(I) Look at p. 226, #49.

Suppose \( z = g(x, y) = x^2y + xy^2 \) is a surface above (its domain) the unit square, \([0, 1] \times [0, 1]\).

(a) Find

\[
\int_0^1 \int_0^1 (x^2 y + xy^2) \, dx \, dy = ???
\]

Inner: [We integrate the inner integral first.]

\[
\int_0^1 (x^2 y + xy^2) \, dx = \left[ \left( \frac{x^3}{3} \right) (y) + \left( \frac{x^2}{2} \right) y^2 \right]_{x=0}^{x=1} = \frac{y}{3} + \frac{y^2}{2}
\]

Outer:

\[
\int_0^1 \left( \frac{y}{3} + \frac{y^2}{2} \right) \, dy = \left[ \frac{1}{3} \left( \frac{y^2}{2} \right) + \frac{1}{2} \left( \frac{y^3}{3} \right) \right]_0^1 = \frac{1}{6} + \frac{1}{6} = \frac{1}{3}
\]

(b) Divide \( g \) by the appropriate constant and form \( f(x, y) \), the associated probability (density) function.

If we divide by \( (1/3) \), then this is the same as multiplying by 3. Thus, we have

\[
f(x, y) = 3(x^2y + xy^2)
\]

and this must have all of the properties attributed to probability density functions. In particular, it is always nonnegative and the integral over its domain is equal to 1.00.

(c) Find the probability:

\[
P \left( 0 \leq x \leq \frac{1}{2} \text{ AND } 0 \leq y \leq \frac{1}{4} \right) = ???
\]

The double integral is

\[
\int_0^{1/4} \left( \int_0^{1/2} 3(x^2y + xy^2) \, dx \right) \, dy.
\]

The order of integration does not matter because the region of interest is a rectangle. Other shapes would make a difference, but rectangles are simple!

Inner:

\[
3 \int_0^{1/2} (x^2 y + xy^2) \, dx = 3 \left[ \frac{x^3 y}{3} + \frac{x^2 y^2}{2} \right]_0^{1/2} = 3 \left( \frac{y}{24} + \frac{y^2}{8} \right)
\]

Outer:

\[
3 \int_0^{1/4} \left( \frac{y}{24} + \frac{y^2}{8} \right) \, dy = 3 \left[ \frac{y^2}{48} + \frac{y^3}{24} \right]_0^{1/4} = 3 \left( \frac{1}{48} \left( \frac{1}{16} \right) + \frac{1}{24} \left( \frac{1}{64} \right) \right) = \frac{3}{512}.
\]
Complete p. 226: #54, 55, 56.

Remember that the Jacobian is $r$.

(#54) We have:

$y: 0 \rightarrow \sqrt{1 - x^2}$

$x: 0 \rightarrow 1$.

We need the region between the two curves $y = 0$ and $y = \sqrt{1 - x^2}$. The second one is the upper half of the unit circle.

The second constraint only allows us to take the portion on the right side of the $y$-axis.

Thus, this region of integration must be the quarter circle in Quadrant I.

Thus, when we translate this region into polar coordinates, we have:

$r: 0 \rightarrow 1$ [Stay inside the circle!]

$\theta: 0 \rightarrow \pi/2$ [Quadrant I only!]

We substitute into the integrand:

$x = r \cos (\theta)$

$y = r \sin (\theta)$

$x^2 + 2xy = (r \cos (\theta))^2 + 2 (r \cos (\theta)) (r \sin (\theta))$

$= r^2 \cos^2 (\theta) + 2r^2 \cos (\theta) \sin (\theta)$

This is our new integrand. Don’t forget that we need that extra factor of $r$ for the Jacobian.

The double integral becomes

$$
\int_0^{\pi/2} \int_0^1 (r^2 \cos^2 (\theta) + 2r^2 \cos (\theta) \sin (\theta)) r \, dr \, d\theta
$$

We can split this into two integrals.

