Problem Set PS02

ISSUED: 9/5/02 **Due: 9/12/02**

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

   (b) How many zeros does the function $f(x) = (x^2 - 2x - 15)e^{-\frac{1}{2}x^2}$ have? Where are they?

2. The functions

$$y_1 = A \sin kx$$

   and

$$y_2 = B \cos kx$$

   are solutions of the differential equation

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

   where k is a positive real constant. Verify by direct substitution that any *linear combination* of the independent solutions of Eq. (1), $Y = y_1 + y_2$, is also a solution of Eq. (1). But the product $Z = y_1 y_2$ is not a solution.

3. Suppose the following *boundary conditions* are imposed on the solutions of Eq. (1), $Y(-L) = 0$, $Y(L) = 0$ and $Y(0) = 1$. What are A, B and k. Note: $A = 0$ and $B = 0$ is a solution (called the trivial solution) but this is not a useful solution since $Y = 0$ for all x is this case.

Exercises

4. 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 $\hat{O}_{xp} \equiv \frac{1}{\hat{x}}\hat{p}_x\hat{x}$. 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) $\psi(x) = kx^2$

5. Suppose that the wavefunction for an electron of some crazy system over the region $(0 < x < \infty)$ is of the form $\psi(x) = xe^{-\alpha x}$, where α is a positive constant.

   (a) Normalize this wavefunction over this region.

   (b) Find the probability that the electron is more than a distance $x = 1/\alpha$ away from $x = 0$.

   (c) Find the probability that the electron is between $x = 1/\alpha$ and $x = 2/\alpha$.

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

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 δx for the wavefunction used in the previous two problems.

Conceptual Problems

8. Can you ever know *exactly* where your shoes are?

9. Use the uncertainty principle to explain why atoms are stable.

10. 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?

11. Why must one normalize wavefunctions.

Computer Problems

12. 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?

13. A quantum object on the range $-\infty < x < \infty$ is described by the set of wavefunctions $\psi_n(x) = \frac{1}{x^{n+1}}$, where $n = 1, 2, 3 \cdots$. 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.

Reflective Exercises

14. 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?

15. Please read the following dictum:

    ‘As one goldfish said to another: “Of course there is a God! Who do you think changes the water?”’

    (a) To what extent is the goldfish’s conception of God a good one.

    (b) In principle, goldfish scientists could, through careful experiment and observation, eventually determine that the waterchanger is simply a human. Would that knowledge in any way change the answer to (a)?

① ⓐ $f(x) = \frac{1}{x}\sin a_n x$ need $\sin a_n L = 0$ and $\sin a_n(-L) = 0$

$\sin a_n(-L) = -\sin a_n L$

$\sin a_n L = 0$ when $a_n L = n\pi$ $n = 1, 2 \ldots$

so $a_n = \frac{n\pi}{L}$ $n = 1, 2, \ldots$

ⓑ $e^{-\frac{1}{2}x^2}$ has no zeros

$x^2 - 2x - 15 = 0$ $x = \frac{-2 \pm \sqrt{4+4(15)}}{2} = \frac{-2 \pm 8}{2} \Rightarrow x = -5,\ x = -3$

zeros at $x = -5$ and $x = -3$

②

$Y = A\sin kx + B\cos kx$

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

so $-k^2 Y + k^2 Y = 0$ ✓

$\frac{d^2Z}{dx^2} = \frac{d^2 AB\cos kx \sin kx}{dx^2} = AB\frac{d}{dx}\left(-k\sin kx^2 + k\cos kx^2\right)$

$= AB(-2k^2\sin kx\cos kx - 2k^2\cos kx\sin kx)$

$= -4ABk^2\sin kx\cos kx$

so $\frac{d^2Z}{dx^2} + k^2 Z = -4ABk^2\sin kx\cos kx + k^2 AB\cos kx\sin kx \neq 0$ ✓

③ $A\cos kL + B\sin kL = 0$ Ⓘ $A\cos k0 + B\sin k0 = 1$ $\boxed{A = 1}$

$A\cos k(-L) + B\sin k(-L) = 0$

$A\cos kL - B\sin kL = 0$ Ⓘⓘ

Ⓘ + Ⓘⓘ = $2A\cos kL = 0$ $A = 1$

$2\cos kL = 0$

$kL = \frac{n\pi}{2}$ $n = 1, 2, \ldots$

$\boxed{k = \frac{n\pi}{2L}}$ Ⓘ − Ⓘⓘ = $2B\sin\frac{2\pi}{2L} = 0$

so $B = 0$

④ ⓐ $\frac{1}{x}\hat{p}\hat{x}e^x = \frac{1}{x}(-i\hbar\frac{d}{dx})xe^x = -\frac{i\hbar}{x}e^x + \frac{-i\hbar}{x}e^x$

$= -i\hbar e^x(1 + \frac{1}{x}) \neq \lambda e^x$ not eigenfunction.

