

Exam 2, Q2 (4/2/20, Sturgeon)
Chem 322: Quantum Mechanics (30 pts total)
Material Covered: Chapter 7 (Engel, 2nd Ed.)

Name _____
(please print)

Exam instructions: This is question 2 of 3 for your “take-home” exam. Question 3 will be available on Friday. During this exam, you may use your textbook, lab notebook, class notes, and/or any other documents you prepared. ***This question is due by 5 pm TODAY...please take a picture/scan and email them to me.***

I agree to follow the guidelines listed above and state that I have neither given nor received any unauthorized aid on this exam.

(signature)

Like all quantum mechanical models, 2-dimensional rotation, sometimes referred to as the rigid rotor, has a Hamiltonian, an acceptable wavefunction, and a resulting eigenvalue or energy. The boundary condition that leads to the quantization is diagrammed in figure 7.5. The Hamiltonian can be written in Cartesian coordinates, but it is more desirable to use spherical polar coordinates.

Please write down the Schrodinger equation in Cartesian coordinates (eq. 7.10)

Please write the Schrodinger equation in spherical polar coordinates (eq. 7.11)

The solution to this differential equation is slightly different from other quantum models. The wavefunction has essentially two related solutions that can be viewed as rotation in the clockwise direction and rotation in the counter-clockwise direction. Write these wavefunctions below (eq. 7.12):

$$\Phi_+(\phi) =$$

$$\Phi_-(\phi) =$$

Example problem 7.4 shows how to determine the normalization constant, $A_{+\phi}$. Please show below how the normalization constant for $A_{-\phi}$, is determined...**show all work**.

Start here: $\Phi_{-}(\phi) =$

$\Phi_{-}^{*}(\phi) =$

(your result should confirm the normalization constant for both wavefunctions is the same)

Having two wavefunction, regardless of how similar they are, could cause some problems. So the way we deal with this is we group the “sign” (+ or -) with the quantum number m_l , hence the wave function then becomes:

$$\Phi_{-}(\phi) = Ae^{-im_l\phi} \dots \text{with } m_l = 0, \pm 1, \pm 2, \pm 3, \dots \text{get it?} \rightarrow \square \text{ (check here)}$$

Take home point:

Q: why is the m_l quantum number \pm where as n and l are just + integers?

A: because rotation can occur in two directions, clockwise and counter-clockwise.

From the form of the 2D rotation wavefunction, we kind of lose the visual aspect of the wavefunction since graphing the square of the above exp wavefunction is not immediately obvious. As you are probably aware, we can write this wavefunction in terms of trigonometric functions that are more visually understandable (**Note we don't want to do this when doing calculations since it is VERY easy to take derivatives of exponential functions!!!**) We do this using the Euler's relationship...have a look at Wikipedia, "Euler's formula, section Relationship to trigonometry"

Write the Euler's relationship here $\rightarrow e^{ix} =$

And the other Euler's relationship $\rightarrow e^{-ix} =$

...recall that the wavefunction has little meaning, but the square of the wavefunction (or better yet in this case, the $\Phi \times \Phi^*$ ← complex conjugate) has great significance and can be visualized. Considering the form of our wavefunction of interest, show how.. $\Phi_-(\phi) = Ae^{-im_l\phi}$ is converted to... $\Phi_-(\phi)^2 = \cos^2(m_l\phi) - \sin^2(m_l\phi)$ $\Phi_-(\phi)^2 \sim \cos^2(m_l\phi) + \sin^2(m_l\phi)$.

Okay, now that we have all the parts, show how the energy is derived by operating on the above wavefunction and solving for E_{m_l} (eq. 7.14).