The first one is

$$
\int_0^{\pi/2} \int_0^1 r^3 \cos^2 (\theta) \, dr \, d\theta = \frac{\pi}{16}.
$$

Since the limits of integration are constants and the integrand is factorable, we can break this into a product.

$$
\left( \int_0^1 r^3 \, dr \right) \left( \int_0^{\pi/2} \cos^2 (\theta) \, d\theta \right)
$$

The first one is $\frac{1}{4}$. The second one requires the trig. identity:

$$
\cos^2 (\theta) = \frac{1}{2} + \frac{\cos (2\theta)}{2}
$$

$$
\int \cos^2 (\theta) \, d\theta = \frac{\theta}{2} + \frac{\sin (2\theta)}{4} + C.
$$
Thus, we have
\[ \int_0^{\pi/2} \cos^2(\theta) \, d\theta = \left[ \frac{\theta}{2} + \frac{\sin(2\theta)}{4} \right]_0^{\pi/2} = \frac{\pi}{4}. \]

Thus, the product of the two integrals is \( \frac{\pi}{16} \).

The second integral is
\[ 2 \int_0^{\pi/2} \int_0^1 (r^3 \cos(\theta) \sin(\theta)) \, dr \, d\theta = \frac{1}{4}. \]

This one is also factorable.
\[ 2 \left( \int_0^1 r^3 \, dr \right) \left( \int_0^{\pi/2} \cos(\theta) \sin(\theta) \, d\theta \right) \]

Again, the first integral is \( \frac{1}{4} \), but the second requires a u-substitution.
\[ u = \sin(\theta), \ du = \cos(\theta) \, d\theta \]
\[ \int_0^{\pi/2} \cos(\theta) \sin(\theta) \, d\theta \Rightarrow \int u \, du = \frac{u^2}{2} + C \]
\[ = \left[ \frac{\sin^2(\theta)}{2} \right]_0^{\pi/2} = \frac{1}{2}. \]

Thus, the integral is
\[ 2 \left( \frac{1}{4} \right) \left( \frac{1}{2} \right) = \frac{1}{4}. \]

The sum of the original two integrals is
\[ \int_0^{\pi/2} \int_0^1 (r^2 \cos^2(\theta) + 2r^2 \cos(\theta) \sin(\theta)) \, r \, dr \, d\theta = \frac{\pi}{16} + \frac{1}{4}. \]

(III) Follow Example 10.7 on p. 235. We know that \( a_0 \) is the Bohr radius (for hydrogen).

Find the average distances for the \( 2s \), \( 2p_y \), and \( 2p_z \) orbitals (on p. 231).

The Jacobian is \( r^2 \sin(\theta) \).

This time, we integrate over all of 3D space.

Since these are wave functions, we must square each of the functions first. We will just write “\( a \)” instead of \( a_0 \) to avoid confusion.

(a) \( 2s \). The square is
\[ |\psi_{2s}|^2 = \frac{1}{16 (2\pi a^3)} \ast \left( 2 - \frac{r}{a} \right)^2 e^{-r/a}. \]
\[ \langle r \rangle = \frac{1}{16 (2\pi a^3)} \int_0^{2\pi} \int_0^\pi \int_0^\infty r \left( 2 - \frac{r}{a} \right)^2 e^{-r/a} r^2 \sin(\theta) \, dr \, d\theta \, d\phi = 6a. \]

We can factor this.
\[ \frac{1}{16 (2\pi a^3)} \left( \int_0^\infty r^3 \left( 2 - \frac{r}{a} \right)^2 e^{-r/a} \, dr \right) \left( \int_0^\pi \sin(\theta) \, d\theta \right) \left( \int_0^{2\pi} d\phi \right) \]
The last two integrals are 2 and 2\pi.

We must expand the integrand of the first one by FOILing out the polynomial terms.

\[
\int_0^\infty r^3 \left( 2 - \frac{r}{a} \right)^2 e^{-r/a} \, dr = \int_0^\infty r^3 \left( 4 - \frac{4r}{a} + \frac{r^2}{a^2} \right) e^{-r/a} \, dr
\]

\[
= \int_0^\infty \left( 4r^3 - \frac{4r^4}{a} + \frac{r^5}{a^2} \right) e^{-r/a} \, dr
\]

We employ another \( u \)-substitution.

\[ u = \frac{r}{a}, \quad du = \left( \frac{1}{a} \right) dr \Rightarrow dr = a \, du, \quad r = au. \]

As \( r \to +\infty \), we have \( u \to +\infty \), since \( a > 0 \).

\[
\int_0^\infty \left( 4u^3 - \frac{4u^4}{a} + \frac{u^5}{a^2} \right) e^{-r/a} \, dr = \int_0^\infty \left( 4(au)^3 - \frac{4(au)^4}{a} + \frac{(au)^5}{a^2} \right) e^{-u} \, a \, du
\]

\[
= a^4 \int_0^\infty \left( 4u^3 - 4u^4 + u^5 \right) e^{-u} \, du
\]

