CHEM 1410 Homework 2 Solutions

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Problem 1: Q.2.4

A wavefunction Ψ is written as a linear combination of eigenfunctions of a chosen operator as

$$\Psi = \sum_n c_n|\phi_n\rangle.$$

Since more combinations of a set of functions are possible than there are functions, there are more wavefunctions than eigenfunctions.

Problem 2: Q.2.8

In order to normalize a function, one must integrate over all of space. The volume element in spherical polar coordinates is:

$$dv = r^2 dr\ sin\theta\ d\theta\ d\phi$$

So, integrating the function $r\ e^{-r}$ gives

$$\int_V r\ e^{-r} dv = \int_0^\infty r^2 \left(r\ e^{-r}\right) dr\ \int_0^\pi sin\theta\ d\theta\ \int_0^{2\pi} d\phi = 4\pi\ \int_0^\infty r^2 \left(r\ e^{-r}\right) dr$$

which is different than if one integrated only along the radial component.

Problem 3: P.2.4

Here, one must remember that operators should be applied to a function starting from the operator which is closest to the function, *i.e.* the right-most operator.

P.2.4.A

$$\frac{d}{dy}\left[y\left(y^2 e^{-2y^3}\right)\right] = \frac{d}{dy} y^3 e^{-2y^3} = 2y\ e^{-2y^3} - 6y^4\ e^{-2y^3} = 2y(1-3y^3)e^{-2y^3}$$

P.2.4.B

$$y\left[\frac{d}{dy}\left(y\ e^{-2y^3}\right)\right] = y\left(e^{-2y^3} - 6y^3\ e^{-2y^3}\right) = y(1-6y^3)e^{-2y^3}$$

P.2.4.C

$$y\frac{\partial}{\partial x}\left[x\frac{\partial}{\partial y} e^{-2(x+y)}\right] = y\frac{\partial}{\partial x}\left[-2x\ e^{-2(x+y)}\right] = 2y(2x-1)e^{-2(x+y)}$$

P.2.4.D

$$x\frac{\partial}{\partial y}\left[y\frac{\partial}{\partial x}e^{-2(x+y)}\right] = x\frac{\partial}{\partial y}\left[-2y\ e^{-2(x+y)}\right] = 2x(2y-1)e^{-2(x+y)}$$

Problem 4: P.2.31

$$\begin{aligned}
\hat{A}^2 f(x) &= \hat{A}\left[\hat{A}f(x)\right] \\
&= \left(x - \frac{d}{dx}\right)\left(x - \frac{d}{dx}\right) f(x) \\
&= \left(x - \frac{d}{dx}\right)\left(xf(x) - \frac{d}{dx}f(x)\right) \\
&= x^2 f(x) - x\frac{d}{dx}f(x) - \frac{d}{dx}xf(x) + \frac{d^2}{dx^2}f(x) \\
&= \left(x^2 - x\frac{d}{dx} - \frac{d}{dx}x + \frac{d^2}{dx^2}\right) f(x) \\
&= \left[(x^2-1) - 2x\frac{d}{dx} + \frac{d^2}{dx^2}\right] f(x)
\end{aligned}$$

Problem 5: Q.3.8

False. Each eigenvalue λ_n corresponds to an eigenfunction ϕ_n (or a set of degenerate eigenfunctions), each of which carry with it a coefficient that defines its contribution to the wavefunction. Since these coefficients generally differ in magnitude, the probability of observing each eigenvalue will be different.

Problem 6

A

The function $1/x$ on the interval $(1, 2)$ is an acceptable wavefuction because:
(1) it is single-valued in the interval,
(2) it has continuous 1st and 2nd derivatives,
(3) and has finite values in the interval.

B

The function $\sqrt{x}$ on the interval $(0, 1)$ is not an acceptable wavefunction because it is not single-valued on the interval.