Chem221a : Solution Set 4

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Problem 1

First, we're going to want to figure out how to write a matrix representation of $\hat{\mathbf{S}} \cdot \hat{\mathbf{n}}$. We'll start by writing out the unit vector $\hat{\mathbf{n}}$ in terms of the angles α and β (just using basic trig and/or definitions of spherical coordinates, however you want to think of it):

$$\hat{\mathbf{n}} = \begin{pmatrix} \cos(\alpha)\sin(\beta) \\ \sin(\alpha)\sin(\beta) \\ \cos(\beta) \end{pmatrix} \tag{1}$$

The operator $\hat{\mathbf{S}}$ is actually a vector of operators, with the $\hat{S}_i$ spin operator in the ith direction. So we can write it as

$$\hat{\mathbf{S}} = \begin{pmatrix} \hat{S}_x \\ \hat{S}_y \\ \hat{S}_z \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix} \tag{2}$$

where the σ_i are the Pauli spin matrices. Note that this is a vector of matrices. When we take the dot product of the $\hat{\mathbf{n}}$ vector (a vector of numbers) with this vector of matrices, we'll end up with a matrix. We'll cheat a little here and use an "implicit" arbitrary state (that is, not show it).

$$\begin{aligned}
\hat{\mathbf{S}} \cdot \hat{\mathbf{n}} &= \frac{\hbar}{2} \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix} \cdot \begin{pmatrix} \cos(\alpha)\sin(\beta) \\ \sin(\alpha)\sin(\beta) \\ \cos(\beta) \end{pmatrix} && (3) \\
&= \frac{\hbar}{2} \left(\cos(\alpha)\sin(\beta)\sigma_x + \sin(\alpha)\sin(\beta)\sigma_y + \cos(\beta)\sigma_z \right) && (4) \\
&= \frac{\hbar}{2} \left(\cos(\alpha)\sin(\beta) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \sin(\alpha)\sin(\beta) \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \cos(\beta) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) && (5) \\
&= \frac{\hbar}{2} \begin{pmatrix} \cos(\beta) & \sin(\beta)(\cos(\alpha) - i\sin(\alpha)) \\ \sin(\beta)(\cos(\alpha) + i\sin(\alpha)) & -\cos(\beta) \end{pmatrix} && (6) \\
&= \frac{\hbar}{2} \begin{pmatrix} \cos(\beta) & \sin(\beta)e^{-i\alpha} \\ \sin(\beta)e^{i\alpha} & -\cos(\beta) \end{pmatrix} && (7)
\end{aligned}$$

We have used the $|\pm\rangle$ basis to represent the spin operator matrices.

Now that we have found a matrix representation of the operator we're interested in, we need to find the representation of the eigenvector associated with the eigenvalue $+\hbar/2$. Let's choose to represent that eigenvector as $\left(\begin{smallmatrix} c_+ \\ c_- \end{smallmatrix}\right)$ in the $|\pm\rangle$ basis.

Dividing both sides of the eigenequation by $\hbar/2$, we obtain

$$\begin{pmatrix} \cos(\beta) - 1 & e^{-i\alpha}\sin(\beta) \\ e^{i\alpha}\sin(\beta) & -(\cos(\beta) + 1) \end{pmatrix} \begin{pmatrix} c_+ \\ c_- \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{8}$$

From the first line of that matrix equation, we obtain

$$0 = c_+(\cos(\beta) - 1) + c_- e^{-i\alpha}\sin(\beta) \tag{9}$$

$$c_- = -\frac{\cos(\beta) - 1}{\sin(\beta)} e^{i\alpha} c_+ \tag{10}$$

This means that we can represent the state with the vector

$$\left|\hat{\mathbf{S}} \cdot \hat{\mathbf{n}}\right\rangle = \begin{pmatrix} A \\ A\frac{1-\cos(\beta)}{\sin(\beta)} e^{i\alpha} \end{pmatrix} \tag{11}$$

where A can be determined by the normalization condition:

$$1 = |A|^2 + \left| A\frac{1 - \cos(\beta)}{\sin(\beta)} e^{i\alpha} \right|^2 \tag{12}$$

$$= A^2 \left(1 + \left(\frac{1 - \cos(\beta)}{\sin(\beta)} \right)^2 \right) \tag{13}$$

$$\frac{1}{A^2} = \frac{\sin^2(\beta) + 1 + \cos^2(\beta) - 2\cos(\beta)}{\sin^2(\beta)} \tag{14}$$

