Problem 1

[15 pts] Different forms of the Laplacian. Show that the following operators (radial part of the Laplacian) are equal. Hint: put an arbitrary function $R(\rho)$ or $R(r)$ to the right of each term and apply the product rule for derivatives.

Part a

Cylindrical coordinates:

\[
\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} = \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} = \frac{1}{\sqrt{\rho}} \frac{\partial^2}{\partial \rho^2} \sqrt{\rho} + \frac{1}{4\rho^2}
\]

Start with

\[
\frac{\partial^2}{\partial \rho^2} R(\rho) + \frac{1}{\rho} \frac{\partial}{\partial \rho} R(\rho) = R''(\rho) + \frac{R'(\rho)}{\rho}
\]

Now, try

\[
\frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} R(\rho) = \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho R'(\rho)
\]

\[
= \frac{1}{\rho} (\rho R''(\rho) + R'(\rho))
\]

\[
= R''(\rho) + \frac{R'(\rho)}{\rho}
\]

Finally, try

\[
\frac{1}{\sqrt{\rho}} \frac{\partial^2}{\partial \rho^2} \sqrt{\rho} R(\rho) + \frac{1}{4\rho^2} R(\rho) = \frac{1}{\rho^2} \frac{\partial}{\partial \rho} \left( \rho^2 R'(\rho) + \frac{1}{2} \rho^{-1} R(\rho) \right) + \frac{R(\rho)}{4\rho^2}
\]

\[
= \rho^{-\frac{1}{2}} \left( \rho^2 R''(\rho) + \frac{1}{2} \rho^{-1} R'(\rho) + \frac{1}{2} \rho^{-\frac{3}{2}} R'(\rho) - \frac{1}{4} \rho^{-\frac{5}{2}} R(\rho) \right) + \frac{R(\rho)}{4\rho^2}
\]

\[
= R''(\rho) + \frac{1}{2} \rho^{-1} R'(\rho) + \frac{1}{2} \rho^{-1} R'(\rho) - \frac{1}{4} \rho^{-2} R(\rho) + \frac{1}{4} \rho^{-2} R(\rho)
\]

\[
= R''(\rho) + \rho^{-1} R'(\rho)
\]

\[
= R''(\rho) + \frac{R'(\rho)}{\rho}
\]

So, \( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} = \frac{1}{\sqrt{\rho}} \frac{\partial^2}{\partial \rho^2} \sqrt{\rho} + \frac{1}{4\rho^2} \).

Part b

Spherical coordinates:

\[
\frac{\partial}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} = \frac{1}{r} \frac{\partial^2}{\partial r^2} r^2
\]

Start with

\[
\frac{\partial}{\partial r^2} R(r) + \frac{2}{r} \frac{\partial}{\partial r} R(r) = R''(r) + \frac{2}{r} R'(r)
\]
Now, try
\[ \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} R(r) = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 R'(r) \]
\[ = \frac{1}{r^2} (r^2 R''(r) + 2r R'(r)) \]
\[ = R''(r) + \frac{2}{r} R'(r) \]

Finally, try
\[ \frac{1}{r} \frac{\partial}{\partial r} r^2 R(r) = \frac{1}{r} \frac{\partial}{\partial r} (r R'(r) + R(r)) \]
\[ = \frac{1}{r} (r R''(r) + R'(r) + R'(r)) \]
\[ = \frac{1}{r} (r R''(r) + 2R'(r)) \]
\[ = R''(r) + \frac{2}{r} R'(r) \]

So,
\[ \frac{\partial}{\partial \rho} + \frac{2}{r} \frac{\partial}{\partial r} = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} = \frac{1}{r} \frac{\partial^2}{\partial \rho^2} r. \]

Problem 2

[30 pts] 2-d particle in an infinite circular well. Let a be the radius of the circular well, and \( V(\rho) = 0 \) for \( \rho < a \) and \( V(\rho) = \infty \) for \( \rho > a \) (free particle confined to a disk).

Part a

Write Schrödinger’s equation for this particle in 2-d cylindrical (polar) coordinates.

The multi-dimensional time-independent Schrödinger’s equation in rectangular coordinates (and specifically in 2 dimensions) is
\[ -\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi = E \psi \]
\[ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \psi(x, y) + V \psi(x, y) = E \psi(x, y) \]

To transform this into polar coordinates (in terms of \( (\rho, \phi) \)), we first must recognize that we want the partial derivatives in terms of \( \frac{\partial^2}{\partial \rho^2} \) and \( \frac{\partial^2}{\partial \phi^2} \), so we must apply the chain rule four times to the Laplacian:
\[ \frac{\partial^2}{\partial x^2} = \frac{\partial}{\partial x} \left( \frac{\partial \rho}{\partial x} \frac{\partial}{\partial \rho} + \frac{\partial \phi}{\partial x} \frac{\partial}{\partial \phi} \right) \]
\[ = \left( \frac{\partial \rho}{\partial x} \right)^2 \frac{\partial^2}{\partial \rho^2} + \frac{\partial^2 \rho}{\partial x^2} \frac{\partial}{\partial \rho} + \left( \frac{\partial \phi}{\partial x} \right)^2 \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2 \phi}{\partial x^2} \frac{\partial}{\partial \phi} \]
and
\[ \frac{\partial^2}{\partial y^2} = \frac{\partial}{\partial y} \left( \frac{\partial \rho}{\partial y} \frac{\partial}{\partial \rho} + \frac{\partial \phi}{\partial y} \frac{\partial}{\partial \phi} \right) \]
\[ = \left( \frac{\partial \rho}{\partial y} \right)^2 \frac{\partial^2}{\partial \rho^2} + \frac{\partial^2 \rho}{\partial y^2} \frac{\partial}{\partial \rho} + \left( \frac{\partial \phi}{\partial y} \right)^2 \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2 \phi}{\partial y^2} \frac{\partial}{\partial \phi} \]
Now, since $\rho = \sqrt{x^2 + y^2}$ and $\phi = \arctan \frac{y}{x} = \arctan (yx^{-1})$, we can easily calculate the partial derivatives:

