Problem Set PS02

ISSUED: 9/6/01 **Due: 9/13/01**

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 $f(x) = e^{-x} \sin a_n x$ has zeros at $x = 0$ and $x = L$.

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

   (c) Find the value of a_n such that $f(x) = (x^2 - a_n)e^{-\frac{1}{2}x^2}$ has zeros at $x = -2$ and $x = 2$. How about at $x = -L$ and and $x = L$.

2. Verify by direct substitution that

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

   and

$$y_4 = De^{-ikx},$$

   are solutions of

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

   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_1 and y_2 can be written in terms of y_3 and y_4. (Hint: remember Euler's identity.)

4. Verify by direct substitution that any *linear combination* of the independent solutions of Eq. (1), $Y = \alpha y_1 + \beta y_2$, is also a solution of Eq. (1). (Note: α and β are constants).

Exercises

5. Suppose some crazy operator, $\hat{O}_{xp}$ is defined using the position operator $\hat{x} = x$ and the $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$ such that $\hat{O}_{xp} \equiv \hat{x}\hat{p}_x$. Which of the follow wavefunctions are eigenfunctions of $\hat{O}_{xp}$. That is, for which of the following is $\hat{O}_{xp}\psi(x) = \lambda\psi(x)$, where the eigenvalue, λ, is a number and <u>not</u> a function of x (give the eigenvalues when appropriate). .
   (a) $\psi(x) = e^x$
   (b) $\psi(x) = xe^{-\alpha x}$
   (c) $\psi(x) = kx^2$

6. Suppose a different operator from the one in the previous problem is defined as $\hat{O}_{px} \equiv \hat{p}_x\hat{x}$. Does $\hat{O}_{px}\psi(x) = \hat{O}_{xp}\psi(x)$ for any of the wavefunction is the previous problem? Guess first then work your answers. Did you guess correctly?

7. The wavefunction that describes a tunneling electron in the "forbidden" region ($0 < x < L$) is of the form $\psi(x) = e^{-\alpha x}$, where α is a positive constant which is proportional to the energy difference between the potential energy of the forbidden region and the energy of the electron. What are the units for α? Normalize this wavefunction over the forbidden region. Find the probability that the tunneling electron has tunnelled less than a distance $x = 1/\alpha$ away from the nucleus. Does this probability depend on L? One concern in the push for smaller and faster silicon based computers is that when so much circuitry is packed into a small region electrons might well tunnel from one place to another thus causing the circuit to behave incorrectly. The barrier between independent conducting pathways should be such that the probability of tunneling across it is very low. Calculate what L should be in units of $1/\alpha$ such that the probability of an electron tunneling half way into the forbidden region is $< 0.01\%$. One thing to note about this problem is that by normalizing over the forbidden region we are considering only those electrons that are tunneling. This is quite likely only a very small percentage of all the electrons.

8. 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 tunneling wavefunction given above, find the average value of $\hat{x}$ and $\hat{x}^2$.

9. 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 δx for the tunneling wavefunction used in the previous two problems.

Conceptual Problems

10. Can you every know *exactly* where your PChem notes are?
11. Use the uncertainty principle to explain why atoms are stable.
12. How does knowing the variance (or standard deviation) and average value of a physical property improve ones picture of what is going on versus only knowledged of the average itself?

Computer Problems

13. 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?
14. A quantum object is confined to the range $0 < x < \infty$ and is described by the set of wavefunctions $\psi_n(x) = x^n K_n(x)$, where $K_n(x)$ is the n^{th} order modified Bessel function of the second kind and $n = 1, 2, 3\cdots$. Use MATHEMATICA to plot $\psi_n(x)$ and $|\psi_n(x)|^2$ and to normalize $\psi_n(x)$ for the cases of $n = 1, 2$ and 3. (Hint: Look-up how to use the `BesselK` function in the MATHEMATICA book or the online help.)

Reflective Exercises

15. 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?
16. Write a short response to the letter to the editor which appeared in the *Fargo Forum* two years ago. Your response may be in support of, in opposition to, or neutral with regard to the author's opinion.

Not all of us worship at the altar of science

Letters to The Forum

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?