$$A^2 = \frac{1}{2} \frac{\sin^2(\beta)}{1 - \cos(\beta)} \tag{15}$$

$$= \frac{1}{2} \frac{\sin^2(\beta)(1 + \cos(\beta))}{(1 - \cos(\beta))(1 + \cos(\beta))} \tag{16}$$

$$= \frac{1}{2} \frac{\sin^2(\beta)(1 + \cos(\beta))}{1 - \cos^2(\beta)} \tag{17}$$

$$= \frac{1}{2}(1 + \cos(\beta)) \tag{18}$$

$$= \cos^2\left(\frac{\beta}{2}\right) \tag{19}$$

$$A = \cos\left(\frac{\beta}{2}\right) \tag{20}$$

We chose A to be real, and the rest was just trig. Now our state vector can be represented as

$$\left|\hat{\mathbf{S}}\cdot\hat{\mathbf{n}}\right\rangle = \begin{pmatrix} \cos\left(\frac{\beta}{2}\right) \\ \cos\left(\frac{\beta}{2}\right)\frac{1-\cos(\beta)}{\sin(\beta)}e^{i\alpha} \end{pmatrix} \tag{21}$$

$$= \begin{pmatrix} \cos\left(\frac{\beta}{2}\right) \\ \cos\left(\frac{\beta}{2}\right)\frac{(1-\cos(\beta))(1+\cos(\beta))}{\sin(\beta)(1+\cos(\beta))}e^{i\alpha} \end{pmatrix} \tag{22}$$

$$= \begin{pmatrix} \cos\left(\frac{\beta}{2}\right) \\ \cos\left(\frac{\beta}{2}\right)\frac{\sin^2(\beta)}{\sin(\beta)(2\cos^2(\beta/2))}e^{i\alpha} \end{pmatrix} \tag{23}$$

$$= \begin{pmatrix} \cos\left(\frac{\beta}{2}\right) \\ \frac{\sin(\beta)}{2\cos(\beta/2)}e^{i\alpha} \end{pmatrix} \tag{24}$$

$$= \begin{pmatrix} \cos\left(\frac{\beta}{2}\right) \\ \frac{2\sin(\beta/2)\cos(\beta/2)}{2\cos(\beta/2)}e^{i\alpha} \end{pmatrix} \tag{25}$$

$$= \begin{pmatrix} \cos\left(\frac{\beta}{2}\right) \\ \sin\left(\frac{\beta}{2}\right)e^{i\alpha} \end{pmatrix} \tag{26}$$

$$\tag{27}$$

Written in terms of kets (and therefore independent of representation) that becomes

$$\left|\hat{\mathbf{S}}\cdot\hat{\mathbf{n}}\right\rangle = \cos\left(\frac{\beta}{2}\right)\left|+\right\rangle + \sin\left(\frac{\beta}{2}\right)e^{i\alpha}\left|-\right\rangle \tag{28}$$

Problem 2

This problem requires us to calculate probabilities and expectation values, which are only defined with respect to a given state. So the first thing we need to do is define our state. Taking the eigenvector solution from the previous problem and setting $\alpha = 0$, we find ourselves with the state vector

$$\left|\psi\right\rangle = \cos\left(\frac{\beta}{2}\right)\left|+\right\rangle + \sin\left(\frac{\beta}{2}\right)\left|-\right\rangle \tag{29}$$

(a) The probability of measuring a value of $+\frac{\hbar}{2}$ for S_x is given by the modulus square of the overlap of the $|S_x;+\rangle$ state (the state to be measured) with our state, $|\psi\rangle$:

$$P\left(S_x = +\frac{\hbar}{2}\right) = |\langle S_x;+|\psi\rangle|^2 \tag{30}$$
$$= \left|\left(\frac{1}{\sqrt{2}}\langle +| + \frac{1}{\sqrt{2}}\langle -|\right)\left(\cos\left(\frac{\beta}{2}\right)|+\rangle + \sin\left(\frac{\beta}{2}\right)|-\rangle\right)\right|^2 \tag{31}$$
$$= \left|\frac{1}{\sqrt{2}}\cos\left(\frac{\beta}{2}\right) + \frac{1}{\sqrt{2}}\sin\left(\frac{\beta}{2}\right)\right|^2 \tag{32}$$
$$= \frac{1}{2}\left|\cos^2\left(\frac{\beta}{2}\right) + \sin^2\left(\frac{\beta}{2}\right) + 2\cos\left(\frac{\beta}{2}\right)\sin\left(\frac{\beta}{2}\right)\right| \tag{33}$$
$$= \frac{1}{2}\left|1+\sin(\beta)\right| \tag{34}$$
$$= \frac{1}{2}\left(1+\sin(\beta)\right) \tag{35}$$

We can drop the absolute value sign at the end because the sine function can't be less than 1.

