Problem Set PS02

ISSUED: 9/7/00 **Due: 9/14/00**

Prof. Darin J. Ulness Name ______________________________

Instructions. Complete all questions before class on the due date. You are encouraged to work together. Be sure to struggle with the problem before seeking help. Many of the exercises are very similar to problems in the book. Understanding the solution to these problems will be helpful in completing the assigned exercises.

Mathematical Exercises

1. The zeros of functions are important points. The zeros of wavefunctions are called *nodes* which you have probably heard about in freshman chemistry.

   (a) Find the values of a_n such that $f(x) = \cos a_n x$ has zeros at $x = -L$ and $x = L$.

   (b) How many zeros does the function $f(x) = xe^{-\frac{1}{2}x^2}$ have?

   (c) How many zeros does the function $f(x) = (4x^2 - 2)e^{-\frac{1}{2}x^2}$ have?

2. Verify by direct substitution that

$$\begin{aligned} y_1 &= A \sin kx, \\ y_2 &= B \cos kx, \\ y_3 &= C_+ e^{ikx}, \end{aligned}$$

   and

$$y_4 = C_- e^{-ikx},$$

   are solutions of

$$\frac{d^2 y}{dx^2} + k^2 y = 0, \tag{1}$$

   where k is a positive real constant.

3. Equation (1) above is called a second order ordinary differential equation (O.D.E.) and the theory of O.D.E.'s states that there are n and only n independent solutions for any n^{th} order O.D.E. Here $n = 2$, so we expect two independent solutions. Therefore y_1, y_2, y_3 and y_4 can not all be independent. Show that y_3 and y_4 can be written in terms of y_1 and y_2. (Hint: remember Euler's identity.)

Exercises

4. Which of the following are eigenfunctions of the momentum operator $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$. That is, for which of the following is $\hat{p}_x \psi(x) = \lambda \psi(x)$, where the eigenvalue, λ, is a number and <u>not</u> a function of x (give the eigenvalues when appropriate). Which are eigenfunctions of the kinetic energy operator $\hat{T} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$(give eigenvalues when appropriate). .

   (a) $\psi(x) = e^x$

(b) $\psi(x) = xe^{-\alpha x}$

(c) $\psi(x) = \sin kx$

(d) $\psi(x) = kx^2$

(e) $\psi(x) = e^{-\frac{1}{2}x^2}$

5. We shall see later that the so-called radial wavefunction for the 1s atomic orbital is of the form $\psi(r) = e^{-\alpha r}$, where α is a positive constant and $0 \leq r \leq \infty$. What are the units for α? Normalize this wavefunction. The radial wavefunction describes the electron's distance from the nucleus. Find the probability that the electron is more than a distance $r = 1/\alpha$ away from the nucleus.

6. Often one is interested in extracting the average value of some property from a wavefunction. This is done using the average value theorem which states that the average value of some observable, $\hat{O}$, is given by

$$\left\langle \hat{O} \right\rangle = \int_{\substack{\text{all}\\ \text{space}}} \psi^*_{\text{norm}} \hat{O} \psi_{\text{norm}}, \tag{1}$$

where the angled brackets denote averaging. Considering the radial wavefunction given above, find the average value of $\hat{r}$ and $\hat{r}^2$.

7. The variance or uncertainty of the average value of an observable is denoted as δO and is given by

$$\delta O = \sqrt{\left\langle \hat{O}^2 \right\rangle - \left\langle \hat{O} \right\rangle^2}. \tag{2}$$

Find δr for the radial wavefunction used in the previous two problems.

Conceptual Problems

8. Can you every know *exactly* where your car keys are?

9. Assume a quantum object is confined an opaque small cube in three dimensional space. Over time the cube grows in size. How does the minimum uncertainty in the position and momentum of the object change?

Computer Problems

10. Use MATHEMATICA to plot the family of functions $f(x) = \sin n\pi x$, where $n = 1, 2, 3 \cdots$ from 0 to 1. Do all your plots share $x = 0$ and $x = 1$ as common zeros?

11. A quantum object is confined to the range $0 < x < \infty$ and is described by the wavefunction $\psi(x) = \frac{J_1(ax)}{ax}$, where $J_1(ax)$ is the first order Bessel function. Use MATHEMATICA to plot $\psi(x)$ and $|\psi(x)|^2$ for $a = 1$ and to normalize $\psi(x)$. (Hint: Look-up how to use the `BesselJ` function in the MATHEMATICA book or the online help.) Would you ever expect to find the quantum object at $x = 0$? Make a histogram of the probability of finding the object in the interval between each successive integer (i.e., find the probability of finding the object between $x = 0$ and $x = 1$, then between $x = 1$ and $x = 2$ etc. up to between $x = 9$ and $x = 10$). When doing this you will get answers that look frightening, but they are just numbers so use the `N[]` command to turn them into decimals.

Reflective Exercises

12. Write a short response to the letter to the editor which appeared in the *Fargo Forum* last year. Your response may be in support of, in opposition to, or neutral with regard to the author's opinion.