\[
\frac{\partial \rho}{\partial x} = \frac{1}{2} (x^2 + y^2)^{-\frac{1}{2}} (2x) = x (x^2 + y^2)^{-\frac{1}{2}} = x (\rho^2)^{-\frac{1}{2}} = \frac{x}{\rho}
\]

\[
\frac{\partial \rho}{\partial y} = \frac{1}{2} (x^2 + y^2)^{-\frac{1}{2}} (2y) = y (x^2 + y^2)^{-\frac{1}{2}} = y (\rho^2)^{-\frac{1}{2}} = \frac{y}{\rho}
\]

\[
\frac{\partial^2 \rho}{\partial x^2} = \frac{\partial}{\partial x} \left( x (x^2 + y^2)^{-\frac{1}{2}} \right) = (x) \left( -\frac{1}{2} \right) (x^2 + y^2)^{-\frac{3}{2}} (2x) + (x^2 + y^2)^{-\frac{1}{2}} = -x^2 (x^2 + y^2)^{-\frac{3}{2}} + (x^2 + y^2)^{-\frac{1}{2}} = -x^2 (\rho^2)^{-\frac{3}{2}} + (\rho^2)^{-\frac{1}{2}} = -\frac{x^2}{\rho^3} + \frac{1}{\rho}
\]

\[
\frac{\partial^2 \rho}{\partial y^2} = \frac{\partial}{\partial y} \left( y (x^2 + y^2)^{-\frac{1}{2}} \right) = (y) \left( -\frac{1}{2} \right) (x^2 + y^2)^{-\frac{3}{2}} (2y) + (x^2 + y^2)^{-\frac{1}{2}} = -y^2 (x^2 + y^2)^{-\frac{3}{2}} + (x^2 + y^2)^{-\frac{1}{2}} = -y^2 (\rho^2)^{-\frac{3}{2}} + (\rho^2)^{-\frac{1}{2}} = -\frac{y^2}{\rho^3} + \frac{1}{\rho}
\]

\[
\frac{\partial \phi}{\partial x} = \left( 1 + \left( \frac{y}{x} \right)^2 \right)^{-1} (-yx^{-2}) = -yx^{-2} \left( 1 + \left( \frac{y}{x} \right)^2 \right)^{-1} = -y (x^2 + y^2)^{-1} = -y (\rho^2)^{-1} = -\frac{y}{\rho^2}
\]
\[
\frac{\partial \phi}{\partial y} = \left( 1 + \left( \frac{y}{x} \right)^2 \right)^{-1} (x^{-1})
\]
\[
= x^{-1} \left( 1 + \left( \frac{y}{x} \right)^2 \right)^{-1}
\]
\[
= \frac{x}{x^2} \left( 1 + \left( \frac{y}{x} \right)^2 \right)^{-1}
\]
\[
= \frac{x (x^2 + y^2)^{-1}}{x}
\]
\[
= x \left( \rho^2 \right)^{-1}
\]
\[
= \frac{x}{\rho^2}
\]

\[
\frac{\partial^2 \phi}{\partial x^2} = \frac{\partial}{\partial x} \left( -y (x^2 + y^2)^{-1} \right)
\]
\[
= y (x^2 + y^2)^{-2} 2x
\]
\[
= 2xy (x^2 + y^2)^{-2}
\]
\[
= 2xy \left( \rho^2 \right)^{-2}
\]
\[
= \frac{2xy}{\rho^4}
\]

\[
\frac{\partial^2 \phi}{\partial y^2} = \frac{\partial}{\partial y} \left( x (x^2 + y^2)^{-1} \right)
\]
\[
= -x (x^2 + y^2)^{-2} 2y
\]
\[
= -2xy (x^2 + y^2)^{-2}
\]
\[
= -2xy \left( \rho^2 \right)^{-2}
\]
\[
= -\frac{2xy}{\rho^4}
\]

We also know that \( x = \rho \cos \phi \) and \( y = \rho \sin \phi \), so substituting back in we get:

\[
\frac{\partial^2}{\partial x^2} = \left( \frac{\partial \rho}{\partial x} \right)^2 \frac{\partial^2}{\partial \rho^2} + \frac{\partial^2}{\partial x^2} \frac{\partial \rho}{\partial \rho} + \left( \frac{\partial \phi}{\partial x} \right)^2 \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2 \phi}{\partial x^2} \frac{\partial \phi}{\partial \phi}
\]
\[
= \left( \frac{\rho \cos \phi}{\rho} \right)^2 \frac{\partial^2}{\partial \rho^2} - \left( \frac{\rho^2 \cos^2 \phi}{\rho^3} - \frac{1}{\rho} \right) \frac{\partial}{\partial \rho} + \left( \frac{\rho \sin \phi}{\rho^2} \right)^2 \frac{\partial^2}{\partial \phi^2} + \left( \frac{2xy}{\rho^4} \right) \frac{\partial}{\partial \phi}
\]
\[
= \left( \cos^2 \phi \right) \frac{\partial^2}{\partial \rho^2} - \left( \frac{1}{\rho} \right) \left( \cos^2 \phi - 1 \right) \frac{\partial}{\partial \rho} + \left( \frac{\sin^2 \phi}{\rho^2} \right) \frac{\partial^2}{\partial \phi^2} + \left( \frac{2xy}{\rho^4} \right) \frac{\partial}{\partial \phi}
\]
\[
= \left( \cos^2 \phi \right) \frac{\partial^2}{\partial \rho^2} - \left( \frac{1}{\rho} \right) \left( -\sin^2 \phi \right) \frac{\partial}{\partial \rho} + \left( \frac{\sin^2 \phi}{\rho^2} \right) \frac{\partial^2}{\partial \phi^2} + \left( \frac{2xy}{\rho^4} \right) \frac{\partial}{\partial \phi}
\]