(b) As a quick reminder, let me show you how ***

$$\left\langle (\Delta S_x)^2 \right\rangle = \left\langle (S_x - \langle S_x\rangle)^2 \right\rangle \tag{36}$$
$$= \left\langle S_x^2 - 2S_x\langle S_x\rangle + \langle S_x\rangle^2 \right\rangle \tag{37}$$
$$= \left\langle S_x^2 \right\rangle - 2\langle S_x\rangle\langle S_x\rangle + \langle S_x\rangle^2 \tag{38}$$
$$= \left\langle S_x^2 \right\rangle - \langle S_x\rangle^2 \tag{39}$$

So we need to calculate $\langle S_x\rangle$ and $\left\langle S_x^2\right\rangle$. Remember that expectation values are determined for a specific state — in our case, we defined the state $|\psi\rangle$ above. So let's calculate these expectation values:

$$\langle S_x\rangle = \langle\psi|S_x|\psi\rangle \tag{40}$$
$$= \begin{pmatrix}\cos(\beta/2) & \sin(\beta/2)\end{pmatrix}\begin{pmatrix}0 & \hbar/2\\ \hbar/2 & 0\end{pmatrix}\begin{pmatrix}\cos(\beta/2)\\ \sin(\beta/2)\end{pmatrix} \tag{41}$$
$$= \hbar\cos\left(\frac{\beta}{2}\right)\sin\left(\frac{\beta}{2}\right) \tag{42}$$

Now for the other calculation:

$$\left\langle S_x^2\right\rangle = \left\langle\psi|S_x^2|\psi\right\rangle \tag{43}$$
$$= \begin{pmatrix}\cos(\beta/2) & \sin(\beta/2)\end{pmatrix}\begin{pmatrix}\hbar^2/4 & 0\\ 0 & \hbar^2/4\end{pmatrix}\begin{pmatrix}\cos(\beta/2)\\ \sin(\beta/2)\end{pmatrix} \tag{44}$$
$$= \frac{\hbar^2}{4}\left(\cos^2\left(\frac{\beta}{2}\right) + \sin^2\left(\frac{\beta}{2}\right)\right) \tag{45}$$
$$= \frac{\hbar^2}{4} \tag{46}$$

Putting these two results together, we find

$$\left\langle (\Delta S_x)^2 \right\rangle = \left\langle S_x^2 \right\rangle - \left\langle S_x \right\rangle^2 \tag{47}$$
$$= \hbar^2 \left(\frac{1}{4} - \sin^2\left(\frac{\beta}{2}\right) \cos^2\left(\frac{\beta}{2}\right) \right) \tag{48}$$
$$= \frac{\hbar^2}{4} \left(1 - \sin^2\left(\frac{\beta}{2}\right) \cos^2\left(\frac{\beta}{2}\right) \right) \tag{49}$$
$$= \frac{\hbar^2}{4} \left(\sin^2\left(\frac{\beta}{2}\right) + \cos^2\left(\frac{\beta}{2}\right) - 4\sin^2\left(\frac{\beta}{2}\right) \right) \tag{50}$$
$$= \frac{\hbar^2}{4} \left(\sin^2\left(\frac{\beta}{2}\right) \left(1 - \cos^2\left(\frac{\beta}{2}\right)\right) + \cos^2\left(\frac{\beta}{2}\right) \left(1 - \sin^2\left(\frac{\beta}{2}\right)\right) \right.$$
$$\left. -2\sin^2\left(\frac{\beta}{2}\right) \cos^2\left(\frac{\beta}{2}\right) \right) \tag{51}$$
$$= \frac{\hbar^2}{4} \left(\sin^4\left(\frac{\beta}{2}\right) + \cos^4\left(\frac{\beta}{2}\right) - 2\cos^2\left(\frac{\beta}{2}\right) \sin^2\left(\frac{\beta}{2}\right) \right) \tag{52}$$
$$= \frac{\hbar^2}{4} \left(\cos^2\left(\frac{\beta}{2}\right) - \sin^2\left(\frac{\beta}{2}\right) \right)^2 \tag{53}$$
$$= \frac{\hbar^2}{4} \cos^2(\beta) \tag{54}$$

Let's check all of these things for the special cases suggested. ***

$\beta = 0$: When $\beta = 0$, we know that $\mathbf{S} \cdot \hat{\mathbf{n}} = S_z$, which means that $|\mathbf{S} \cdot \hat{\mathbf{n}}\rangle = |+\rangle$. We know that for $|+\rangle$, we have 50% probability of measuring S_x as $+\hbar/2$ and that the dispersion in S_x is $\frac{\hbar^2}{4}$. Both of these are confirmed by plugging $\beta = 0$ into our equations.

