## Chem 542 Problem Set 3

1. Transformation of variables between cartesian to cylindrical coordinates means:

$$
\frac{\partial}{\partial \mathrm{x}}=\cos (\phi) \frac{\partial}{\partial \mathrm{r}}-\frac{\sin (\phi)}{\mathrm{r}} \frac{\partial}{\partial \phi}
$$

and

$$
\frac{\partial}{\partial y}=\sin (\phi) \frac{\partial}{\partial r}+\frac{\cos (\phi)}{r} \frac{\partial}{\partial \phi}
$$

Now we are going to figure out what $\frac{\partial^{2}}{\partial \mathrm{x}^{2}}$ and $\frac{\partial^{2}}{\partial \mathrm{y}^{2}}$ are. First, determine $\frac{\partial^{2}}{\partial \mathrm{x}^{2}}$ via the FOIL method:

$$
\begin{gathered}
\text { (A - B) } \\
\frac{\partial^{2}}{\partial \mathrm{x}^{2}}=\frac{\partial}{\partial \mathrm{x}} \frac{\partial}{\partial \mathrm{x}}=\left(\cos (\phi) \frac{\partial}{\partial \mathrm{r}}-\frac{\sin (\phi)}{\mathrm{r}} \frac{\partial}{\partial \phi}\right) \cdot\left(\cos (\phi) \frac{\partial}{\partial \mathrm{r}}-\frac{\sin (\phi)}{\mathrm{r}} \frac{\partial}{\partial \phi}\right)
\end{gathered}
$$

Now you just must be careful that you do the "FOIL" method correctly; here it is:

$$
\begin{array}{ccccc}
\mathbf{A A}^{\prime} & +\quad \mathbf{A B}^{\prime} & +\quad \mathbf{B A}^{\prime} & + & \mathbf{B B}^{\prime} \\
\frac{\partial^{2}}{\partial \mathrm{x}^{2}}=\cos (\phi) \frac{\partial}{\partial \mathrm{r}} \cdot \cos (\phi) \frac{\partial}{\partial \mathrm{r}}+\cos (\phi) \frac{\partial}{\partial \mathrm{r}} \cdot\left(\frac{-\sin (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi}+\left(\frac{-\sin (\phi)}{\mathrm{r}}\right) \cdot \frac{\partial}{\partial \phi} \cos (\phi) \frac{\partial}{\partial \mathrm{r}}+\left(\frac{-\sin (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi} \cdot\left(\frac{-\sin (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi}
\end{array}
$$

Now we are going to now simplify it.
a. Why can you simplify the $\mathbf{A A}$ ' term as:

$$
\cos (\phi) \frac{\partial}{\partial r} \cos (\phi) \frac{\partial}{\partial r}=\cos ^{2}(\phi) \frac{\partial^{2}}{\partial \mathrm{r}^{2}}
$$

b. Why can't you simplify the AB' term as:

$$
\cos (\phi) \frac{\partial}{\partial \mathrm{r}}\left(\frac{-\sin (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi}=\left(\frac{-\cos (\phi) \sin (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \mathrm{r}} \frac{\partial}{\partial \phi}
$$

but you can as:

$$
\cos (\phi) \frac{\partial}{\partial r}\left(\frac{-\sin (\phi)}{r}\right) \frac{\partial}{\partial \phi}=-\cos (\phi) \sin (\phi) \frac{\partial}{\partial r}\left(\frac{1}{r}\right) \frac{\partial}{\partial \phi}
$$

C. Why can't you simplify the BA' term as:

$$
-\left(\frac{\sin (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi} \cos (\phi) \frac{\partial}{\partial \mathrm{r}}=\left(\frac{-\sin (\phi) \cos (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi} \frac{\partial}{\partial \mathrm{r}}
$$

d. Why can't you simplify the BB' term as:

$$
\left(\frac{-\sin (\phi)}{r}\right) \frac{\partial}{\partial \phi}\left(\frac{-\sin (\phi)}{r}\right) \frac{\partial}{\partial \phi}=\frac{\sin ^{2}(\phi)}{r^{2}} \frac{\partial^{2}}{\partial \phi^{2}}
$$

but you can as:

$$
\left(\frac{-\sin (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi}\left(\frac{-\sin (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi}=\left(\frac{\sin (\phi)}{\mathrm{r}^{2}}\right) \frac{\partial}{\partial \phi} \sin (\phi) \frac{\partial}{\partial \phi}
$$