WEDNESDAY, AUGUST 25, 1999

Letters to The Forum

Not all of us worship at the altar of science

In order to graduate from Fargo-Moorhead colleges it is necessary to study at least one year of natural sciences. Six credits of natural sciences are required to satisfy the liberal arts requirements. This policy applies to all majors regardless if you study nursing or philosophy. Why should students who are not interested in sciences be forced to study sciences?

Why is there so much emphasis on sciences in society? Why do universities, which are independent from other institutions, follow the path of "admiration" of science and force students, who have other values, to conform?

It is possible to graduate from college without ever having taken a philosophy class. Wouldn't it be more logical to make students think in order to become responsible citizens than force them to study science? Isn't our world ruled by scientists?

In former times when other parts of culture like morality and art had equal value with science people had a little bit broader world view than we have today. Isn't it time to think of the consequences that brought us science in all parts of our lives?

I think it is time to become aware of the value that we have as human beings and to start thinking about our future.

Susanne Steinfeld
Moorhead

13. Please read the attached article by M. Singham which appeared in the June 2000 edition of *Physics Today.* The article is directed at physics teachers and students, but applies equally well to chemistry.

    (a) What are some reasons to accept what I teach in PChem as true?

    (b) What are some reasons to not accept what I teach in PChem as true?

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①

(a) $f(-L) = \cos(a_n L)$, $f(L) = \cos(a_n L)$ $\rightarrow$ $\boxed{a_n = \frac{n\pi}{2L} \quad n = \pm1, \pm3, \pm5 \ldots}$

(b) $f(x) = \underbrace{x}_{1\text{ zero}}\ \underbrace{e^{-\frac{x^2}{2}}}_{\text{no zeros}}$ so 1 zero at $x=0$

(c) $f(x) = \underbrace{(4x^2-2)}_{2\text{ zeros}}\ \underbrace{e^{-\frac{x^2}{2}}}_{\text{no zeros}}$ $\quad 4x^2-2=0$, $x^2 = \frac{1}{2} \Rightarrow x = \pm\sqrt{\frac{1}{2}}$

so $\boxed{2 \text{ zeros at } \pm\sqrt{\frac{1}{2}}}$

②

$$\frac{d^2y_1}{dx^2} + k^2 y_1 = -k^2 A\sin kx + k^2 A\sin kx = 0 \checkmark$$

$$\frac{d^2y_2}{dx^2} + k^2 y_2 = -k^2 B\cos kx + k^2 B\cos kx = 0 \checkmark$$

$$\frac{d^2y_3}{dx^2} + k^2 y_3 = -k^2 C_+ e^{ikx} + k^2 C_+ e^{ikx} = 0 \checkmark$$

$$\frac{d^2y_4}{dx^2} + k^2 y_4 = -k^2 C_- e^{-ikx} + k^2 C_- e^{-ikx} = 0 \checkmark$$

③

$$y_3 = C_+ e^{ikx} = C_+(\cos kx + i\sin kx)$$

$$y_3 = \underbrace{C_+\cos kx}_{\frac{C_+}{B}y_2} + \underbrace{iC_+\sin kx}_{\frac{C_+}{A}y_1} = \boxed{\frac{C_+}{B}y_2 + i\frac{C_+}{A}y_1}$$

$$y_4 = C_- e^{-ikx} = C_-(\cos kx - i\sin kx)$$

$$= \underbrace{C_-\cos kx}_{\frac{C_-}{B}y_2} - \underbrace{iC_-\sin kx}_{-i\frac{C_-}{A}y_1} = \boxed{\frac{C_-}{B}y_2 - i\frac{C_-}{A}y_1}$$

④

(a) $\hat{p}_x \psi(x) = -i\hbar\frac{\partial}{\partial x}e^x = -i\hbar e^x$ $\quad \boxed{\lambda = -i\hbar}$

(b) $\hat{p}_x \psi(x) = -i\hbar\frac{\partial}{\partial x}xe^{-\alpha x} = -i\hbar(x\alpha e^{-\alpha x} + e^{-\alpha x})$ not eigenfunction

(c) $\hat{p}_x \psi(x) = -i\hbar\frac{\partial}{\partial x}\sin kx = -i\hbar k\cos kx$ not eigenfunction

(d) $\hat{p}_x \psi(x) = -i\hbar\frac{\partial}{\partial x}kx^2 = -i\hbar 2kx$ not eigenfunction

(e) $\hat{p}_x \psi(x) = -i\hbar\frac{\partial}{\partial x}e^{-\frac{x^2}{2}} = +i\hbar\frac{x}{2}e^{-\frac{x^2}{2}}$ not eigenfunction

(a) $\hat{T}\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}e^x = -\frac{\hbar}{2m}e^x$ $\quad \boxed{\lambda = \frac{\hbar^2}{2m}}$

(b) $\hat{T}\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}xe^{-\alpha x} = -\frac{\hbar^2}{2m}(\alpha^2 xe^{-\alpha x} + 2\alpha e^{-\alpha x})$ not eigenfunction