$\beta = \pi/2$: When $\beta = \pi/2$, $\mathbf{S} \cdot \hat{\mathbf{n}} = S_x$, so $|\mathbf{S} \cdot \hat{\mathbf{n}}; +\rangle = |S_x; +\rangle$. In this state, we have 100% probability of measuring S_x as $+\hbar/2$, and therefore the dispersion in S_x is 0. Of course, this matches the general equations we derived when $\beta = \pi/2$.

$\beta = \pi$: Finally, when $\beta = \pi$, our ket $|\mathbf{S} \cdot \hat{\mathbf{n}}\rangle = |-\rangle$. As with the first of these special cases, the probability is 50%, and the dispersion is $\frac{hbar^2}{4}$. Again, this matches our results.

Problem 3

The transformation matrix which connects the S_z diagonal basis to the S_x diagonal basis is the matrix P which takes any vector α_z represented in the S_z basis and gives its representation α_x in the S_x basis.

As an example, we know that the vector represented as $\frac{1}{\sqrt{2}} \left(\begin{smallmatrix} 1 \\ 1 \end{smallmatrix}\right)$ in the S_z basis is represented as $\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)$ in the S_x basis. This means that we have the equation

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = P \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \tag{55}$$

For the other eigenvector of S_x, we similarly obtain the equation

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} = P \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} \tag{56}$$

From these two equations, we can determine the elements of the matrix P:

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \tag{57}$$

This matrix equation is equivalent to the equations:

$$\sqrt{2} = P_{11} + P_{12} \tag{58}$$

$$P_{21} = -P_{22} \tag{59}$$

Similarly, we use the other matrix equation to give us

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} \tag{60}$$

$$P_{11} = P_{12} \tag{61}$$

$$\sqrt{2} = P_{21} - P_{22} \tag{62}$$

Putting equations (58) and (61) together, we find

$$P_{11} = P_{12} = \frac{1}{\sqrt{2}} \tag{63}$$

Similarly, we can put equations (59) and (62) together to obtain

$$P_{21} = \frac{1}{\sqrt{2}} \tag{64}$$

$$P_{22} = -\frac{1}{\sqrt{2}} \tag{65}$$

Putting all of this together, we end up with the transformation matrix P:

$$P = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \tag{66}$$

To check that this is correct, let's check what happens when we try to diagonalize the S_x matrix. The first step in that check it to find the inverse of the matrix P. However, P is both unitary and Hermitian, which means that it is its own inverse (which you can easily verify by finding P^2). So the diagonalization follows:

$$D = P^{-1} S_x P \tag{67}$$

$$= \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 0 & \hbar/2 \\ \hbar/2 & 0 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \tag{68}$$

$$= \begin{pmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{pmatrix} \tag{69}$$

Finally, let's show how this relates to the expression $\sum_r \left|b^{(r)}\right\rangle \left\langle a^{(r)}\right|$. This general expression for a change of basis connects eigenstates in the initial basis, $\{\left|a^{(r)}\right\rangle\}$, to the kets of the same eigenvalue in the new basis, $\{\left|b^{(r)}\right\rangle\}$. So, writing this for the specific case we're examining:

$$U = \sum_r \left|a^{(r)}\right\rangle \left\langle b^{(r)}\right| \tag{70}$$

$$= |S_x;+\rangle \langle +| + |S_x;-\rangle \langle -| \tag{71}$$

To see how this compares to our matrix representation, let's operate this on an arbitrary ket $|\psi\rangle = c_+ |+\rangle + c_- |-\rangle$:

$$U|\psi\rangle = (|S_x;+\rangle \langle +| + |S_x;-\rangle \langle -|)\,(|\psi\rangle = c_+ |+\rangle + c_- |-\rangle) \tag{72}$$

$$= c_+ |S_x;+\rangle + c_- |S_x;-\rangle \tag{73}$$

We know how to represent the kets $|S_x;\pm\rangle$ in the $|\pm\rangle$ basis:

$$U|\psi\rangle = \frac{1}{\sqrt{2}} \left(c_+ \left(|+\rangle + |-\rangle\right) + c_- \left(|+\rangle - |-\rangle\right)\right) \tag{74}$$

$$= \frac{1}{\sqrt{2}} \left((c_+ + c_-)\,|+\rangle + (c_+ - c_-)\,|-\rangle\right) \tag{75}$$

