Chem. 562
Spring 2012

Name ____________________________

Please put your name on all pages.

Exam 1

7:45

1. This exam contains 7 pages of questions and instructions, as well as two pages of equations and a page of tables.
2. Show your work and make your reasoning clear.
3. You have 1.5 hours to work on the exam.

1.__________/25

2.__________/25

3.__________/15

4.__________/10

5.__________/25

Total_______/100

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1. Consider the wavefunction

$$\Psi(\phi) = \frac{1}{2}\psi_2(\phi) + c_3\psi_3(\phi) + \frac{1}{\sqrt{3}}\psi_4(\phi)$$

where $\psi_2(\phi)$, $\psi_3(\phi)$, and $\psi_4(\phi)$ are the normalized eigenfunctions for the particle-on-a-ring with quantum numbers m_ℓ=+2, +3, and +4, respectively.

1a. (10 pts.) Calculate c_3.

Ψ must be normalized.

$$|\Psi|^2 = 1 = \frac{1}{4} + c_3^2 + \frac{1}{3} = 1$$ 5

$$c_3^2 = 1 - \frac{1}{4} - \frac{1}{3} = \frac{12}{12} - \frac{3}{12} - \frac{4}{12}$$

$$= \frac{5}{12}$$

$$\therefore c_3 = \sqrt{\frac{5}{12}}$$ 5

1b. (10 pts) Calculate $\langle \ell_z \rangle$ in units of $\hbar$.

$$\langle \ell_z \rangle = \int \Psi^* \hat{\ell}_z \Psi \, d\tau \quad \text{and} \quad \ell_z \psi_m = m\hbar$$ 5

$$= 2\hbar c_1^2 + 3\hbar c_2^2 + 4\hbar c_4^2$$

$$= 2\hbar \cdot \frac{1}{4} + 3\hbar \frac{5}{12} + 4\hbar \frac{1}{3}$$

$$\frac{6}{12} + \frac{15}{12} + \frac{16}{12}$$

$$= \frac{1}{2}\hbar + \frac{5}{4}\hbar + \frac{4}{3}\hbar$$ 5

$$= \frac{37}{12}\hbar$$

$$\frac{37}{12}$$

1c. (5 pts.) If we were to measure ℓ_z just once, what is the most likely value that we would obtain and explain why (in one sentence)? 5

We would measure $\underset{3}{\underline{3\hbar}}$ because $\underset{2}{\underline{|c_3|^2}}$ is the largest probability

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2a. (5 pts.) In a single sentence, explain why quantum mechanical operators must be Hermitian.

Because Hermetian operators give real eigenvalues.

2b. (10 pts.) Mathematically prove that quantum mechanical operators are Hermitian. Start by using the equation $\hat{A}\psi = a\,\psi$

$$\int \psi^* \hat{A} \psi = a \int \psi^* \psi = a \qquad \hat{A}^* \psi^* = a^* \psi^*$$

$$\int \psi \hat{A}^* \psi^* = a^* \int \psi \psi^* = a^*$$

because $a = a^*$ must be true

$$\int \psi^* A \psi = \int \psi \hat{A}^* \psi^*$$

definition of Hermetian.

2c. (10 pts). The x-projection of a dipole is given by $\mu_x = \mu_0 \sin(\theta)\cos(\varphi)$. In spherical harmonics (provided at the end of your exam), is the x-axis component of the dipole proportional to $(Y_{1,+1} + Y_{1,-1})$ or $(Y_{1,+1} - Y_{1,-1})$. Mathematically justify your answer.

expand using Euler's formula $e^{\pm i\phi} = \cos\phi \pm i\sin\phi$

0

$$Y_{1,+1} = -\left(\frac{3}{8\pi}\right)^{1/2} \sin\theta \left(\cos\phi + i\sin\phi\right)$$

since we want to keep $\cos\phi$ and loose $\sin\phi$,

3 something

$$Y_{1,-1} = +\left(\frac{3}{8\pi}\right)^{1/2} \sin\theta \left(\cos\phi - i\sin\phi\right)$$