(c) $\hat{T}\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\sin kx = +\frac{\hbar^2 k^2}{2m}\sin kx$ $\quad \boxed{\lambda = \frac{\hbar^2 k^2}{2m}}$

(d) $\hat{T}\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}kx^2 = -\frac{\hbar^2}{m}$ not eigenfunction

(e) $\hat{T}\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}e^{-\frac{x^2}{2}} = -\frac{\hbar}{2m}\left(\frac{x^2}{2}e^{-\frac{x^2}{2}} + \frac{1}{2}e^{-\frac{x^2}{2}}\right)$ not eigenfunction

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⑤

$$N = \sqrt{\int_0^\infty e^{-2\alpha r}dr} = \sqrt{\frac{1}{-2\alpha}e^{-2\alpha r}\Big|_0^\infty} = \sqrt{\frac{1}{2\alpha}}$$

so $\boxed{\psi_{norm} = \sqrt{2\alpha}\,e^{-\alpha r}}$ $\quad \boxed{\alpha \text{ has units of } \frac{1}{\text{distance}}}$

$$P(r>a) = \int_a^\infty |\psi_{norm}|^2 dr = 2\alpha\int_a^\infty e^{-2\alpha r} = -\frac{2\alpha}{2\alpha}e^{-2\alpha r}\Big|_a^\infty$$

$$= \boxed{e^{-2}}$$

⑥

$$\langle r \rangle = \int_0^\infty \sqrt{2\alpha}e^{-\alpha r}\, r\, \sqrt{2\alpha}e^{-\alpha r}dr = 2\alpha\int_0^\infty re^{-2\alpha r}dr = 2\alpha\frac{re^{-2\alpha r}}{-2\alpha}\Big|_0^\infty - 2\alpha\int_0^\infty \frac{-1}{2\alpha}e^{-2\alpha r}dr$$

$u = r \quad v = \frac{1}{-2\alpha}e^{-2\alpha r}$

$du = dr \quad dv = e^{-2\alpha r}dr$

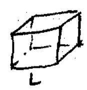
$$= \boxed{\frac{1}{2\alpha}}$$

$$2\alpha\int_0^\infty e^{-\alpha r}r^2e^{-\alpha r}dr \xrightarrow{\text{mathematica}} \frac{1}{2\alpha^2}$$

⑦ from ⑥

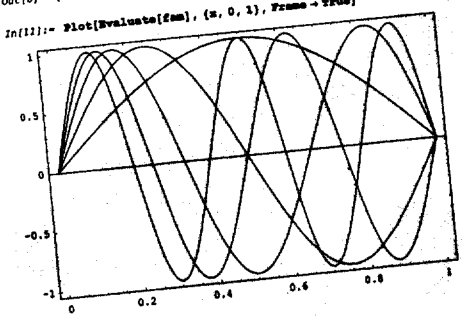
$$\delta r = \sqrt{\frac{1}{2\alpha^2} - \frac{1}{2\alpha}} = \boxed{\sqrt{\frac{1-\alpha}{2\alpha^2}}}$$

⑧ yes, but only for an instant then you have no idea where they went

⑨  $L\uparrow \quad \delta\vec{x}\downarrow,\ \delta\hat{p}\uparrow$

⑩

```
In[8]:= fam = Table[Sin[n Pi x], {n, 1, 5}]
Out[8]= {Sin[π x], Sin[2 π x], Sin[3 π x], Sin[4 π x], Sin[5 π x]}
In[11]:= Plot[Evaluate[fam], {x, 0, 1}, Frame → True]
```

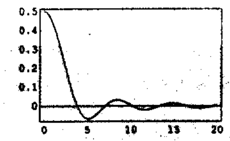


Out[11]= -Graphics-

(11)

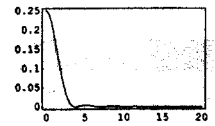
In[60]:= unorm = BesselJ[1, x] / x;

In[62]:= Plot[unorm, {x, 0, 20}, PlotRange → All, Frame → True]



Out[62]= - Graphics -

In[65]:= Plot[unorm^2, {x, 0, 20}, PlotRange → All, Frame → True]



Out[65]= - Graphics -

In[69]:= n = Sqrt[Integrate[unorm^2, {x, 0, Infinity}]]

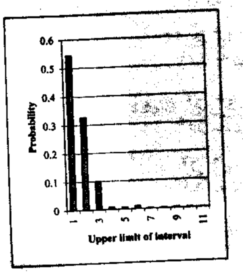
Out[69]= $\frac{2}{\sqrt{3\pi}}$

In[71]:= norm = 1 / n unorm;

In[75]:= Table[N[Integrate[norm^2, {x, i, i + 1}]], {i, 0, 10}]

Out[75]= {0.542905, 0.326061, 0.0998647, 0.0075519, 0.00589246, 0.0085665, 0.00172915, 0.000846939, 0.00224573, 0.000755273, 0.000198626}

0.542905
0.326061
0.099865
0.007552
0.005892
0.008567
0.001729
0.000847
0.002246
0.000755
0.000199



(12)+(13) your words