Now the equivalent process using our matrix representation:

$$U|\psi\rangle = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \begin{pmatrix} c_+ \\ c_- \end{pmatrix} \tag{76}$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} c_+ + c_- \\ c_+ - c_- \end{pmatrix} \tag{77}$$

And that's the same thing!

Problem 4

(a) This is relatively straightforward once we put this into bra-ket notation:

$$\sum_{i=1}^{\infty} \psi_i^*(x)\psi_i(x') = \sum_{i=1}^{\infty} \langle \psi_i | x \rangle \langle x' | \psi_i \rangle \tag{78}$$

$$= \sum_{i=1}^{\infty} \langle x' | \psi_i \rangle \langle \psi_i | x \rangle \tag{79}$$

$$= \langle x' | \left(\sum_{i=1}^{\infty} |\psi_i\rangle \langle \psi_i| \right) |x\rangle \tag{80}$$

$$= \langle x' | x \rangle \tag{81}$$

$$= \delta(x - x') \tag{82}$$

(b) Running through these Shankar exercises:

(i) 1.10.1

First, let's show where the absolute value comes from. Remember that the Dirac delta function is even. So if $a < 0$, we have $\delta(ax) = \delta(-|a|\,x) = \delta(|a|\,x)$. If $a > 0$, we obviously have $\delta(ax) = \delta(|a|\,x)$.

Now let's use the hint. We'll define $u = |a|\,x$, so we have

$$\int \mathrm{d}u\,\delta(u) = \int \mathrm{d}|a|\,x\,\delta(|a|\,x) \tag{83}$$

$$= |a| \int \mathrm{d}x\,\delta(|a|\,x) \tag{84}$$

$$\int \mathrm{d}u\,\delta(u)/\,|a| = \int \mathrm{d}x\,\delta(|a|\,x) \tag{85}$$

Once we integrate over u, the name of the variable doesn't really matter. So we'll rename it x.

$$\int \mathrm{d}x\,\delta(x)/\,|a| = \int \mathrm{d}x\,\delta(ax) \tag{86}$$

So $\delta(x)/\,|a| = \delta(ax)$.

(ii) 1.10.2

For this one, we'll basically just have to expand the function as a Taylor series, and use the result from the previous problem. When the argument to a delta function has multiple zeros $\{x_i\}$, we can think of it as being nonzero when $x = x_1$ or x_2 or $\ldots$. This is the same as what we'd get if we said the delta function was the sum of delta function from the contribution at $x_1, x_2, \ldots$. Therefore, we sum over all the possible roots, and then take the Taylor series expansion around each one of these roots:

$$\delta(f(x)) \approx \sum_i \delta\left(f(x_i) + \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x=x_i}(x - x_i)\right) \tag{87}$$

$$= \sum_i \delta\left(0 + \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x=x_i}(x - x_i)\right) \tag{88}$$

$$= \sum_i \delta(x - x_i)\left(\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x=x_i}\right)^{-1} \tag{89}$$

(iii) 1.10.3

There are a number of ways of looking at this problem. The one I would suggest is to say that if the Dirac delta function is the derivative of the theta (or Heaviside)[1] function, then the Heaviside function is the antiderivative of the Dirac delta function. So we write

$$\theta(x - x') = \int_{-\infty}^{x} \mathrm{d}x\,\delta(x - x') \tag{90}$$

[1] A number of you referred to this as the "Heavyside" function. This is incorrect. The name is not because it is "heavy on one side" or something like that. It is named for the much underappreciated English physicist (and arguably mathematician) Oliver Heaviside. Give the poor fellow credit, since he really doesn't get as much as he deserves.

Now, let's consider what the antiderivative of the Dirac delta function will look like. For any value less than x', the Dirac delta is zero, and so the Heaviside function is zero up to that point. But one the integral has passed through the value of x' (i.e., $x > x'$) the Dirac delta takes on the value of the function multiplying it at the value x'. In this case, the function multiplying it just 1, which has a value of 1 at x' (and everywhere else). So for $x > x'$ the integral becomes 1, and we see that this satisfies the definition of the Heaviside function.

