Don't panic! Problems 2 and 3 look long, but most of it is just story-telling. You need to do just a small fraction of the steps. But do read and process the text in between the actual problems. The reward is that you get a better idea of the relation between the discrete and continuously valued observables and the associated operators.

Reminder: now that we are dealing with continuous variables, you will often need some integral formulas. You can find these either in Griffiths (inside back cover), or online; feel free to use wolframalpha. When doing integrals, it is best to write down general formulas before plugging in specific values; for example, you should write $\int_0^\pi \sin(x)dx = -\cos(x)|_0^\pi = 2$. However, sometimes integrals can be evaluated explicitly only for certain values of their range. For example, there's no nice formula for $\int_a^b e^{-x^2}dx$ for general a and b, but `wolframalpha` will tell you that $\int_{-\infty}^{\infty} e^{-x^2}dx = \sqrt{\pi}$.

1. Griffiths 3rd ed., Problem 1.16, all the subproblems that weren't on the previous homework: c, e, g, h.

   Optional, not graded, but highly recommended: revisit problem 1.3 in Griffiths, which you did on the previous HW. Use your work to verify that you were not lied to in class. (At least not about Gaussians.)

2. *From Discrete to "Continuous" Matrix Elements of Operators...*

   The matrix form of an operator depends on what basis we work in. For example, you are familiar with the fact that the operator corresponding to the x-component of the spin of a spin 1/2 particle is

   $$\hat{s_x} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{1}$$

   in the $\{|\pm z\rangle\}$ basis, i.e., when that matrix is going to multiply a column vector $\begin{pmatrix} a \\ b \end{pmatrix}$ that represents the state $a\,|{+z}\rangle + b\,|{-z}\rangle$. Yet, the exact same operator takes the matrix form

   $$\hat{s_x} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2}$$

   if we work in the $\{|\pm x\rangle\}$ basis (meaning, we intend for this matrix to multiply a column vector $\begin{pmatrix} a \\ b \end{pmatrix}$ that represents the state $a\,|{+x}\rangle + b\,|{-x}\rangle$.)

Completely generally, the components A_{ij} of the matrix of an operator $\hat{A}$, in the arbitrary basis $\{|i\rangle\}$ are

$$A_{ij} = \langle i|\hat{A}|j\rangle \ . \tag{3}$$

a. Use Eq. (3) to compute all four components of $\hat{s_z}$ in the $\{|\pm x\rangle\}$ basis.

b. Now let us boldly apply the same formula in the setting of continuously valued observables like position,

$$\hat{x} = \int dx\, x\ |x\rangle\langle x| \ , \tag{4}$$

and momentum, $\hat{p} = \int dp\, p\ |p\rangle\langle p|$. Here $|x\rangle$ are the δ-function normalized position eigenstates, $\langle x'|x\rangle = \delta(x - x')$; and similarly for $|p\rangle$. All integrals run from $-\infty$ to $+\infty$ unless otherwise noted. Use Eq. (3) to show that the matrix elements of $\hat{x}$ in the position basis $\{|x\rangle\}$ are given by

$$\langle x|\hat{x}|x'\rangle = x\,\delta(x - x') \ . \tag{5}$$

c. Use Eq. (3) to show that the matrix elements of $\hat{p}$ in the position basis $\{|x\rangle\}$ are given by

$$\langle x|\hat{p}|x'\rangle = \frac{1}{2\pi\hbar}\int dp\, p\, e^{ip(x-x')/\hbar} \ . \tag{6}$$

d. To understand what this strange integral means, consult your lecture notes from Oct. 17, where we proved that for a general state $|\psi\rangle$,

$$\langle x|\hat{p}|\psi\rangle = -\mathrm{i}\hbar\,\frac{d}{dx}\,\langle x|\psi\rangle \ . \tag{7}$$

Use this result to show that the integral in Eq. (6) must evaluate to

$$\langle x|\hat{p}|x'\rangle = -\mathrm{i}\hbar\,\frac{d}{dx}\delta(x - x') \ . \tag{8}$$

The derivative of the δ function, like the δ function itself, is not really a well-defined function but a distribution (but in your derivation, just treat it like a function).

e. Using integration by parts, prove that for any (reasonable) function $f(x)$,

$$\int f(x)\,\frac{d}{dx}\delta(x-x')\,dx = -g(x')\ , \tag{9}$$

where $g(x) = \frac{df}{dx}$.

f. As a consistency check, use Eqs. (8) and (9) to derive Eq. (7). *Hint:* starting from the LHS of Eq. (7), insert the identity operator in the form $\mathbb{I} = \int dx'\,|x'\rangle\,\langle x'|$.