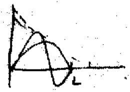
It is possible to graduate from college without ever having taken a philosophy class. Wouldn't it be more logical to make students think in order to become responsible citizens than force them to study science? Isn't our world ruled by scientists?

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

① ⓐ Want



e^{-x} is never zero so we only need to focus on the $\sin a_n x$ factor

$\sin a_n x$ is always zero at $x=0$

for $\sin a_n x$ to be zero at $x=L$, $a_n L = n\pi$ $n=\pm1,\pm2$.

$\Rightarrow \boxed{a_n = \frac{n\pi}{L}}$ $n=\pm1,\pm2\cdots$

ⓑ $e^{-\frac{x^2}{2}}$ is never zero so focus on x^2-1

This can be factored $x^2-1 = (x+1)(x+1)$

$\Rightarrow$ zeros at $\boxed{x=\pm1}$

ⓒ want $f(-2)=f(2)=0$

again $e^{-\frac{x^2}{2}}$ is never zero so consider x^2-a_n

$x^2-a_n\Big|_{x=\pm2} = 4-a_n=0 \Rightarrow \boxed{a_n=4}$

$x^2-a_n\Big|_{x=\pm L} = L^2-a_n=0 \Rightarrow a_n=L^2$

②

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

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

$\frac{d^2y_3}{dx^2}+k^2y_2 = -k^2Ce^{ikx} + k^2Ce^{ikx} = 0$ ✓

$\frac{d^2y_4}{dx^2}+k^2y_4 = -k^2De^{-ikx} + k^2Ce^{-ikx} = 0$ ✓

③ from Euler's identities

$\cos kx = \frac{1}{2}(e^{ikx}+e^{-ikx})$, $\sin kx = \frac{1}{2i}(e^{ikx}-e^{-ikx})$

$y_1 = A\sin kx = \frac{A}{2i}(e^{ikx}-e^{-ikx}) = \frac{A}{2i}\left(\frac{y_3}{C}-\frac{y_4}{D}\right)$ ✓

$y_2 = B\cos kx = \frac{B}{2}(e^{ikx}+e^{-ikx}) = \frac{B}{2}\left(\frac{y_3}{C}+\frac{y_4}{C}\right)$ ✓

④ $\frac{d^2Y}{dx^2}+k^2Y = -k^2\alpha A\sin kx - k^2\beta B\cos kx + k^2(\alpha A\sin kx + \beta B\cos kx)$

$= 0$ ✓

⑤ ⓐ $\hat{O}_{xp}e^x = x\left(-i\hbar\frac{d}{dx}\right)e^x = -i\hbar xe^x$ not eigenfunction

ⓑ $\hat{O}_{xp}\,xe^{-\alpha x} = x\left(-i\hbar\frac{d}{dx}\right)xe^{-\alpha x} = +i\hbar\alpha x^2e^{-\alpha x} - i\hbar xe^{-\alpha x}$ not eigenfunction

ⓒ $\hat{O}_{xp}\,kx^2 = x\left(-i\hbar\frac{d}{dx}\right)kx^2 = 2i\hbar kx^2$ eigenfunction $\lambda = -2i\hbar$

⑥ ⓐ $\hat{O}_{px}e^x = -i\hbar\frac{d}{dx}xe^x = -i\hbar xe^x - i\hbar e^x$

ⓑ $\hat{O}_{px}\,xe^{-\alpha x} = -i\hbar\frac{d}{dx}x^2e^{-\alpha x} = +\alpha i\hbar x^2e^{-\alpha x} - 2i\hbar xe^{-\alpha x}$

ⓒ $\hat{O}_{px}\,kx^2 = -i\hbar\frac{d}{dx}kx^3 = 3i\hbar kx^2$

none of these are the same as in ⑤

⑦ α has units of $\frac{1}{\text{length}}$

$N = \sqrt{\int_0^L|e^{-\alpha x}|^2dx} = \sqrt{\int_0^L e^{-2\alpha x}dx} = \sqrt{\frac{-1}{2\alpha}(e^{-2\alpha L}-1)}$

$\psi_{norm} = \frac{1}{\sqrt{\frac{1}{2\alpha}(1-e^{-2\alpha L})}}e^{-\alpha x}$