What happens when $x = x'$? Good question. Let's not go there.

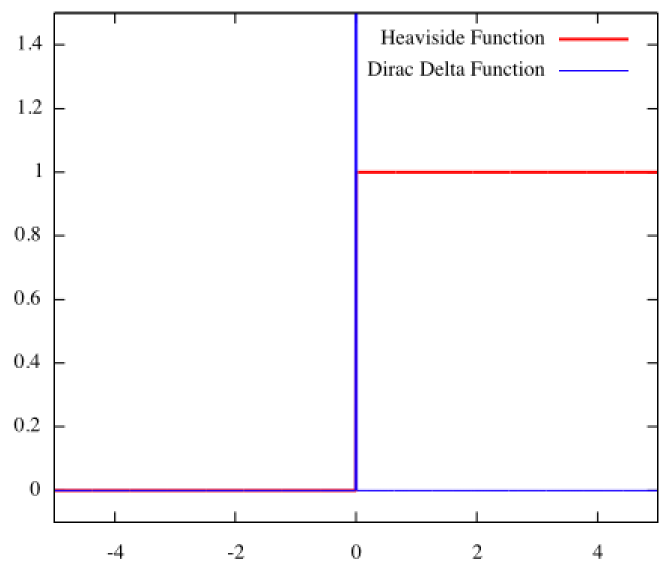

Figure 1: Plots of the Dirac delta function and the Heaviside function.

Problem 5

Although this problem isn't enumerated as a multipart problem, I'll break it down into two subsections: one where we only use the definition of $\langle x|p\rangle$ and one where we only use the fact that the operator $\hat{p}$ acts as $\frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}$ in the $\{|x\rangle\}$-representation.

(a) First, we forget what we know about the representations of operators. We'll just use the completeness relation along with the definition of $\langle x|p\rangle$ and the definition of eigenvalues. Within this, there are (at least) three ways of doing this; I'll only show one for the first expression, but I'll show all three for the second.

(i)

$$\langle x'|\hat{x}\hat{p}|\psi\rangle = x' \langle x'|\hat{p}|\psi\rangle \tag{91}$$
$$= x' \int_{\mathbb{R}} \mathrm{d}p \, \langle x'|p\rangle \langle p|\hat{p}|\psi\rangle \tag{92}$$
$$= x' \int_{\mathbb{R}} \mathrm{d}p \, p \, \langle x'|p\rangle \langle p|\psi\rangle \tag{93}$$
$$= x' \int_{\mathbb{R}} \mathrm{d}p \, p \frac{1}{\sqrt{2\pi\hbar}} e^{ipx'/\hbar} \langle p|\psi\rangle \tag{94}$$

Now we use the fact that $e^{ipx'/\hbar} \langle p|\psi\rangle = \frac{\mathrm{d}}{\mathrm{d}x'} \left(\frac{\hbar}{ip} e^{ipx'/\hbar} \langle p|\psi\rangle \right)$. That gives us

$$\langle x'|\hat{x}\hat{p}|\psi\rangle = x' \int_{\mathbb{R}} \mathrm{d}p \, \frac{\mathrm{d}}{\mathrm{d}x'} p \frac{\hbar}{ip} \frac{1}{\sqrt{2\pi\hbar}} e^{ipx'/\hbar} \langle p|\psi\rangle \tag{95}$$
$$= x' \frac{\mathrm{d}}{\mathrm{d}x'} \int_{\mathbb{R}} \mathrm{d}p \, \frac{\hbar}{i} \frac{1}{\sqrt{2\pi\hbar}} \langle p|\psi\rangle \tag{96}$$
$$= x' \frac{\mathrm{d}}{\mathrm{d}x'} \frac{\hbar}{i} \int_{\mathbb{R}} \mathrm{d}p \, \langle x'|p\rangle \langle p|\psi\rangle \tag{97}$$
$$= x' \frac{\mathrm{d}}{\mathrm{d}x'} \frac{\hbar}{i} \langle x'|\psi\rangle \tag{98}$$
$$= x' \frac{\hbar}{i} \frac{\mathrm{d}}{\mathrm{d}x'} \psi(x') \tag{99}$$

(ii) *First method.* The first way to do this is essentially the same as what we did above. To be honest, I find this a little sketchy, but I think it's okay. The others methods are definitely safe.