When \( n \) is a positive integer, then we have the short-cut formula:

\[
\int_0^\infty u^n e^{-u} \, du = n!
\]

Thus, our substituted integral is easy to evaluate.

\[
a^4 \int_0^\infty \left( 4u^3 - 4u^4 + u^5 \right) e^{-u} \, du = a^4 (4 \cdot 3! - 4 \cdot 4! + 5!) = 48a^4.
\]

We now multiply the other factors together.

\[
\langle r \rangle = \frac{1}{16 (2\pi a^3)} (48a^4) (2) (2\pi) = 6a. \checkmark
\]

(b) \( 2p_y \).

\[
\left| \psi_{2p_y} \right|^2 = \frac{1}{16 (2\pi a^5)} \cdot r^2 e^{-r/a} \sin^2 (\theta) \sin^2 (\phi).
\]

\[
\langle r \rangle = \frac{1}{16 (2\pi a^5)} \int_0^{2\pi} \int_0^\pi \int_0^\infty r \cdot r^2 e^{-r/a} \sin^2 (\theta) \sin^2 (\phi) \cdot r^2 \sin (\theta) \, dr \, d\theta \, d\phi = 5a.
\]

\[
\langle r \rangle = \frac{1}{16 (2\pi a^5)} \left( \int_0^\infty r^5 e^{-r/a} \, dr \right) \left( \int_0^\pi \sin^3 (\theta) \, d\theta \right) \left( \int_0^{2\pi} \sin^2 (\phi) \, d\phi \right)
\]

Using the same steps as before, the first integral is

\[
\int_0^\infty r^5 e^{-r/a} \, dr = (5!) a^6 = 120a^6.
\]
The second one is tricky.
We use the trig. identity $\sin^2(\theta) = 1 - \cos^2(\theta)$.

\[
\int_0^\pi \sin^3(\theta) \, d\theta = \int_0^\pi (1 - \cos^2(\theta)) \sin(\theta) \, d\theta \\
= \int_0^\pi \sin(\theta) \, d\theta - \int_0^\pi \cos^2(\theta) \sin(\theta) \, d\theta
\]

The second part requires $u = \cos(\theta)$, $du = -\sin(\theta) \, d\theta \Rightarrow \sin(\theta) \, d\theta = -du$.

\[
\int_0^\pi \sin^3(\theta) \, d\theta = \left[ -\cos(\theta) \right]_0^\pi + \left[ \frac{\cos^3(\theta)}{3} \right]_0^\pi = \frac{4}{3}.
\]

The last integral requires the reduction of power formula.

\[
\sin^2(\phi) = \frac{1}{2} - \frac{\cos(2\phi)}{2} \Rightarrow \int \sin^2(\phi) \, d\phi = \frac{\phi}{2} - \frac{\sin(2\phi)}{4} + C.
\]

Thus, we have

\[
\int_0^{2\pi} \sin^2(\phi) \, d\phi = \left[ \frac{\phi}{2} - \frac{\sin(2\phi)}{4} \right]_0^{2\pi} = \pi.
\]

We multiply all the pieces together.

\[
\langle r \rangle = \frac{1}{16 (2\pi a^5)} \left( 120a^6 \right) \left( \frac{4}{3} \right) (\pi) = 5a. \checkmark
\]

(c) $2p_z$

\[
|\psi_{2p_z}|^2 = \frac{1}{16 (2\pi a^5)} * r^2 e^{-r/a} \cos^2(\theta).
\]

\[
\langle r \rangle = \frac{1}{16 (2\pi a^5)} \int_0^{2\pi} \int_0^\pi \int_0^\infty r^2 e^{-r/a} \cos^2(\theta) r^2 \sin(\theta) \, dr \, d\theta \, d\phi = 10a.
\]

\[
\langle r \rangle = \frac{1}{16 (2\pi a^5)} \left( \int_0^\infty r^5 e^{-r/a} \, dr \right) \left( \int_0^\pi \cos^2(\theta) \, d\theta \right) \left( \int_0^{2\pi} \, d\phi \right) \\
= \frac{1}{16 (2\pi a^5)} \left( 120a^6 \right) \left( \frac{2}{3} \right) (2\pi) = 5a.
\]

We should expect the average distance for all the $2p$ orbitals to be the same. They technically should have the same quantum energy.