and

\[
\frac{\partial^2}{\partial y^2} = \left( \frac{\partial \rho}{\partial y} \right)^2 \frac{\partial^2}{\partial \rho^2} + \frac{\partial^2}{\partial y^2} \frac{\partial \rho}{\partial \rho} + \left( \frac{\partial \phi}{\partial y} \right)^2 \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2 \phi}{\partial y^2} \frac{\partial \phi}{\partial \phi}
\]
\[
= \left( \frac{\rho \sin \phi}{\rho} \right)^2 \frac{\partial^2}{\partial \rho^2} - \left( \frac{\rho^2 \sin^2 \phi}{\rho^3} - \frac{1}{\rho} \right) \frac{\partial}{\partial \rho} + \left( \frac{\rho \cos \phi}{\rho^2} \right)^2 \frac{\partial^2}{\partial \phi^2} - \left( \frac{2xy}{\rho^4} \right) \frac{\partial}{\partial \phi}
\]
\[= (\sin^2 \phi) \frac{\partial^2}{\partial \rho^2} - \left( \frac{1}{\rho} \right) \left( \cos^2 \phi - 1 \right) \frac{\partial}{\partial \rho} + \left( \frac{\cos^2 \phi}{\rho^2} \right) \frac{\partial^2}{\partial \phi^2} - \left( \frac{2xy}{\rho^4} \right) \frac{\partial}{\partial \phi} \]

And the Laplacian becomes:

\[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} = (\cos^2 \phi) \frac{\partial^2}{\partial \rho^2} - \left( \frac{1}{\rho} \right) \left( -\sin^2 \phi \right) \frac{\partial}{\partial \rho} + \left( \frac{\sin^2 \phi}{\rho^2} \right) \frac{\partial^2}{\partial \phi^2} + \left( \frac{2xy}{\rho^4} \right) \frac{\partial}{\partial \phi} \]

Substituting back into Schrödinger’s equation, we get:

\[-\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} \right) \psi(\rho, \phi) + V \psi(\rho, \phi) = E \psi(\rho, \phi)\]

**Part b**

Do a separation of variables \(\psi(\rho, \phi) = R(\rho)\Phi(\phi)\) to obtain radial and azimuthal equations.

Using the polar coordinate form from part (a), and separating into \(R(\rho)\) and \(\Phi(\phi)\), we get:

\[-\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} \right) R(\rho)\Phi(\phi) + VR(\rho)\Phi(\phi) = ER(\rho)\Phi(\phi)\]

\[-\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} \right) R(\rho) = \frac{\hbar^2}{2m} \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} \Phi(\phi) + V \]

\[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} \]

\[-\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} \right) R(\rho) - \frac{\hbar^2}{2m} \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} \Phi(\phi) + V = 2m (E - V)\]

Here, to go further, we need to be able to separate \(V\). If \(V\) is not separable, then we cannot complete the separation of variables. However, we know that \(V(\rho) = 0\), and if \(V\) is separable, then \(V = V(\rho) V(\phi)\), so \(V\) must be zero (and therefore constant). So, we can define \(k\) so that \(\hbar^2 k^2 = 2m(E - V)\), because \(E - V = T = \frac{\rho^2}{2m} = \frac{\hbar^2 k^2}{2m}\).

So, we have:

\[\left( \frac{\rho^2}{R(\rho)} \frac{\partial^2}{\partial \rho^2} + \frac{\rho}{R(\rho)} \frac{\partial}{\partial \rho} \right) R(\rho) + \frac{1}{\Phi(\phi)} \frac{\partial^2}{\partial \phi^2} \Phi(\phi) = -\rho^2 k^2\]

\[\left( \frac{\rho^2}{R(\rho)} \frac{\partial^2}{\partial \rho^2} + \frac{\rho}{R(\rho)} \frac{\partial}{\partial \rho} \right) R(\rho) + \rho^2 k^2 + \frac{1}{\Phi(\phi)} \frac{\partial^2}{\partial \phi^2} \Phi(\phi) = 0\]

So:

\[\left( \frac{\rho^2}{R(\rho)} \frac{\partial^2}{\partial \rho^2} + \frac{\rho}{R(\rho)} \frac{\partial}{\partial \rho} \right) R(\rho) + \rho^2 k^2 = \frac{1}{\Phi(\phi)} \frac{\partial^2}{\partial \phi^2} \Phi(\phi) = k^2\]
So, we have for $R(\rho)$:

$$
\left( \frac{\rho^2}{R(\rho)} \frac{\partial^2}{\partial \rho^2} + \frac{\partial}{\partial \rho} \frac{\partial}{\partial \rho} \right) R(\rho) + \rho^2 k^2 = k^2 \phi
$$

$$
\left( \rho^2 \frac{\partial^2}{\partial \rho^2} + \rho \frac{\partial}{\partial \rho} \right) R(\rho) + \rho^2 k^2 R(\rho) = k^2 R(\rho)
$$

$$
\left( \rho^2 \frac{\partial^2}{\partial \rho^2} + \rho \frac{\partial}{\partial \rho} \right) R(\rho) + \rho^2 k^2 R(\rho) - k^2 R(\rho) = 0
$$