$$\langle x'|\hat{p}\hat{x}|\psi\rangle = \int_{\mathbb{R}} \mathrm{d}p \, \langle x'|\hat{p}|p\rangle \langle p|\hat{x}|\psi\rangle \tag{100}$$
$$= \int_{\mathbb{R}} \mathrm{d}p \, p e^{ix'p/\hbar} \langle p|\hat{x}|\psi\rangle \tag{101}$$
$$= \int_{\mathbb{R}} \mathrm{d}p \, p \frac{\mathrm{d}}{\mathrm{d}x'} \left(\frac{\hbar}{ip} e^{ix'p/\hbar} \langle p|\hat{x}|\psi\rangle \right) \tag{102}$$
$$= \frac{\hbar}{i} \frac{\mathrm{d}}{\mathrm{d}x'} \int_{\mathbb{R}} \mathrm{d}p \, \langle x'|p\rangle \langle p|\hat{x}|\psi\rangle \tag{103}$$
$$= \frac{\hbar}{i} \frac{\mathrm{d}}{\mathrm{d}x'} (\langle x'|\hat{x}|\psi\rangle) \tag{104}$$
$$= \frac{\hbar}{i} \frac{\mathrm{d}}{\mathrm{d}x'} (x'\psi(x')) \tag{105}$$
$$= \frac{\hbar}{i} \left(\psi(x') + x' \frac{\mathrm{d}}{\mathrm{d}x'} \psi(x') \right) \tag{106}$$

Second method. The next way to solve this is very similar to the above, but makes use of the derivative of the delta function.

$$\langle x'|\hat{p}\hat{x}|\psi\rangle = \int_{\mathbb{R}} \mathrm{d}p \int_{\mathbb{R}} \mathrm{d}x \, \langle x'|\hat{p}|p\rangle \langle p|\hat{x}|x\rangle \langle x|\psi\rangle \tag{107}$$

$$= \int_{\mathbb{R}} \mathrm{d}p \, p \int_{\mathbb{R}} \mathrm{d}x \, x \, \langle x'|p\rangle \langle p|x\rangle \langle x|\psi\rangle \tag{108}$$

$$= \int_{\mathbb{R}} \mathrm{d}p \, p \int_{\mathbb{R}} \mathrm{d}x \, x \frac{1}{\sqrt{2\pi\hbar}} e^{ipx'/\hbar} \langle p|x\rangle \langle x|\psi\rangle \tag{109}$$

$$= \int_{\mathbb{R}} \mathrm{d}p \, p \int_{\mathbb{R}} \mathrm{d}x \, x \frac{\mathrm{d}}{\mathrm{d}x'} \left(\frac{1}{\sqrt{2\pi\hbar}} \frac{\hbar}{ip} e^{ipx'/\hbar} \langle p|x\rangle \langle x|\psi\rangle \right) \tag{110}$$

$$= \frac{\hbar}{i} \int_{\mathbb{R}} \mathrm{d}p \int_{\mathbb{R}} \mathrm{d}x \, x \frac{\mathrm{d}}{\mathrm{d}x'} \left(\langle x'|p\rangle \langle p|x\rangle \langle x|\psi\rangle \right) \tag{111}$$

$$= \frac{\hbar}{i} \int_{\mathbb{R}} \mathrm{d}x \, x \frac{\mathrm{d}}{\mathrm{d}x'} \langle x'|x\rangle \langle x|\psi\rangle \tag{112}$$

$$= \frac{\hbar}{i} \int_{\mathbb{R}} \mathrm{d}x \, \frac{\mathrm{d}}{\mathrm{d}x'} \delta(x'-x) x \psi(x) \tag{113}$$

Now we'll use another fact which Prof. Neumark gave us regarding delta functions: $\int \mathrm{d}x \, \frac{\mathrm{d}}{\mathrm{d}x'} \delta(x'-x) f(x) = f'(x')$. Identifying $f(x) = x\psi(x)$, this gives us

$$\langle x'|\hat{p}\hat{x}|\psi\rangle = \frac{\hbar}{i} \left(\psi(x') + x' \frac{\mathrm{d}}{\mathrm{d}x'} \psi(x') \right) \tag{114}$$

Third method. The last way I'll show to solve this uses integration by parts. This is a more general method that can be more widely applied, but takes a little more thinking for this specific problem.