## Answers:

a. Because $\frac{\partial}{\partial r}$ doesn't operate on $\cos (\phi)$, so it "slips" past the derivative.
b. Because $\frac{1}{\mathrm{r}}$ cannot slip past the $\frac{\partial}{\partial \mathrm{r}}$ operator, but $\sin (\phi)$ can.
c. Because $\cos (\phi)$ cannot pass through the $\frac{\partial}{\partial \phi}$ operator.
d. Because $\sin (\phi)$ cannot pass through the $\frac{\partial}{\partial \phi}$ operator, but $\frac{1}{\mathrm{r}}$ can.
2. Using the "rules" from question 1, can you determine what $\frac{\partial^{2}}{\partial \mathrm{x}^{2}}$ is in cylindrical coordinates?

## Answer:

$$
\cos ^{2}(\phi) \frac{\partial^{2}}{\partial \mathrm{r}^{2}}-\cos (\phi) \sin (\phi) \frac{\partial}{\partial \mathrm{r}} \cdot\left(\frac{1}{\mathrm{r}}\right) \frac{\partial}{\partial \phi}-\left(\frac{\sin (\phi)}{\mathrm{r}}\right) \cdot \frac{\partial}{\partial \phi} \cos (\phi) \frac{\partial}{\partial \mathrm{r}}+\left(\frac{\sin (\phi)}{\mathrm{r}^{2}}\right) \frac{\partial}{\partial \phi} \cdot \sin (\phi) \frac{\partial}{\partial \phi}
$$

3. Using the "rules" from question 1, can you determine what $\frac{\partial^{2}}{\partial \mathrm{y}^{2}}$ is in cylindrical coordinates? You must show your work on this one.

Answer: Starting with:

$$
\frac{\partial^{2}}{\partial \mathrm{y}^{2}}=\frac{\partial}{\partial \mathrm{y}} \frac{\partial}{\partial \mathrm{y}}=\left(\sin (\phi) \frac{\partial}{\partial \mathrm{r}}+\frac{\cos (\phi)}{\mathrm{r}} \frac{\partial}{\partial \phi}\right) \cdot\left(\sin (\phi) \frac{\partial}{\partial \mathrm{r}}+\frac{\cos (\phi)}{\mathrm{r}} \frac{\partial}{\partial \phi}\right)
$$

This leads to:

$$
\begin{aligned}
& \frac{\partial^{2}}{\partial \mathrm{y}^{2}}=\sin (\phi) \frac{\partial}{\partial \mathrm{r}} \sin (\phi) \frac{\partial}{\partial \mathrm{r}}+\sin (\phi) \frac{\partial}{\partial \mathrm{r}} \frac{\cos (\phi)}{\mathrm{r}} \frac{\partial}{\partial \phi}+\frac{\cos (\phi)}{\mathrm{r}} \frac{\partial}{\partial \phi} \sin (\phi) \frac{\partial}{\partial \mathrm{r}}+\frac{\cos (\phi)}{\mathrm{r}} \frac{\partial}{\partial \phi} \frac{\cos (\phi)}{\mathrm{r}} \frac{\partial}{\partial \phi}= \\
& \frac{\partial^{2}}{\partial \mathrm{y}^{2}}=\sin ^{2}(\phi) \frac{\partial^{2}}{\partial \mathrm{r}^{2}}+\sin (\phi) \cos (\phi) \frac{\partial}{\partial \mathrm{r}}\left(\frac{1}{\mathrm{r}}\right) \frac{\partial}{\partial \phi}+\left(\frac{\cos (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi} \sin (\phi) \frac{\partial}{\partial \mathrm{r}}+\left(\frac{\cos (\phi)}{\mathrm{r}^{2}}\right) \frac{\partial}{\partial \phi} \cos (\phi) \frac{\partial}{\partial \phi}
\end{aligned}
$$

My only question to you is, did you notice that I gave you the answer on the next page before or after you worked the question?