And for $\Phi(\phi)$:

$$
\frac{\partial^2}{\partial \phi^2} \Phi(\phi) = k^2 \phi
$$

$$
\frac{\partial^2}{\partial \phi^2} \Phi(\phi) = k^2 \Phi(\phi)
$$

Letting $\Phi(\phi) = e^{ik\phi}$, we get:

$$
\frac{\partial^2}{\partial \phi^2} \Phi(\phi) = k^2 \Phi(\phi)
$$

$$
-\hat{L}_2^2 \Phi(\phi) = k^2 \Phi(\phi)
$$

$$
-\hat{L}_2^2 \Phi(\phi) = k^2 \Phi(\phi)
$$

$$
-\hat{L}_2^2 \Phi(\phi) = h^2 k^2 \Phi(\phi)
$$

$$
-\hat{L}_2^2 \Phi(\phi) = h^2 k^2 \Phi(\phi)
$$

**Part c**

Show that $\Phi = e^{im\phi}$ is a solution of the azimuthal equation. Using boundary conditions at $\phi = 0$ and $\phi = 2\pi$, show that $m = 0, \pm 1, \pm 2, \ldots$

If $\Phi(\phi) = e^{im\phi}$ then we have:

$$
-\hat{L}_2^2 \Phi(\phi) = h^2 k^2 \Phi(\phi)
$$

$$
-\left( h^2 \frac{\partial^2}{\partial \phi^2} \right) \Phi(\phi) = h^2 k^2 \Phi(\phi)
$$

$$
-\frac{\partial^2}{\partial \phi^2} e^{im\phi} = k^2 \Phi(\phi)
$$

$$
-\frac{\partial^2}{\partial \phi^2} e^{im\phi} = k^2 \Phi(\phi)
$$

$$
m^2 = k^2
$$

$$
m = k
$$

If for $\phi = 0$ and $\phi = 2\pi$ we want $e^{im0} = e^{im2\pi} = 1$. Taking $e^{im2\pi} = \cos(2\pi m) + i \sin(2\pi m) = 1$. This is only true when $m \in \mathbb{Z}$. In that case, $i \sin(2\pi m) = 0$ and $\cos(2\pi m) = 1$.

**Part d**

Show that the radial equation is the Bessel equation of order $m$ with the substitution $x = k\rho$, where $E = \hbar^2 k^2 / 2m$. See [http://mathworld.wolfram.com/BesselFunctionoftheFirstKind.html](http://mathworld.wolfram.com/BesselFunctionoftheFirstKind.html) Equation (1). The solutions are called Bessel functions $J_m(k\rho)$ of order $m$. 

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The Bessel function is:

\[ x^2 \frac{d^2 y}{dx^2} + x \frac{dy}{dx} + (x^2 - n^2) y = 0 \]

The radial equation is:

\[
\left( \rho^2 \frac{\partial^2}{\partial \rho^2} + \frac{\partial}{\partial \rho} \right) R(\rho) + \rho^2 k^2 R(\rho) - m^2 R(\rho) = 0 \\
\rho^2 \frac{\partial^2}{\partial \rho^2} R(\rho) + \rho \frac{\partial}{\partial \rho} R(\rho) + (\rho^2 k^2 - m^2) R(\rho) = 0
\]

To get the radial equation from the Bessel equation, we substitute in \( x = k \rho \) and recognize that \( \frac{dy}{dx} = \frac{d\rho}{dx} \) and \( \frac{d^2 y}{dx^2} = \frac{d}{dx} \left( \frac{d\rho}{dx} \frac{dy}{d\rho} \right) \) into the Bessel equation:

\[
k^2 \rho^2 \left( \frac{d\rho}{dx} \right)^2 \frac{d^2 y}{d\rho^2} + k \rho \left( \frac{d\rho}{dx} \frac{dy}{d\rho} \right) + (k^2 \rho^2 - n^2) y = 0
\]

Now we know that \( \rho = \frac{x}{k} \), and so \( \frac{d\rho}{dx} = \frac{1}{k} \) and \( \frac{d^2 \rho}{dx^2} = 0 \). Plugging these in, we get:

\[
k^2 \rho^2 \left( \frac{1}{k} \right)^2 \frac{d^2 y}{d\rho^2} + 0 + k \rho \left( \frac{1}{k} \frac{dy}{d\rho} \right) + (k^2 \rho^2 - n^2) y = 0
\]

If \( y(\rho) = R(\rho) \) and \( n = m \), then we have:

\[
\rho^2 \frac{d^2 R}{d\rho^2} + \rho \frac{dR}{d\rho} + (k^2 \rho^2 - n^2) R = 0
\]

\[
\frac{d^2 R}{d\rho^2} + \frac{1}{\rho} \frac{dR}{d\rho} + \left( k^2 - \frac{m^2}{\rho^2} \right) R = 0
\]

**Part e**

Apply the boundary condition \( \psi(a) = 0 \) to determine the values of \( k \) for each \( m \). For each value of \( m \) there is a series of radial modes \( k_{mn} \) indexed by \( n \) (the number of nodes).