$$\langle x'|\hat{p}\hat{x}|\psi\rangle = \int_{\mathbb{R}} \mathrm{d}p \, p \int_{\mathbb{R}} \mathrm{d}x \, x \, \langle x'|p\rangle \langle p|x\rangle \langle x|\psi\rangle \tag{115}$$

$$= \int_{\mathbb{R}} \mathrm{d}p \, p \int_{\mathbb{R}} \mathrm{d}x \, x \frac{1}{2\pi\hbar} e^{ipx'/\hbar} e^{-ipx/\hbar} \psi(x) \tag{116}$$

$$= \frac{1}{2\pi\hbar} \int_{\mathbb{R}} \mathrm{d}p \, p e^{ipx'/\hbar} \int_{\mathbb{R}} \mathrm{d}x \, x e^{-ipx/\hbar} \psi(x) \tag{117}$$

Now we do the integral over x by parts. The formula for integration by parts is

$$\int_a^b \mathrm{d}x \, u(x) v'(x) = u(x)v(x)\big|_a^b - \int_a^b \mathrm{d}x \, u'(x) v(x) \tag{118}$$

For this particular integral, we choose $u(x) = x\psi(x)$ and $v'(x) = e^{-ipx\hbar}$. That means that $u'(x) = x\psi'(x) + \psi(x)$ and that $v(x) = \frac{-\hbar}{ip} e^{-ipx/\hbar}$. One of the tricks is that the wavefunction is assumed to be bound — so the $u(x)v(x)$ term goes to zero at $\pm\infty$.[2] This

[2] Technically ***

gives us

$$\langle x'|\hat{p}\hat{x}|\psi\rangle = \frac{1}{2\pi\hbar}\int_{\mathbb{R}} \mathrm{d}p\, p e^{ipx'/\hbar}\left(0 - \int_{\mathbb{R}} \mathrm{d}x\, \frac{-\hbar}{ip} e^{-ipx/\hbar}\left(x\psi'(x) + \psi(x)\right)\right) \tag{119}$$

$$= \frac{1}{2\pi\hbar}\frac{\hbar}{i}\int_{\mathbb{R}} \mathrm{d}p \int_{\mathbb{R}} \mathrm{d}x\, e^{ipx'/\hbar} e^{-ipx/\hbar}\left(x\psi'(x) + \psi(x)\right) \tag{120}$$

$$= \frac{\hbar}{i}\int_{\mathbb{R}} \mathrm{d}p \int_{\mathbb{R}} \mathrm{d}x\, \langle x'|p\rangle \langle p|x\rangle \langle x| \left(|\psi\rangle + x\, |\psi'_x\rangle\right) \tag{121}$$

We have defined a state $|\psi'_x\rangle$ which, in a position representation, is the first derivative of $\psi(x)$.

$$\langle x'|\hat{p}\hat{x}|\psi\rangle = \frac{\hbar}{i}\int_{\mathbb{R}} \mathrm{d}x\, \langle x'|x\rangle \langle x| \left(|\psi\rangle + x\, |\psi'_x\rangle\right) \tag{122}$$

$$= \frac{\hbar}{i}\int_{\mathbb{R}} \mathrm{d}x\, \delta(x' - x) \langle x| \left(|\psi\rangle + x\, |\psi'_x\rangle\right) \tag{123}$$

$$= \frac{\hbar}{i} \langle x'| \left(|\psi\rangle + x'\, |\psi'_x\rangle\right) \tag{124}$$

$$= \frac{\hbar}{i}\left(\psi(x') + x' \frac{\mathrm{d}}{\mathrm{d}x'}\psi(x')\right) \tag{125}$$

(b) This time, we forget about the tricks we used above, and just use what we know about the representations of the operators. You've probably calculated the commutator $[\hat{x}, \hat{p}]$ before; this is essentially the same calculation.

(i)

$$\langle x'|\hat{x}\hat{p}|\psi\rangle = x' \langle x'|\hat{p}|\psi\rangle \tag{126}$$

$$= x' \frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x'} \langle x'|\psi\rangle \tag{127}$$

$$= \frac{\hbar}{i} x' \frac{\mathrm{d}}{\mathrm{d}x'}\psi(x') \tag{128}$$

(ii)

$$\langle x'|\hat{p}\hat{x}|\psi\rangle = \frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x'} \langle x'|\hat{x}|\psi\rangle \tag{129}$$

$$= \frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x'} \left(x' \langle x'|\psi\rangle\right) \tag{130}$$

$$= \frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x'} \left(x'\psi(x')\right) \tag{131}$$

$$= \frac{\hbar}{i}\left(\psi(x') + x' \frac{\mathrm{d}}{\mathrm{d}x'}\psi(x')\right) \tag{132}$$

Not surprisingly, these are the same results that we had found with the previous method.