It turns out that $\frac{\partial^{2}}{\partial \mathrm{x}^{2}}+\frac{\partial^{2}}{\partial \mathrm{y}^{2}}=$

$$
\begin{aligned}
& \cos ^{2}(\phi) \frac{\partial^{2}}{\partial \mathrm{r}^{2}}-\cos (\phi) \sin (\phi) \frac{\partial}{\partial \mathrm{r}} \cdot\left(\frac{1}{\mathrm{r}}\right) \frac{\partial}{\partial \phi}-\left(\frac{\sin (\phi)}{\mathrm{r}}\right) \cdot \frac{\partial}{\partial \phi} \cos (\phi) \frac{\partial}{\partial \mathrm{r}}+\left(\frac{\sin (\phi)}{\mathrm{r}^{2}}\right) \frac{\partial}{\partial \phi} \cdot \sin (\phi) \frac{\partial}{\partial \phi}+ \\
& \sin ^{2}(\phi) \frac{\partial^{2}}{\partial \mathrm{r}^{2}}+\sin (\phi) \cos (\phi) \frac{\partial}{\partial \mathrm{r}} \cdot\left(\frac{1}{\mathrm{r}}\right) \frac{\partial}{\partial \phi}+\left(\frac{\cos (\phi)}{\mathrm{r}}\right) \cdot \frac{\partial}{\partial \phi} \sin (\phi) \frac{\partial}{\partial \mathrm{r}}+\left(\frac{\cos (\phi)}{\mathrm{r}^{2}}\right) \frac{\partial}{\partial \phi} \cdot \cos (\phi) \frac{\partial}{\partial \phi}
\end{aligned}
$$

Note that two middle terms cancel:

$$
-\cos (\phi) \sin (\phi) \frac{\partial}{\partial r} \cdot\left(\frac{1}{r}\right) \frac{\partial}{\partial \phi}+\sin (\phi) \cos (\phi) \frac{\partial}{\partial r} \cdot\left(\frac{1}{r}\right) \frac{\partial}{\partial \phi}=0
$$

Which leaves: $\frac{\partial^{2}}{\partial \mathrm{x}^{2}}+\frac{\partial^{2}}{\partial \mathrm{y}^{2}}=$

$$
\cos ^{2}(\phi) \frac{\partial^{2}}{\partial \mathrm{r}^{2}}-\left(\frac{\sin (\phi)}{\mathrm{r}}\right) \cdot \frac{\partial}{\partial \phi} \cos (\phi) \frac{\partial}{\partial \mathrm{r}}+\left(\frac{\sin (\phi)}{\mathrm{r}^{2}}\right) \frac{\partial}{\partial \phi} \cdot \sin (\phi) \frac{\partial}{\partial \phi}+
$$

$$
\sin ^{2}(\phi) \frac{\partial^{2}}{\partial \mathrm{r}^{2}}+\left(\frac{\cos (\phi)}{\mathrm{r}}\right) \cdot \frac{\partial}{\partial \phi} \sin (\phi) \frac{\partial}{\partial \mathrm{r}}+\left(\frac{\cos (\phi)}{\mathrm{r}^{2}}\right) \frac{\partial}{\partial \phi} \cdot \cos (\phi) \frac{\partial}{\partial \phi}
$$