We have:

\[
\rho^2 \frac{d^2 R}{d\rho^2} + \frac{dR}{d\rho} + (k^2 \rho^2 - m^2) R = 0
\]

\[
\frac{d^2 R}{d\rho^2} + \frac{1}{\rho} \frac{dR}{d\rho} + \left( k^2 - \frac{m^2}{\rho^2} \right) R = 0
\]

The solution to this part can be found in the table from the web site in part (f). Taking \( \psi(a) = 0 \), we get \( J_m(x_{nm}) = 0 \). These values are given in Table 1.
ProblemSet #6

\(n\) \(J_0(x_n0) = 0 \quad J_1(x_n1) = 0 \quad J_2(x_n2) = 0 \quad J_3(x_n3) = 0 \quad J_4(x_n4) = 0 \quad J_5(x_n5) = 0\)

<table>
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<th>(J_0(x_n0))</th>
<th>(J_1(x_n1))</th>
<th>(J_2(x_n2))</th>
<th>(J_3(x_n3))</th>
<th>(J_4(x_n4))</th>
<th>(J_5(x_n5))</th>
</tr>
</thead>
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<tr>
<td>1</td>
<td>2.4048</td>
<td>3.8317</td>
<td>5.1356</td>
<td>6.3802</td>
<td>7.5883</td>
<td>8.7715</td>
</tr>
<tr>
<td>2</td>
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<td>7.0156</td>
<td>8.4172</td>
<td>9.7610</td>
<td>11.0647</td>
<td>12.3386</td>
</tr>
</tbody>
</table>

Table 1: The \(n\)th values of \(x\) where \(J_m(x) = 0\).

Part f

Show that the energy levels are \(E_{nm} = \frac{\hbar^2 x_{nm}^2}{2ma^2}\), where \(x_{nm}\) is the \(n\)-th zero of \(J_m(x)\). Using the values of \(x\) where the \(J_m(x) = 0\) (see http://mathworld.wolfram.com/BesselFunctionZeros.html), fill in the numerical value of each energy level in figure 1. Draw the node lines for each mode.

Since \(x_{nm} = ka\), from part (d), and \(E = \frac{\hbar^2 k^2}{2m}\), we have \(E_{nm} = \frac{\hbar^2 x_{nm}^2}{2ma^2}\).

Part g

For an electron, what radius \(a\) would give a transition of \(\lambda = 121.5\) nm from the first excited state to the ground state?

The first excited state occurs at \(n = 1, m = 1\), and the transition energy, \(\Delta E = \frac{\hbar c}{\lambda} = \frac{1.24 \times 10^3 \text{eV nm}}{121.5 \text{nm}} = 10.21 \text{eV}\). Using \(E_{nm} = \frac{\hbar^2 x_{nm}^2}{2ma^2}\), we can also find

\[
\Delta E = E_{11} - E_{10} = 10.21 \text{eV} = \frac{\hbar^2 x_{11}^2}{2m_e a^2} - \frac{\hbar^2 x_{10}^2}{2m_e a^2} = \frac{\hbar^2}{2m_e a^2} (x_{11}^2 - x_{10}^2)
\]

\[
a = \sqrt{\frac{\hbar^2}{2m_e \Delta E} (x_{11}^2 - x_{10}^2)}
\]

\[
a = \sqrt{\frac{\hbar^2}{2m_e 10.21 \text{eV}} (5.52^2 - 3.83^2)}
\]

\[
a = 0.243 \text{ nm}
\]

Problem 3

[20 pts] Show the following functions \(Y_{lm}(\theta, \phi)\) are solutions of the differential equations:

\[\hat{L}_z Y_{lm} \equiv -i\hbar \frac{\partial}{\partial \phi} Y_{lm} = \hbar m Y_{lm}\]

and

\[\hat{L}^2 Y_{lm} \equiv \left( \frac{-\hbar^2}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \left( -\hbar^2 \frac{\partial^2}{\partial \phi^2} \right) \right) Y_{lm} = \hbar^2 l(l + 1) Y_{lm}\]

(In other words, they are eigenfunctions of \(\hat{L}^2\) and \(\hat{L}_z\)).
Part a

\( Y_{00} = 1 \)

In this case, we have \( m = 0 \) and first:

\[
\hat{L}_z Y_{00} = -i\hbar \frac{\partial}{\partial \phi} Y_{00} = \hbar (0) Y_{00}
\]

\[
\hat{L}_z (1) = -i\hbar \frac{\partial}{\partial \phi} (1) = \hbar (0) (1)
\]

\[
\hat{L}_z (1) \equiv 0 = 0
\]

And next \( l = 0 \) and:

\[
\hat{L}^2 Y_{00} = \left( \frac{-\hbar^2}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \left( -\hbar^2 \frac{\partial^2}{\partial \phi^2} \right) \right) Y_{00} = \hbar^2 0 (0 + 1) Y_{00}
\]

\[
\hat{L}^2 (1) = \left( \frac{-\hbar^2}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} (1) + \frac{1}{\sin^2 \theta} \left( -\hbar^2 \frac{\partial^2}{\partial \phi^2} \right) (1) \right) = 0
\]

\[
\hat{L}^2 (1) \equiv 0 = 0
\]

Part b

\( Y_{10} = \cos \theta \)
Figure 2: Nodes and Energy Levels filled in for Problem 2, Part f ($x_{nm}^2$ on the y-axis, $m$ on the x-axis)

For this, we have $m = 0$ and:

\[ \hat{L}_z Y_{10} = -i\hbar \frac{\partial}{\partial \phi} Y_{10} = \hbar \left( 0 \right) Y_{10} \]

\[ \hat{L}_z \cos \theta = -i\hbar \frac{\partial}{\partial \phi} \cos \theta = \hbar \left( 0 \right) \cos \theta \]

\[ \hat{L}_z \cos \theta = 0 = 0 \]