$P(x<\frac{1}{\alpha}) = \frac{2\alpha}{1-e^{-2\alpha L}}\int_0^{1/\alpha}e^{-2\alpha x}dx$

$= \frac{2\alpha}{(1-e^{-2\alpha L})}\left(\frac{1}{2\alpha}(1-e^{-2})\right)$

$= \frac{(1-e^{-2})}{(1-e^{-2\alpha L})}$

⑦ cont

$P(x>\frac{L}{2}) = \frac{2\alpha}{1-e^{-2\alpha L}}\int_{\frac{L}{2}}^{L}e^{-2\alpha x}dx = \frac{e^{-L\alpha}-e^{-2L\alpha}}{1-e^{-2\alpha L}}$

in units of α

$P(x>\frac{L}{2}) = \frac{e^{-L}-e^{-2L}}{1-e^{-2L}} < 0.0001$

$L > 9.210$ (Mathematica)

⑧ $\langle\hat{x}\rangle = \frac{2\alpha}{1-e^{-2\alpha L}}\int_0^L e^{-\alpha x}xe^{-\alpha x}dx = 2\alpha\,\frac{\frac{1}{4a^2}-\frac{e^{-2aL}(1+2aL)}{4a^2}}{1-e^{-2L}}$

$\langle\hat{x}^2\rangle = \frac{2\alpha}{1-e^{-2\alpha L}}\int_0^L e^{-\alpha x}x^2e^{-\alpha x}dx = 2\alpha\,\frac{\frac{1}{4a^3}-\frac{e^{-2aL}(1+2aL+2a^2L^2)}{4a^3}}{1-e^{-2L}}$

⑨ $\sqrt{\langle x^2\rangle+\langle x\rangle^2}$

$\frac{1}{16a^4(-1+e^{2L})^2}\left(e^{-4(-1+a)L}\left(-(-1+e^{2aL}-2aL)^2+4ae^{2(-1+a)L}(-1+e^{2L})(-1+e^{2aL}-2aL-2a^2L^2)\right)\right)$

⑩ You can only know where your PChem notes are for an instant, but then you are completely uncertain of their momentum so the next instant you would have no idea where they are.

⑪ If the electron collapses to the nucleus it would be confined to an extremely small region of space and if we know the electron is stuck to the nucleus then we have some knowledge of its momentum – more than what is allowed by the uncertainty principle.

⑫ Variance provides information on the spread of a property about its average

⑬

```
In[59]:= Plot[Evaluate[Table[Sin[i Pi x], {i, 1, 8}]], {x, 0, 1}, Frame → True]
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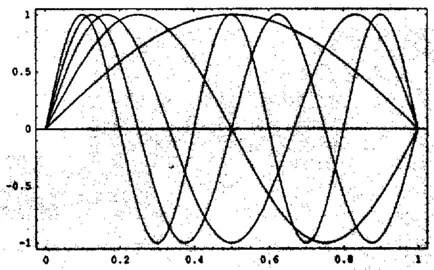

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Out[59]= -Graphics-
```

⑭

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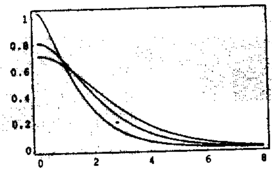
In[146]:= norms = Table[Integrate[(BesselK[n, x] x^n)^2, {x, 0, Infinity}], {n, 1, 3}]
```

Out[146]= $\left\{\frac{3\pi^2}{32}, \frac{315\pi^2}{512}, \frac{51975\pi^2}{4096}\right\}$

```
In[142]:= Plot[Evaluate[Table[1 / Sqrt[norms[[n]]] BesselK[n, x] x^n, {n, 1, 3}]],
            {x, 0, 8}, Frame → True]
```



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Out[142]= -Graphics-
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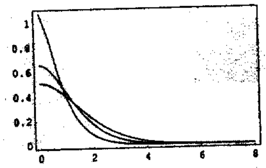
```
In[143]:= Plot[Evaluate[Table[(1 / Sqrt[norms[[n]]] BesselK[n, x] x^n)^2, {n, 1, 3}]],
            {x, 0, 8}, Frame → True]
```



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Out[143]= -Graphics-
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⑮ your words

⑯ your words