Now we will break the sum into different parts to simplify it. I will re-represent $\frac{\partial^{2}}{\partial \mathrm{x}^{2}}+\frac{\partial^{2}}{\partial \mathrm{y}^{2}}$ as:

solve in 4 a

$$
\left[\begin{array}{l}
-\left(\frac{\sin (\phi)}{\mathrm{r}}\right) \cdot \frac{\partial}{\partial \phi} \cos (\phi) \frac{\partial}{\partial \mathrm{r}} \\
+\left(\frac{\cos (\phi)}{\mathrm{r}}\right) \cdot \frac{\partial}{\partial \phi} \sin (\phi) \frac{\partial}{\partial \mathrm{r}} \\
\text { solve in } 4 \mathrm{~b}, \mathrm{c}, \mathrm{~d}
\end{array}+\right.
$$


4. a. Can you simplify the sum of the two leading terms to remove the angle parts:

$$
\cos ^{2}(\phi) \frac{\partial^{2}}{\partial \mathrm{r}^{2}}+\sin ^{2}(\phi) \frac{\partial^{2}}{\partial \mathrm{r}^{2}}=?
$$

Hint, it's really easy- what is the simplest trig identity you know?
b. Now let's deal with these two "middle" terms. We can show that if you add them together then:

$$
-\left(\frac{\sin (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi} \cos (\phi) \frac{\partial}{\partial \mathrm{r}}+\left(\frac{\cos (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi} \sin (\phi) \frac{\partial}{\partial \mathrm{r}}=\frac{1}{\mathrm{r}} \frac{\partial}{\partial \mathrm{r}}
$$

How? Let's start by acting $\Psi(\mathrm{r}) \cdot \Psi(\phi)$ on the first term above:

$$
-\left(\frac{\sin (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi} \cos (\phi) \frac{\partial \Psi(\mathrm{r}) \cdot \Psi(\phi)}{\partial \mathrm{r}}=-\left(\frac{\sin (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi} \cos (\phi) \cdot \Psi(\phi) \frac{\partial \Psi(\mathrm{r})}{\partial \mathrm{r}}
$$

Can you show that the expression above can be simplified to:

$$
\left(\frac{\sin ^{2}(\phi)}{\mathrm{r}}\right) \Psi(\phi) \frac{\partial \Psi(\mathrm{r})}{\partial \mathrm{r}}-\left(\frac{\sin (\phi) \cos (\phi)}{\mathrm{r}}\right) \frac{\partial \Psi(\phi)}{\partial \phi} \frac{\partial \Psi(\mathrm{r})}{\partial \mathrm{r}}
$$

C. Likewise show that the second term in pt. b reduces to:

$$
\begin{aligned}
\left(\frac{\cos (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi} & \sin (\phi) \frac{\partial \Psi(\mathrm{r}) \cdot \Psi(\phi)}{\partial \mathrm{r}} \\
& =\left(\frac{\cos ^{2}(\phi)}{\mathrm{r}}\right) \Psi(\phi) \frac{\partial \Psi(\mathrm{r})}{\partial \mathrm{r}}+\left(\frac{\cos (\phi) \sin (\phi)}{\mathrm{r}}\right) \frac{\partial \Psi(\phi)}{\partial \phi} \frac{\partial \Psi(\mathrm{r})}{\partial \mathrm{r}}
\end{aligned}
$$

d. Now can you show that:

$$
\left[-\left(\frac{\sin (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi} \cos (\phi) \frac{\partial}{\partial \mathrm{r}}+\left(\frac{\cos (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi} \sin (\phi) \frac{\partial}{\partial \mathrm{r}}\right] \Psi(\mathrm{r}) \cdot \Psi(\phi)=\frac{1}{\mathrm{r}} \frac{\partial \Psi(\mathrm{r}) \cdot \Psi(\phi)}{\partial \mathrm{r}}
$$