And next $l = 1$ and:

\[ \hat{L}^2 Y_{10} = \left( \frac{-\hbar^2}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \left( -\hbar^2 \frac{\partial^2}{\partial \phi^2} \right) \right) Y_{10} = \hbar^2 \left( 1 + 1 \right) Y_{10} \]

\[ \hat{L}^2 \cos \theta = \left( \frac{-\hbar^2}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} \cos \theta + \frac{1}{\sin^2 \theta} \left( -\hbar^2 \frac{\partial^2}{\partial \phi^2} \right) \cos \theta \right) = \hbar^2 \left( 1 + 1 \right) \cos \theta \]

\[ \hat{L}^2 \cos \theta = \frac{-\hbar^2}{\sin \theta} \frac{\partial}{\partial \theta} (-\sin^2 \theta) + 0 = 2\hbar^2 \cos \theta \]

\[ \hat{L}^2 \cos \theta = \frac{-\hbar^2}{\sin \theta} (-2 \sin \theta \cos \theta) = 2\hbar^2 \cos \theta \]

\[ \hat{L}^2 \cos \theta = 2\hbar^2 \cos \theta = 2\hbar^2 \cos \theta \]

**Part c**

\[ Y_{1\pm 1} = \sin \theta e^{\pm i\phi} \]
For this, we have \( m = \pm 1 \) and:

\[
\hat{L}_z Y_{1\pm 1} = -i\hbar \frac{\partial}{\partial \phi} Y_{1\pm 1} = \hbar (\pm 1) Y_{1\pm 1}
\]

\[
\hat{L}_z \sin \theta e^{\pm i\phi} = -i\hbar \frac{\partial}{\partial \phi} \sin \theta e^{\pm i\phi} = \hbar (\pm 1) \sin \theta e^{\pm i\phi}
\]

\[
\hat{L}_z \sin \theta e^{\pm i\phi} = -i\hbar \sin \theta \pm i e^{\pm i\phi} = \hbar (\pm 1) \sin \theta e^{\pm i\phi}
\]

\[
\hat{L}_z \sin \theta e^{\pm i\phi} = \pm \hbar \sin \theta e^{\pm i\phi} = \pm \hbar \sin \theta e^{\pm i\phi}
\]

And next \( l = 1 \) and:

\[
\hat{L}_z^2 Y_{1\pm 1} = \left( -\frac{\hbar^2}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \left( -\hbar^2 \frac{\partial^2}{\partial \phi^2} \right) \right) Y_{1\pm 1} = \hbar^2 (1 + 1) Y_{1\pm 1}
\]

\[
\hat{L}_z^2 \sin \theta e^{\pm i\phi} = \left( -\frac{\hbar^2}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} \sin \theta e^{\pm i\phi} + \frac{1}{\sin^2 \theta} \left( -\hbar^2 \frac{\partial^2}{\partial \phi^2} \right) \sin \theta e^{\pm i\phi} \right) = \hbar^2 \sin \theta e^{\pm i\phi}
\]

\[
\hat{L}_z^2 \sin \theta e^{\pm i\phi} = \left( -\frac{\hbar^2}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \cos \theta e^{\pm i\phi} + \frac{1}{\sin^2 \theta} \left( -\hbar^2 \frac{\partial^2}{\partial \phi^2} \sin \theta e^{\pm i\phi} \right) \right) = \hbar^2 \sin \theta e^{\pm i\phi}
\]

\[
\hat{L}_z^2 \sin \theta e^{\pm i\phi} = \left( \hbar^2 e^{\pm i\phi} \left( \sin^2 \theta + \cos^2 \theta \right) + \hbar^2 e^{\pm i\phi} \right) = 2\hbar^2 \sin \theta e^{\pm i\phi}
\]

\[
\hat{L}_z^2 \sin \theta e^{\pm i\phi} = \hbar^2 e^{\pm i\phi} \left( \sin^2 \theta - \cos^2 \theta + 1 \right) = 2\hbar^2 \sin \theta e^{\pm i\phi}
\]

\[
\hat{L}_z^2 \sin \theta e^{\pm i\phi} = \hbar^2 e^{\pm i\phi} \left( \sin^2 \theta - \cos^2 \theta + \sin^2 \theta + \cos^2 \theta \right) = 2\hbar^2 \sin \theta e^{\pm i\phi}
\]

\[
\hat{L}_z^2 \sin \theta e^{\pm i\phi} = \hbar^2 e^{\pm i\phi} \sin^2 \theta = 2\hbar^2 \sin \theta e^{\pm i\phi}
\]

\[
Y_{2\pm 1} = \sin \theta \cos \theta e^{\pm i\phi}
\]

For this, we have \( m = \pm 1 \) and:

\[
\hat{L}_z Y_{2\pm 1} = -i\hbar \frac{\partial}{\partial \phi} Y_{2\pm 1} = \hbar (\pm 1) Y_{2\pm 1}
\]

\[
\hat{L}_z \sin \theta \cos \theta e^{\pm i\phi} = -i\hbar \frac{\partial}{\partial \phi} \sin \theta \cos \theta e^{\pm i\phi} = \hbar (\pm 1) \sin \theta \cos \theta e^{\pm i\phi}
\]

\[
\hat{L}_z \sin \theta \cos \theta e^{\pm i\phi} = -i\hbar \sin \theta \cos \theta (\pm i) e^{\pm i\phi} = \hbar (\pm 1) \sin \theta \cos \theta e^{\pm i\phi}
\]

\[
\hat{L}_z \sin \theta \cos \theta e^{\pm i\phi} = \pm \hbar \sin \theta \cos \theta e^{\pm i\phi} = \pm \hbar \sin \theta \cos \theta e^{\pm i\phi}
\]