subtract: $Y_{1,+1} - Y_{1,-1}$

5 something right

→ 7/10

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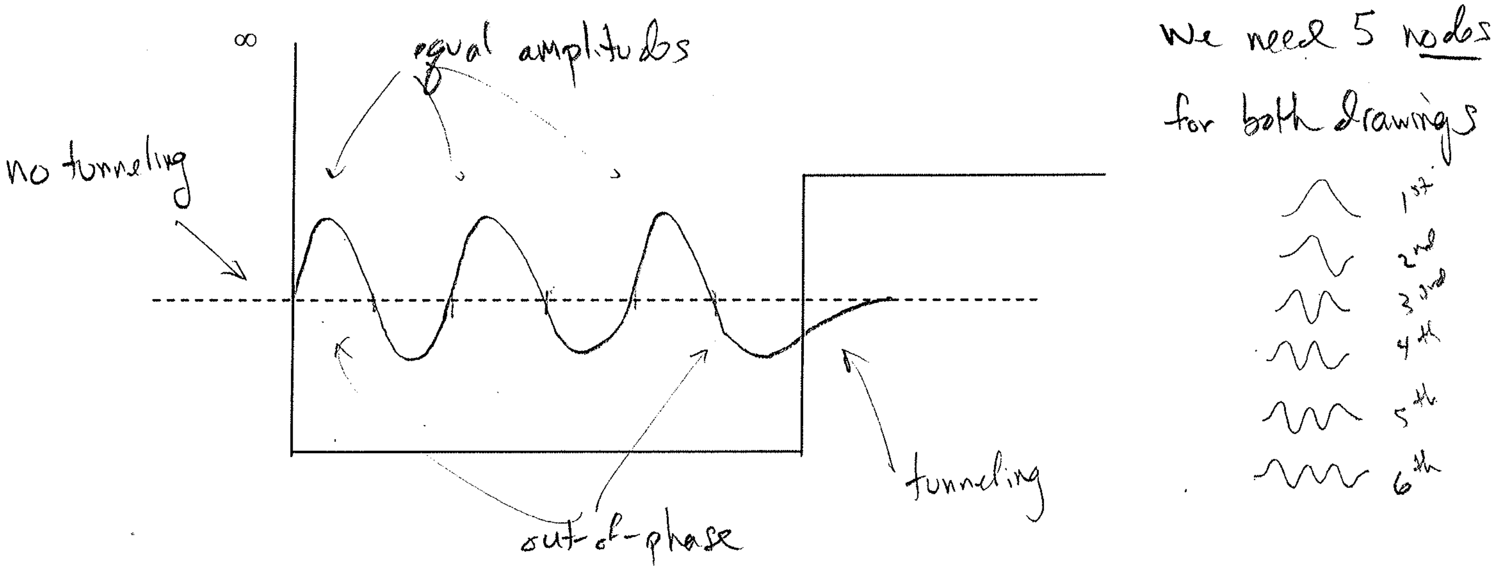
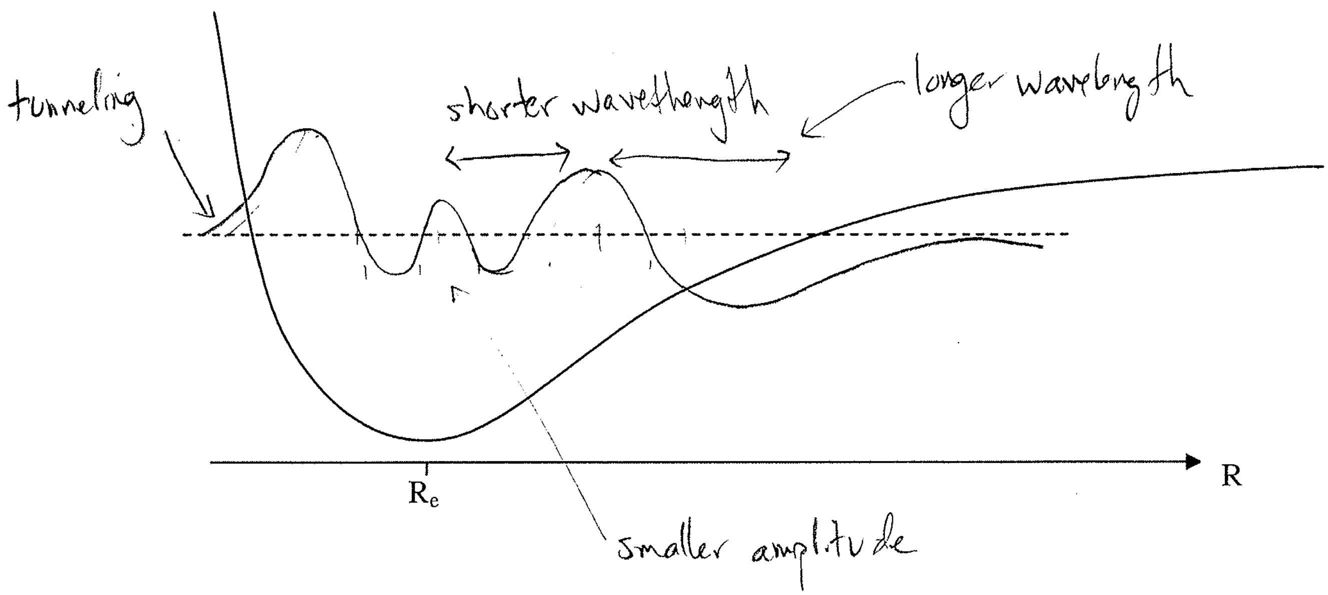
3a. (10 pts.) For each of the potential below, the dashed line is at the energy of the 6th eigenstate from the bottom of the well. Draw the wavefunction. You will be graded on the proper portrayal of the intensity, wavelength and shape of the wavefunction. So, be precise! You can point out important features if you are having problems drawing them accurately.