Hint: for pt. b\&c use the product rule.
Answers: a. First just factor: $\cos ^{2}(\phi) \frac{\partial^{2}}{\partial \mathrm{r}^{2}}+\sin ^{2}(\phi) \frac{\partial^{2}}{\partial \mathrm{r}^{2}}$ as $\left(\cos ^{2}(\phi)+\sin ^{2}(\phi)\right) \frac{\partial^{2}}{\partial \mathrm{r}^{2}}$ and note that: $\cos ^{2}(\phi)+\sin ^{2}(\phi)=1$. Thus $\cos ^{2}(\phi) \frac{\partial^{2}}{\partial \mathrm{r}^{2}}+\sin ^{2}(\phi) \frac{\partial^{2}}{\partial \mathrm{r}^{2}}=\frac{\partial^{2}}{\partial \mathrm{r}^{2}}$.
b. The first step is to operate on: $\frac{\partial}{\partial \phi} \cos (\phi) \cdot \Psi(\phi)$ which uses the product rule: $\frac{\partial}{\partial \phi} \cos (\phi)$. $\Psi(\phi)=-\sin (\phi) \Psi(\phi)+\cos (\phi) \frac{\partial \Psi(\phi)}{\partial \phi}$. Insert this into the equation:
$-\left(\frac{\sin (\phi)}{\mathrm{r}}\right)\left(-\sin (\phi) \Psi(\phi)+\cos (\phi) \frac{\partial \Psi(\phi)}{\partial \phi}\right) \frac{\partial \Psi(\mathrm{r})}{\partial \mathrm{r}}$ which simplifies to the answer.
c. Likewise $\left(\frac{\cos (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi} \sin (\phi) \frac{\partial \Psi(\mathrm{r}) \cdot \Psi(\phi)}{\partial \mathrm{r}}=\left(\frac{\cos (\phi)}{\mathrm{r}}\right) \frac{\partial}{\partial \phi} \sin (\phi) \cdot \Psi(\phi) \frac{\partial \Psi(\mathrm{r})}{\partial \mathrm{r}}=$

$$
\begin{aligned}
& \left(\frac{\cos (\phi)}{\mathrm{r}}\right)\left(\cos (\phi) \cdot \Psi(\phi)+\sin (\phi) \cdot \frac{\partial \Psi(\phi)}{\partial \phi}\right) \frac{\partial \Psi(\mathrm{r})}{\partial \mathrm{r}}= \\
& \frac{\cos ^{2}(\phi)}{\mathrm{r}} \Psi(\phi) \frac{\partial \Psi(\mathrm{r})}{\partial \mathrm{r}}+\frac{\cos (\phi) \sin (\phi)}{\mathrm{r}} \frac{\partial \Psi(\phi)}{\partial \phi} \frac{\partial \Psi(\mathrm{r})}{\partial \mathrm{r}}
\end{aligned}
$$

d. Combining the terms in pt. b\&c:

$$
\begin{gathered}
\left(\frac{\sin ^{2}(\phi)}{\mathrm{r}}\right) \Psi(\phi) \frac{\partial \Psi(\mathrm{r})}{\partial \mathrm{r}}-\left(\frac{\sin (\phi) \cos (\phi)}{\mathrm{r}}\right) \frac{\partial \Psi(\phi)}{\partial \phi} \frac{\partial \Psi(\mathrm{r})}{\partial \mathrm{r}}+\left(\frac{\cos ^{2}(\phi)}{\mathrm{r}}\right) \Psi(\phi) \frac{\partial \Psi(\mathrm{r})}{\partial \mathrm{r}} \\
+\left(\frac{\cos (\phi) \sin (\phi)}{\mathrm{r}}\right) \frac{\partial \Psi(\phi)}{\partial \phi} \frac{\partial \Psi(\mathrm{r})}{\partial \mathrm{r}}= \\
\\
\frac{\left(\sin ^{2}(\phi)+\cos ^{2}(\phi)\right)}{\mathrm{r}} \Psi(\phi) \frac{\partial \Psi(\mathrm{r})}{\partial \mathrm{r}}=\frac{\Psi(\phi)}{\mathrm{r}} \frac{\partial \Psi(\mathrm{r})}{\partial \mathrm{r}}
\end{gathered}
$$