ⓑ $\frac{1}{x}\hat{p}\hat{x}\, xe^{-\alpha x} = \frac{1}{x}(-i\hbar\frac{d}{dx})x^2 e^{-\alpha x}$

$= \frac{-i\hbar}{x}\left((-\alpha)x^2 e^{-\alpha x} + 2xe^{-\alpha x}\right)$

$= i\hbar\, xe^{-\alpha x} - 2i\hbar\, e^{-\alpha x} \neq \lambda xe^{-\alpha x}$ not eigenfunction

ⓒ $\frac{1}{x}\hat{p}\hat{x}\, kx^2 = \frac{-i\hbar}{x}\frac{\partial}{\partial x}kx^3 = \frac{1}{x}k3x^2 = 3kx \neq \lambda kx^2$ not eigenfunction.

⑤ ⓐ $\int_0^\infty x^2 e^{-2\alpha x}dx \xrightarrow{\text{mathematica}} \frac{1}{4\alpha^3}$

So $\psi_{norm} = 2\sqrt{\alpha^3}\, x e^{-\alpha x}$

ⓑ $4\alpha^3\int_{1/\alpha}^{\infty} x^2 e^{-2\alpha x}dx \xrightarrow{\text{mathematica}} \frac{5}{e^2}$

ⓒ $4\alpha^3\int_{1/\alpha}^{3/\alpha} x^2 e^{-2\alpha x}dx \xrightarrow{\text{mathematica}} \frac{5}{e^2} - \frac{5}{2e}$

⑥ $\langle x\rangle = \int_{-\infty}^{\infty}\psi^*_{norm}\, x\, \psi_{norm} = 4\alpha^3\int_0^\infty x e^{-\alpha x}\, x\, x e^{-\alpha x}dx = \frac{3}{2\alpha}$

$\langle x^2\rangle = \int_{-\infty}^{\infty}\psi^*_{norm}\, x^2\, \psi_{norm} = 4\alpha^3\int_0^\infty x e^{-\alpha x}x^2 x e^{-\alpha x}dx = \frac{3}{\alpha^2}$

⑦ $\delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\frac{3}{a^2} - \frac{9}{4a^2}} = \frac{\sqrt{3}}{2a}$

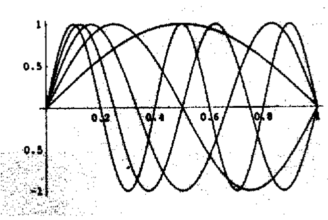
⑧ You can know exactly where your shoes are but if you do you lose all information about how fast your shoes are going.

⑨ see last year's solution key

⑩ see last year's solution key

⑪ one must normalize wavefunctions in order to interprete them as probability distributions

⑫



⑬ Untitled-4

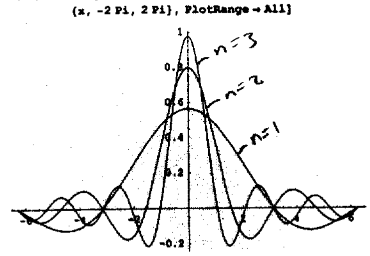
In[37]:= Integrate[(Sin[n x] / x) ^2, {x, -Infinity, Infinity}]

Out[37]= If[Im[n] == 0, n π Sign[n], $\int_{-\infty}^{\infty}\frac{\mathrm{Sin}[n\,x]^2}{x^2}dx$]

Sign[n] mean the sign of n. For example Sign[-5] = −1, sign[5] = +1

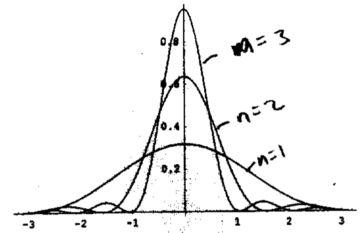
so $\psi_{norm,n} = \frac{1}{\sqrt{n\pi}}\frac{1}{x^{n+1}}$

In[46]:= Plot[Evaluate[Table[1 / Sqrt[n Pi] Sin[n x] / x, {n, 1, 3}]], {x, -2 Pi, 2 Pi}, PlotRange → All]



Out[46]= - Graphics -

In[48]:= Plot[Evaluate[Table[(1 / Sqrt[n Pi] Sin[n x] / x) ^2, {n, 1, 3}]], {x, -Pi, Pi}, PlotRange → All]



Out[48]= - Graphics -

⑭
⑮ } your words