3c. (5 pts) Is it MORE, LESS or EQUALLY likely to find the particle at R<Re than R>R_e ? Explain.

Less likely, because slope is steeper.

~~Less~~ Particle spends most "time" on shallow shelf.

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4. (10 pts.) The Schrodinger equation for a particle-on-a-sphere is

$$\frac{-\hbar^2}{2m}\frac{1}{r^2}\Lambda^2\psi(\theta,\phi) = E\psi(\theta,\phi)$$

Show that the wavefunction is separable $\psi(\theta,\phi) = \Theta(\theta)\Phi(\phi)$ by re-writing the Schrodinger equation into the form $f(\theta) + f(\phi) = 0$. Label $f(\theta)$ and $f(\phi)$ in your answer.

+2

$$-\frac{\hbar^2}{2mr^2}\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right]\Theta(\theta)\Phi(\phi) = E\Theta(\theta)\Phi(\phi)$$

multiply by $\sin^2\theta$ & move coeffic. +3

$$\left[\frac{\partial^2}{\partial\phi^2} + \sin\theta\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right]\Theta(\theta)\Phi(\phi) = -\frac{2Emr^2}{\hbar^2}\sin^2\theta\,\Theta(\theta)\Phi(\phi)$$

$$\Theta(\theta)\frac{\partial^2}{\partial\phi^2}\Phi(\phi) + \Phi(\phi)\sin\theta\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\Theta(\theta) = -\frac{2mr^2E}{\hbar^2}\sin^2\theta\,\Theta(\theta)\Phi(\phi)$$

+5

divide by $\Theta(\theta)\Phi(\phi)$ and rearrange

$$\underbrace{\frac{1}{\Phi(\phi)}\frac{\partial^2}{\partial\phi^2}\Phi(\phi)}_{f(\phi)} + \underbrace{\frac{\sin\theta}{\Theta(\theta)}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\Theta(\theta) + \frac{2mr^2E}{\hbar^2}\sin^2\theta}_{f(\theta)} = 0$$