Therefore you can state that the operator is $\frac{1}{\mathrm{r}} \frac{\partial}{\partial \mathrm{r}}$
5. Last one. In question 4 we have simplified all the terms but the last two:

$$
\left(\frac{\sin (\phi)}{\mathrm{r}^{2}}\right) \frac{\partial}{\partial \phi} \cdot \sin (\phi) \frac{\partial}{\partial \phi}+\left(\frac{\cos (\phi)}{\mathrm{r}^{2}}\right) \frac{\partial}{\partial \phi} \cdot \cos (\phi) \frac{\partial}{\partial \phi}
$$

Try acting on this operator with a wavefunction $\Psi(r) \cdot \Psi(\phi)$ to show that it is equal to:

$$
\Psi(\mathrm{r})\left(\frac{1}{\mathrm{r}^{2}} \frac{\partial^{2} \Psi(\phi)}{\partial \phi^{2}}\right)
$$

Hint, you're going to use the product rule again.
Answer: Well, do what it says:

$$
\begin{aligned}
& \left(\frac{\sin (\phi)}{\mathrm{r}^{2}}\right) \frac{\partial}{\partial \phi} \cdot \sin (\phi) \frac{\partial \Psi(\mathrm{r}) \cdot \Psi(\phi)}{\partial \phi}+\left(\frac{\cos (\phi)}{\mathrm{r}^{2}}\right) \frac{\partial}{\partial \phi} \cdot \cos (\phi) \frac{\partial \Psi(\mathrm{r}) \cdot \Psi(\phi)}{\partial \phi}= \\
& \Psi(\mathrm{r})\left(\frac{\sin (\phi)}{\mathrm{r}^{2}}\right) \frac{\partial}{\partial \phi} \cdot \sin (\phi) \frac{\partial \Psi(\phi)}{\partial \phi}+\Psi(\mathrm{r})\left(\frac{\cos (\phi)}{\mathrm{r}^{2}}\right) \frac{\partial}{\partial \phi} \cdot \cos (\phi) \frac{\partial \Psi(\phi)}{\partial \phi}
\end{aligned}
$$

Now you have to use the product rule:

$$
\begin{aligned}
& \Psi(\mathrm{r})\left(\frac{\sin (\phi)}{\mathrm{r}^{2}}\right)\left(\cos (\phi) \frac{\partial \Psi(\phi)}{\partial \phi}+\sin (\phi) \frac{\partial^{2} \Psi(\phi)}{\partial \phi^{2}}\right)+\Psi(\mathrm{r})\left(\frac{\cos (\phi)}{\mathrm{r}^{2}}\right)\left(-\sin (\phi) \frac{\partial \Psi(\phi)}{\partial \phi}+\cos (\phi) \frac{\partial^{2} \Psi(\phi)}{\partial \phi^{2}}\right)= \\
& \Psi(\mathrm{r})\left(\frac{\sin (\phi) \cos (\phi)}{\mathrm{r}^{2}} \frac{\partial \Psi(\phi)}{\partial \phi}+\frac{\sin ^{2}(\phi)}{\mathrm{r}^{2}} \frac{\partial^{2} \Psi(\phi)}{\partial \phi^{2}}\right)+\Psi(\mathrm{r})\left(\frac{-\sin (\phi) \cos (\phi)}{\mathrm{r}^{2}} \frac{\partial \Psi(\phi)}{\partial \phi}+\frac{\cos ^{2}(\phi)}{\mathrm{r}^{2}} \frac{\partial^{2} \Psi(\phi)}{\partial \phi^{2}}\right)= \\
& \Psi(\mathrm{r})\left(\frac{\sin ^{2}(\phi)}{\mathrm{r}^{2}} \frac{\partial^{2} \Psi(\phi)}{\partial \phi^{2}}\right)+\Psi(\mathrm{r})\left(\frac{\cos ^{2}(\phi)}{\mathrm{r}^{2}} \frac{\partial^{2} \Psi(\phi)}{\partial \phi^{2}}\right)=\Psi(\mathrm{r})\left(\frac{\sin ^{2}(\phi)+\cos ^{2}(\phi)}{\mathrm{r}^{2}} \frac{\partial^{2} \Psi(\phi)}{\partial \phi^{2}}\right)=\Psi(\mathrm{r})\left(\frac{1}{\mathrm{r}^{2}} \frac{\partial^{2} \Psi(\phi)}{\partial \phi^{2}}\right)
\end{aligned}
$$