And next \( l = 2 \) and:

\[
\hat{L}_z^2 Y_{2\pm 1} = \left( -\frac{\hbar^2}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \left( -\hbar^2 \frac{\partial^2}{\partial \phi^2} \right) \right) Y_{2\pm 1} = \hbar^2 (2 + 1) Y_{2\pm 1}
\]

\[
\hat{L}_z^2 \sin \theta \cos \theta e^{\pm i\phi} = \left( -\frac{\hbar^2}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \cos \theta e^{\pm i\phi} + \frac{1}{\sin^2 \theta} \left( -\hbar^2 \frac{\partial^2}{\partial \phi^2} \sin \theta \cos \theta e^{\pm i\phi} \right) \right) = \hbar^2 6 \sin \theta \cos \theta e^{\pm i\phi}
\]

\[
\hat{L}_z^2 \sin \theta \cos \theta e^{\pm i\phi} = \left( -\frac{\hbar^2}{\sin \theta} e^{\pm i\phi} \frac{\partial}{\partial \theta} \sin \theta (\sin^2 \theta + \cos^2 \theta) + \frac{1}{\sin^2 \theta} \hbar^2 \cos \theta e^{\pm i\phi} \right) = \hbar^2 6 \sin \theta \cos \theta e^{\pm i\phi}
\]

\[
\hat{L}_z^2 \sin \theta \cos \theta e^{\pm i\phi} = \left( -\frac{\hbar^2}{\sin \theta} e^{\pm i\phi} \frac{\partial}{\partial \theta} \sin \theta (1 - 2 \sin^2 \theta) + \frac{1}{\sin^2 \theta} \hbar^2 \cos \theta e^{\pm i\phi} \right) = \hbar^2 6 \sin \theta \cos \theta e^{\pm i\phi}
\]

\[
\hat{L}_z^2 \sin \theta \cos \theta e^{\pm i\phi} = \left( -\frac{\hbar^2}{\sin \theta} e^{\pm i\phi} \frac{\partial}{\partial \theta} \sin \theta (\sin - 2 \sin^3 \theta) + \frac{1}{\sin^2 \theta} \hbar^2 \cos \theta e^{\pm i\phi} \right) = \hbar^2 6 \sin \theta \cos \theta e^{\pm i\phi}
\]
\[ \hat{L}^2 \sin \theta \cos \theta e^{\pm i\phi} = \left( -\frac{\hbar^2}{\sin \theta} e^{\pm i\phi} (\cos \theta - 6 \sin^2 \theta \cos \theta) + \frac{1}{\sin \theta} \hbar^2 \cos \theta e^{\pm i\phi} \right) = \hbar^2 6 \sin \theta \cos \theta e^{\pm i\phi} \]

\[ \hat{L}^2 \sin \theta \cos \theta e^{\pm i\phi} = (\hbar^2 e^{\pm i\phi} (-\cos \theta + 6 \sin^2 \theta \cos \theta) + \hbar^2 e^{\pm i\phi} \cos \theta) = \hbar^2 6 \sin^2 \theta \cos \theta e^{\pm i\phi} \]

\[ \hat{L}^2 \sin \theta \cos \theta e^{\pm i\phi} = \hbar^2 \cos \theta e^{\pm i\phi} (-1 + 6 \sin^2 \theta + 1) = \hbar^2 6 \sin^2 \theta \cos \theta e^{\pm i\phi} \]

\[ \hat{L}^2 \sin \theta \cos \theta e^{\pm i\phi} = \hbar^2 6 \sin^2 \theta \cos \theta e^{\pm i\phi} = \hbar^2 6 \sin^2 \theta \cos \theta e^{\pm i\phi} \]

**Problem 4**

Show that the corresponding orbitals in rectangular coordinates from Problem 5 are also solutions of
\[ \nabla^2 r Y_{lm} = 0 \] (where \( \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \)). Note that the real and imaginary parts of each solution can be used as separate solutions.

**Part a**

\[ Y_{00} = 1 \]

This is constant with respect to \( x, y \) and \( z \), so the second derivatives for each of these will be zero. The Laplacian will require that second partial derivatives be taken. So \( \nabla^2 r Y_{00} = 0 \).

**Part b**

\[ r Y_{10} = z \]

This is linear with respect to \( z \), and constant with respect to \( x \) and \( y \), so the second derivatives for each of these will be zero. The Laplacian will require that second partial derivatives be taken. So \( \nabla^2 r Y_{10} = 0 \).

**Part c**

\[ r Y_{1\pm 1} = x \pm iy \]

This is linear with respect to \( x \) and \( y \), and constant with respect to \( z \), so the second derivatives for each of these will be zero. The Laplacian will require that second partial derivatives be taken. So \( \nabla^2 r Y_{1\pm 1} = 0 \).

**Part d**

\[ r^2 Y_{2\pm 1} = z (x \pm iy) \]

The first derivatives of this function with respect to \( x, y, \) or \( z \) are constant with respect to \( x, y \) or \( z \), so the second derivatives with respect to \( x, y \) and \( z \) will be zero. The Laplacian will require that second partial derivatives be taken. So \( \nabla^2 r Y_{2\pm 1} = 0 \).

**Problem 7.9**

If \( n = 3 \):
Part a

What are the possible values of \( l \)?

\( l \) can be 0, 1, or 2.

Part b

For each value of \( l \) in part (a), list the possible values of \( m \).

For \( l = 0 \), \( m = 0 \). For \( l = 1 \), \( m = 0, \pm 1 \). For \( l = 2 \), \( m = 0, \pm 1, \pm 2 \).

Part c

Using the fact that there are two quantum states for each combination of values of \( l \) and \( m \) because of electron spin, find the total number of electron states with \( n = 3 \).

For \( l = 0 \), \( m = 0 \), there are 2 states. For \( l = 0 \), \( m = 0, \pm 1 \), there are 6 states. For \( l = 2 \), \( m = 0, \pm 1, \pm 2 \), there are 10 states. This totals to 18 states.

