The thing to remember is that when considering differential operators, they act on everything to the right, including the arbitrary function which is implicitly assumed to be there (but usually not explicitly written.)

(c) Keeping in mind the comments at the end of the last part we can easily evaluate these commutators as follows:

$$[i\frac{\mathrm{d}}{\mathrm{d}x}, x]\psi(x) = i\frac{\mathrm{d}}{\mathrm{d}x}(x\psi(x)) - ix\frac{\mathrm{d}}{\mathrm{d}x}\psi(x) = i\psi(x)$$

Since this holds for an arbitrary function $\psi(x)$ the following operator expression is true:

$$[i\frac{\mathrm{d}}{\mathrm{d}x}, x] = i$$

Note the similarity with the commutation relation for position and momentum. It is easy to see that if we represent the position operator $\widehat{x}$ by x then we should represent the momentum operator $\widehat{p}$ by $-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}$.

Similarly we can calculate the other commutator where we will now only implicitly consider an arbitrary function $\psi(x)$:

$$[\frac{\mathrm{d}^2}{\mathrm{d}x^2}, x] = \frac{\mathrm{d}^2}{\mathrm{d}x^2}x - x\frac{\mathrm{d}^2}{\mathrm{d}x^2} = \frac{\mathrm{d}}{\mathrm{d}x} + \frac{\mathrm{d}}{\mathrm{d}x}x\frac{\mathrm{d}}{\mathrm{d}x} - x\frac{\mathrm{d}^2}{\mathrm{d}x^2} = \frac{\mathrm{d}}{\mathrm{d}x} + \frac{\mathrm{d}}{\mathrm{d}x} + x\frac{\mathrm{d}^2}{\mathrm{d}x^2} - x\frac{\mathrm{d}^2}{\mathrm{d}x^2} = 2\frac{\mathrm{d}}{\mathrm{d}x}$$

If that is not clear then write it out with the operators explicitly acting on an arbitrary function $\psi(x)$.