are the negative of eachother, so when added you get 0 .
6. Calculate the 1 s and 1 p kinetic energy (in eV ) for an electron in a 1 nm sphere. Discuss whether this is a lot of energy or not so much (perhaps compare it to the temperature necessary to reach the same thermal energy). Hint: you have to be careful about finding the zero's of a Bessel vs. spherical Bessel function.

Answer: From class, we saw that the energy was related to:

$$
\mathrm{J}_{0 \text { or } 1}(k \cdot a)=0
$$

where $k \cdot a$ provides 0's for the spherical Bessel functions. The $1^{\text {st }}$ zero for the 1 -s state is at 3.14 , and for the $1-p$ state it is 4.49 , see:
https://quantummechanics.ucsd.edu/ph130a/130 notes/node226.html.
Hence, the energy of the 1-s state is:

$$
k \cdot a=\sqrt{\frac{2 m E}{\hbar^{2}}} a=3.14
$$

Using a of 1 nm , etc., we find an energy of $6.02 \times 10^{-20} \mathrm{~J}$, or 0.38 eV . Similarly, for the $1-$ $p$ state we find $E=1.23 \times 10^{-19} \mathrm{~J}$, or 0.77 eV . This is a very large amount of energy, as it corresponds to a thermal temperature of 4400 K .
7. A certain one-particle, one-dimensional system has a wave function given by

$$
\psi=a e^{-i b t} e^{-b m x^{2} / \hbar}
$$

where $a$ and $b$ are constants and $m$ is the particle's mass. Given that the timedependent Schrodinger equation is:

$$
-\frac{\hbar}{i} \frac{\partial}{\partial t} \psi=-\frac{\hbar^{2}}{2 m} \frac{\partial^{2}}{\partial x^{2}} \psi+\hat{V} \psi=E \psi
$$

a. Please find the potential energy function V.
b. While you're at it, find $E$ (energy) for this system.

Answer: a. Starting with:

$$
-\frac{\hbar}{i} \frac{\partial}{\partial t} \psi=-\frac{\hbar}{i} \frac{\partial}{\partial t} a e^{-i b t} e^{-b m x^{2} / \hbar}=\hbar b \cdot a e^{-i b t} e^{-b m x^{2} / \hbar}
$$

Factoring out $\psi$ gives:

$$
-\frac{\hbar}{i} \frac{\partial}{\partial t} \psi=\hbar b \cdot \psi
$$

And on the other side:

$$
-\frac{\hbar^{2}}{2 m} \frac{\partial^{2}}{\partial x^{2}} a e^{-i b t} e^{-b m x^{2} / \hbar}=-\frac{\hbar^{2}}{2 m} a e^{-i b t}\left\{\frac{2 b m e^{-b m x^{2} / \hbar}}{\hbar}\left(\frac{2 b m x^{2}}{\hbar}-1\right)\right\}
$$

Simplification gives:

$$
\begin{aligned}
-\frac{\hbar^{2}}{2 m} a e^{-i b t} & \left\{\frac{2 b m e^{-b m x^{2} / \hbar}}{\hbar}\left(\frac{2 b m x^{2}}{\hbar}-1\right)\right\} \\
& =-\frac{\hbar^{2}}{2 m} a e^{-i b t}\left\{\frac{4 b^{2} m^{2} x^{2} e^{-b m x^{2} / \hbar}}{\hbar^{2}}-\frac{2 b m e^{-b m x^{2} / \hbar}}{\hbar}\right\}
\end{aligned}
$$