3. *. . . and back*

Eqs. (5) and (8) are the closest thing to a "matrix" representation of $\hat{x}$ and $\hat{p}$ in the continuous basis $\{|x\rangle\}$. To make this look like an actual matrix, we have to discretize position, so let us replace Eq. (4) by

$$\hat{x} = \sum_{i=-\infty}^{\infty} x_i\,|i\rangle\,\langle i| \tag{10}$$

Here $x_i = i\Delta x$; Δx is some small length scale; i runs over all integers (negative, positive, and 0); and the discrete basis states are conventionally orthonormal: $\langle i|j\rangle = \delta_{ij}$. Physically, you can think of $|i\rangle$ as the state in which the particle is localized to the interval $[x_i, x_{i+1})$. Then Eq. (5) becomes

$$\langle i|\hat{x}|j\rangle = x_i\,\delta_{ij}\ . \tag{11}$$

This is much more like a matrix. It is still infinite-dimensional, but now it is a discrete kind of infinity, with rows and columns labeled by integers. So it is easy to think of it as a matrix whose rows and columns just keep on going in all directions.

The momentum matrix elements are a little trickier. We would like a discrete version of Eq. (8) that limits to Eq. (8) as $\Delta x \to 0$. This is easiest if we consider a general state $|\psi\rangle$ and its position space wavefunction $\psi(x) = \langle x|\psi\rangle$, which we imagine is smooth.

(a) Show that in the limit as $\Delta x \to 0$,

$$\psi(x) \approx \frac{\langle i|\psi\rangle}{\sqrt{\Delta x}}\ . \tag{12}$$

(b) Using the standard calculus definition of the derivative, show that

$$\frac{d}{dx}\psi \approx \frac{1}{2\Delta x}\left(\frac{\langle i+1|\psi\rangle}{\sqrt{\Delta x}} - \frac{\langle i-1|\psi\rangle}{\sqrt{\Delta x}}\right) . \tag{13}$$

(c) Now most of our work is done, and I will take you through the remaining steps, leaving just one tiny problem for you at the end. Let $|\chi\rangle = \hat{p}\,|\psi\rangle$. By the same logic that led to Eq. (12), we can again express this wavefunction in terms of the discrete basis $|i\rangle$ as

$$\chi(x) \approx \frac{\langle i|\chi\rangle}{\sqrt{\Delta x}} . \tag{14}$$

We showed in class that the two wavefunctions are related by

$$\chi(x) = \langle x|\chi\rangle = -\mathrm{i}\hbar\frac{d}{dx}\psi(x) . \tag{15}$$

The previous three equations together imply

$$\langle i|\chi\rangle \approx -\mathrm{i}\hbar\,\frac{\langle i+1|\psi\rangle - \langle i-1|\psi\rangle}{2\Delta x} . \tag{16}$$

So far we required $\psi(x)$ to be smooth, but linearity requires that the above result holds even if we choose $|\psi\rangle = |j\rangle$. Recalling that $|\chi\rangle = \hat{p}\,|\psi\rangle$, we thus obtain the matrix elements of the momentum operator in the position basis:

$$p_{ij} = \langle i|\hat{p}|j\rangle \approx -\mathrm{i}\hbar\,\frac{\langle i+1|j\rangle - \langle i-1|j\rangle}{2\Delta x} . \tag{17}$$

Write p_{ij} in terms of a difference of Kronecker deltas. (This is the only part of the problem that you need to do.) Now you have the momentum operator in manifest, discrete matrix form.