Problem 7.10

Determine the minimum angle that \( L \) can make with the z-axis when the angular momentum quantum number is:

Part a

\( l = 4 \)

The minimum angle that \( L \) can make with the z-axis is given by

\[
\cos \theta = \frac{L_z}{L} = \frac{m \hbar}{\hbar \sqrt{l(l+1)}} = \frac{m}{\sqrt{l(l+1)}}
\]

when \( m = \pm l \). This gives us:

\[
\cos \theta = \frac{4}{\sqrt{4(4+1)}} = \frac{4}{\sqrt{20}}
\]

\[
\theta = \arccos \frac{4}{\sqrt{20}} = 0.464 = 26.6^\circ
\]

Part b

\( l = 2 \)
Once again, the minimum angle that \( L \) can make with the z-axis is given by

\[
\cos \theta = \frac{L_z}{L} = \frac{m \hbar}{\hbar \sqrt{l(l+1)}} = \frac{m}{\sqrt{l(l+1)}},
\]

when \( m = \pm l \). This gives us:

\[
\cos \theta = \frac{2}{\sqrt{2(2+1)}} = \frac{2}{\sqrt{6}}
\]

\[
\theta = \arccos \frac{2}{\sqrt{6}} = 0.615 = 35.3^\circ
\]

**Problem 7.15**

Show that if \( V \) is a function only of \( r \), then \( dL/dt = 0 \), i.e. that \( L \) is conserved.

If \( V \) is a function only of \( r \), where \( r = |\vec{r}| \), then \( V \) scales linearly with the distance from the center of the potential well, and work is done only when the distance from the center of the potential well changes. This implies that the force must also be directed radially, or no work would be done. So, we know that \( \vec{F} \parallel \vec{r} \). Also, we have:

\[
\frac{d\vec{L}}{dt} = \frac{d}{dt} (\vec{r} \times \vec{p})
\]

\[
= \frac{d\vec{r}}{dt} \times \vec{p} + \vec{r} \times \frac{d\vec{p}}{dt}
\]

\[
= \frac{d\vec{r}}{dt} \times \vec{p} + \vec{r} \times \vec{F}
\]

\[
= \frac{d\vec{r}}{dt} \times \vec{p} + \vec{r} \times \nabla V
\]

\[
= \frac{d\vec{r}}{dt} \times \vec{p} + \vec{r} \times \left( \frac{\partial V}{\partial r} \hat{r} + \frac{\partial V}{\partial \theta} \hat{\theta} \right)
\]

\[
= \frac{d\vec{r}}{dt} \times \vec{p} + \vec{r} \times \left( \frac{\partial V}{\partial r} \hat{r} + 0 \right)
\]

\[
= \frac{d\vec{r}}{dt} \times \vec{p} + \vec{r} \times \frac{\partial V}{\partial r} \hat{r}
\]

\[
= \frac{d\vec{r}}{dt} \times \vec{p} + 0
\]

But, \( m \frac{d^2 \vec{r}}{dt^2} = \vec{F} \), so \( \frac{d\vec{L}}{dt} = \vec{r} \times \vec{F} \). But, \( \vec{F} \parallel \vec{r} \), so \( \frac{d\vec{L}}{dt} = 0 \).

Or, we could do:

\[
\frac{d\vec{L}}{dt} = \frac{d}{dt} (\vec{r} \times \vec{p})
\]

\[
= \frac{d\vec{r}}{dt} \times \vec{p} + \vec{r} \times \frac{d\vec{p}}{dt}
\]

\[
= \frac{d\vec{r}}{dt} \times \vec{p} + \vec{r} \times \vec{F}
\]

\[
= \frac{d\vec{r}}{dt} \times \vec{p} + \vec{r} \times \nabla V
\]

\[
= \frac{d\vec{r}}{dt} \times \vec{p} + \vec{r} \times \left( \frac{\partial V}{\partial r} \hat{r} + \frac{\partial V}{\partial \theta} \hat{\theta} \right)
\]

\[
= \frac{d\vec{r}}{dt} \times \vec{p} + \vec{r} \times \left( \frac{\partial V}{\partial r} \hat{r} + 0 \right)
\]

\[
= \frac{d\vec{r}}{dt} \times \vec{p} + \vec{r} \times \frac{\partial V}{\partial r} \hat{r}
\]

\[
= \frac{d\vec{r}}{dt} \times \vec{p} + 0
\]
\[
\frac{d\vec{r}}{dt} \times m \frac{d\vec{r}}{dt} = m \left( \frac{d\vec{r}}{dt} \times \frac{d\vec{r}}{dt} \right) = 0
\]

**Problem 7.16**

What are the possible values of \( n \) and \( m \) if:

**Part a**

\( l = 3 \)

In this case, \( n \geq 4 \), and \( -3 \leq m \leq 3 \), with \( n, m \in \mathbb{Z} \).

**Part b**

\( l = 4 \)

In this case, \( n \geq 5 \), and \( -4 \leq m \leq 4 \), with \( n, m \in \mathbb{Z} \).

**Part c**

\( l = 0 \)

In this case, \( n \geq 1 \), with \( n \in \mathbb{Z} \), and \( m = 0 \).

**Part d**

Compute the minimum possible energy for parts (a) through (c).

The minimum binding energy is given by

\[
E_n = -\left( \frac{kZe^2}{\hbar} \right)^2 \frac{\mu}{2n^2} = -13.6 \frac{Z^2}{n^2} \text{ eV}
\]

where \( Z = 1 \). The minimum (most negative) value for \( E_n \) will occur when \( n \) takes on the largest possible value.

For part (a), we have:

\[
E_4 = -13.6 \frac{1}{4^2} \text{ eV} = -0.85 \text{ eV}
\]

For part (b), we have:

\[
E_5 = -13.6 \frac{1}{5^2} \text{ eV} = -0.544 \text{ eV}
\]

And for part (c), we have:

\[
E_1 = -13.6 \frac{1}{1^2} \text{ eV} = -13.6 \text{ eV}
\]