Factoring out $\psi$ gives:

$$
-2 b^{2} m x^{2} \cdot \psi+\hbar b \cdot \psi
$$

Now going back to the original $-\frac{\hbar}{i} \frac{\partial}{\partial t} \psi=-\frac{\hbar^{2}}{2 m} \frac{\partial^{2}}{\partial x^{2}} \psi+\hat{V} \psi$ expression:

$$
\hbar b \cdot \psi=-2 b^{2} m x^{2} \cdot \psi+\hbar b \cdot \psi+\hat{V} \psi
$$

We can simply solve for V :

$$
\hbar b \cdot \psi+2 b^{2} m x^{2} \cdot \psi-\hbar b \cdot \psi=\hat{V} \psi
$$

Therefore $\hat{V}=2 b^{2} m x^{2}$
b. Since $-\frac{\hbar}{i} \frac{\partial}{\partial t} \psi=\widehat{H} \psi=E \psi$, and that $-\frac{\hbar}{i} \frac{\partial}{\partial t} \psi=\hbar b \cdot \psi=E \psi$, clearly the energy is $\hbar b$.
8. Let's say that the last problem was secretly about the Harmonic oscillator, for which the potential energy operator is: $\hat{V}=\frac{1}{2} k_{f} x^{2}$. Can you determine what "b" actually is in terms of the angular frequency: $\omega=\sqrt{\frac{k_{f}}{m}}$, and show that the energy is: $E=\frac{1}{2} \hbar \omega$ ?

Answer: If $\hat{V}=\frac{1}{2} k_{f} x^{2}=2 b^{2} m=\frac{1}{2} k_{f}$, then $b=\frac{1}{2} \sqrt{\frac{k_{f}}{m}}=\frac{1}{2} \omega$, and thus $\hat{V}=2 b^{2} m x^{2}=$ $2 \frac{\omega^{2}}{4} m x^{2}=\frac{1}{2} m \omega^{2} x^{2}$. Likewise the energy is $E=\frac{1}{2} \hbar \sqrt{\frac{k_{f}}{m}}=\frac{1}{2} \hbar \omega$.
9. Write the following complex numbers in the $x+i y$ form.
a. $(2+3 i)^{2}$
b. $\frac{1+3 i}{1-2 i}$

Answer: a. Just square the expression:

$$
(2+3 i) \cdot(2+3 i)=4+6 i+6 i+9 i 2=4-9+12 i=-5+12 i
$$

b. Try the same approach as last time:

$$
\frac{1+3 i}{1-2 i} \frac{(1+2 i)}{(1+2 i)}=\frac{1+2 i+3 i+6 i^{2}}{1+2 i-2 i-4 i^{2}}=\frac{-5+5 i}{5}=-1+i
$$

10. Although you should be aware that imaginary numbers are expressed as: a+ib, they may also come in the form: $r e^{i \theta}$ where x is the real axis and y is the imaginary as shown here. Can you transform the following into that form?
a. $1+2 \mathrm{i}$
b. 1-i
c. $\frac{1}{1+i}$.

Hint: the last one requires some additional effort.


Answer: a. Here you can see that the length and angle are defined by standard trigonometric relationships: $r=\sqrt{1^{2}+2^{2}}=\sqrt{5} ; \theta=\operatorname{atan}\left(\frac{2}{1}\right)=1.107$. Thus, the point is $\sqrt{5} \cdot e^{1.107 \cdot \theta}=\sqrt{5} \cdot e^{i \cdot 0.35 \pi \cdot \theta}$.
b. $\sqrt{2} \cdot e^{-0.7845 \cdot \theta}=\sqrt{2} \cdot e^{-i \cdot \frac{\pi}{4} \cdot \theta}$
C. $\frac{1}{(1+i)} \frac{1-i}{(1-i)}=\frac{1-i}{1-i+i-i^{2}}=\frac{1-i}{2}=\frac{1}{2}-\frac{1}{2} i$.

Therefore the answer is $\frac{\sqrt{2}}{2} \cdot e^{-0.7845 \cdot \theta}=\frac{\sqrt{2}}{2} \cdot e^{-i \cdot \frac{\pi}{4} \cdot \theta}$.