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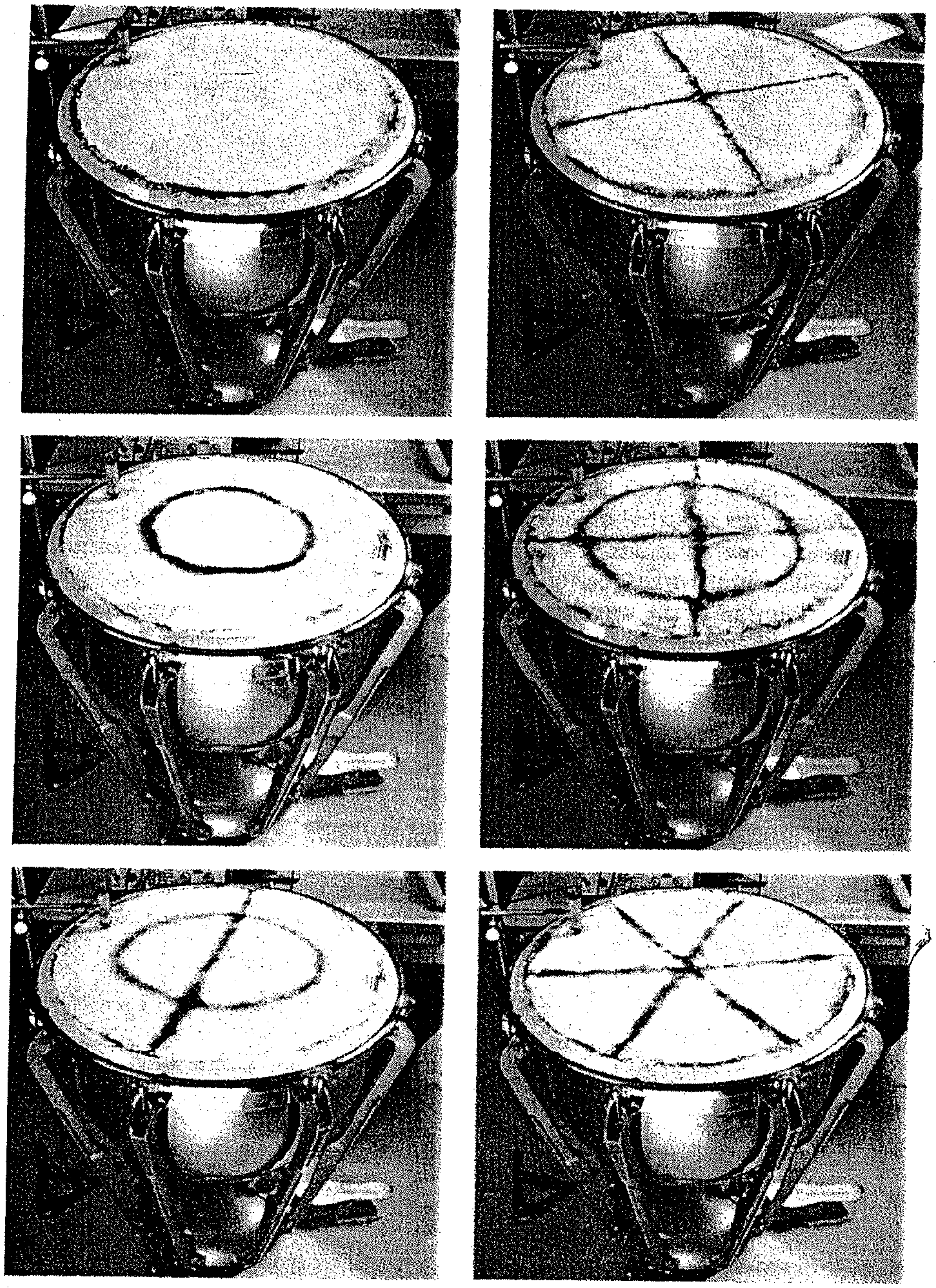
5. Shown below are a series of pictures of a vibrating drumhead with powder sprinkled on it. In each picture, the drumhead is being beaten at a particular frequency using a computer controlled hammer (upper left corner of the figures). The powder is dispersed in different patterns for each frequency. Answer the questions on the following page.

2-5 A Vibrating Membrane **63**



Powder that is sprinkled on a vibrating drumhead will collect at the nodes, where the vibrations are the weakest. The above photographs illustrate six of the normal modes of a circular drumhead.

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5a (5 pts). In one sentence, explain why the powder appears in lines and circles, rather than all over the place.

There are nodes.

5b (5 pts). If this were a quantum mechanical system (a particle-in-a-circular-plane), how many quantum numbers would you need to describe the system? And what coordinate system would you use (Cartesian, cylindrical, spherical or a combination)?

Two q.n. Cylindrical.

5c (5 pts). Write a 2-dimensional quantum mechanical wavefunction that is consistent with the observations in the pictures. Use a diameter D. No need to normalize

The wavefxn must be seperable because the lines and circles ~~or~~ can be manipulated independently of one another.

One must be P. on. Ring., the other P.I.B.

$$\Psi(\theta, r) = \Theta(\theta)\, R(r) = \frac{1}{(2\pi)^{1/2}} e^{im_\ell \phi} \left(\frac{2}{L}\right)^{1/2} \cos \frac{n\pi x}{D}$$

5e (5 pts). Write an expression for the energy that would describe any of these pictures. if ~~it~~ ~~was~~ they represented a particle w/ mass m

$$E = E_{ring} + E_{PIB} = \frac{m_\ell^2 \hbar^2}{2mr^2} + \frac{h^2 n^2}{8mD^2}$$

5d (5 pts). What values would the quantum numbers have for the picture in the lower left hand corner?

ring quantum number has 1 node, so $m_\ell = 1$.

box has two nodes, so $n = 3$.