Quantum Chemistry by Levine

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Sep 2023

1 Chapter 5 Angular Momentum

5.1
(a) no.
(b) yes
(c) yes
(d) yes
(e) yes
for all well-behaved functions

5.2
(a)$[\hat{A},\hat{B}]=\hat{A}\hat{B}-\hat{B}\hat{A}=-[\hat{B},\hat{A}]$
(b)$[\hat{A},\hat{A}^n]=\hat{A}^{n+1}-\hat{A}^{n+1}=0$
(c)$[k\hat{A},\hat{B}]=k\hat{A}\hat{B}-\hat{B}k\hat{A}=k[\hat{A},\hat{B}]$
(d)$[\hat{A},\hat{B}+\hat{C}]=\hat{A}(\hat{B}+\hat{C})-(\hat{B}+\hat{C})\hat{A}=[\hat{A},\hat{B}]+[\hat{A},\hat{C}]$
(e)$[\hat{A},\hat{B}C]=\hat{A}\hat{B}\hat{C}-\hat{B}\hat{C}\hat{A}$

5.3
$[\hat{x},\hat{p_x}^3]=p_x[\hat{x},\hat{p_x}^2]+[\hat{x},\hat{p_x}]\hat{p_x}^2$
$=-i\hbar\frac{\partial}{\partial x}(2\hbar^2\frac{\partial}{\partial x})+i\hbar(-\hbar^2\frac{\partial^2}{\partial x^2})$

5.4
for a harmonic oscillator:
$<x>=0$
for energy level $n=0$, it has energy $E=\frac{hv}{2}$
from which $<T>=\frac{hv}{4}$
$<V>=\frac{1}{2}kx^2=\frac{hv}{4}$
So $<x^2>=\frac{hv}{2k}=\frac{h}{8\pi^2\nu m}$
$(\triangle x)^2=<x^2>-<x>^2=\frac{h}{8\pi^2\nu m}$
So:
$\triangle x=\sqrt{\frac{h}{8\pi^2\nu m}}$

similarly:
$< p_x >= 0$
Given $< T >= \frac{p_x^2}{2m} = \frac{hv}{4}$
$< p_x^2 >= \frac{hvm}{2}$
$\triangle p_x = \sqrt{< p_x^2 > - < p_x >^2} = \sqrt{\frac{hvm}{2}}$
So:
$\triangle x \triangle p_x = \frac{h}{4\pi} = \frac{\hbar}{2}$

5.5
Given the non-stationary state: $\Psi = \sqrt{105/l^7}x^2(l-x)$
We need to calculate 4 values: $< x >, < x^2 >, < p_x >, < p_x^2 >$
$< x >= \int_{-\inf} \inf \Psi^* x \Psi d\tau = \frac{5l}{8}$
$< x^2 >= \int_{-\inf}^{\inf} \Psi^* x^2 \Psi d\tau = \frac{5l^2}{12}$
$< p_x >= \int_{-\inf}^{\inf} \Psi^* (-i\hbar \frac{\partial}{\partial x}) \Psi d\tau = 0$
$< p_x^2 >= \int_{-\inf}^{\inf} \Psi^* (-i\hbar \frac{\partial}{\partial x})^2 \Psi d\tau = \frac{14\hbar^2}{l^2}$
$\triangle x = \sqrt{< x^2 > - < x >^2} = \sqrt{\frac{5}{192}l}$
$\triangle p_x = \sqrt{< p_x^2 > - < p_x >^2} = \sqrt{14}\frac{\hbar}{l}$
So:
$\triangle x \triangle p_x = \sqrt{\frac{5}{192}l}\sqrt{14}\frac{\hbar}{l} > \frac{\hbar}{2}$

5.6
Given Ψ is the eigenfunction, the only measurement value can be eigenvalue a
So it is expected there is no deviation.
$\triangle A =< A^2 > - < A >^2$
where:
$< A^2 >= \int_{-\inf}^{\inf} \Psi^* A^2 \Psi = a^2$
$< A >^2 = a^2$
So: $\triangle A = \sqrt{< A^2 > - < A >^2} = 0$

5.7
$(\triangle A)^2 = \int_{-\inf}^{\inf} \Psi (A - < A >)^2 \Psi d\tau$
$= \int_{-\inf}^{\inf} \Psi A^2 \Psi d\tau - 2 < A > \int_{-\inf}^{\inf} \Psi A \Psi d\tau + < A >^2 =< A^2 > - < A >^2$

5.8
All the combinations HH, HT, TH, TT
So $< w >= 1$
where w takes value $2, 1, 0$
w^2 can take $4, 1, 0$ at different possibilities

$< w^2 >= 4 * \frac{1}{4} + 1 * \frac{1}{2} + 0 * \frac{1}{4} = 1.5$
So:
$\sigma w = \sqrt{< w^2 > - < w >^2} = \sqrt{0.5}$

5.9
(a)vector
(b)vector
(c)scalar
(d)scalar
(e)vector
(f)scalar

5.10
$A = (3, -2, 6), B = (-1, 4, 4)$
$|A| = 7, |B| = \sqrt{33}$
$A + B = (-2, 3, 10), A - B = (4, -6, 2)$
$AB = 13$
$A * B = (-32, -18, 10)$
$cos\theta = \frac{AB}{|A||B|} = \frac{13}{7\sqrt{33}}$

5.11
two diagonal lines are $(1, 1, 1), (-1, 1, -1)$
$cos\theta = \frac{-1}{3}$

5.13
$grad\, f = \overrightarrow{i}(4x - 5yz) + \overrightarrow{j}(-5xz) + \overrightarrow{-5xy + 2z}$
$\nabla f = 4 + 0 + 2 = 6$

5.14
(a) $div \cdot grad\, g(x, y, z) = div\dot{(}\overrightarrow{i}(\frac{\partial}{\partial x}) + \overrightarrow{j}(\frac{\partial}{\partial y}) + \overrightarrow{k}(\frac{\partial}{\partial z}))$
$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$
(b)$div \cdot \overrightarrow{r} = (\overrightarrow{i}\frac{\partial}{\partial x} + \overrightarrow{j}\frac{\partial}{\partial y} + \overrightarrow{k}\frac{\partial}{\partial z})(\overrightarrow{i}x + \overrightarrow{j}y + \overrightarrow{k}z) = 1 + 1 + 1 = 3$

5.15
(a)$|B| = \sqrt{13}$
(b) with each axis:
$cos\alpha = \frac{(3,-2,0,1)(1,0,0,0)}{\sqrt{13}} = \frac{3}{\sqrt{13}}$
$cos\alpha = \frac{(3,-2,0,1)(0,1,0,0)}{\sqrt{13}} = \frac{-2}{\sqrt{13}}$

$cos\alpha = \frac{(3,-2,0,1)(0,0,1,0)}{\sqrt{13}} = 0$
$cos\alpha = \frac{(3,-2,0,1)(0,0,0,1)}{\sqrt{13}} = \frac{1}{\sqrt{13}}$

5.16

(a) no
(b) yes
(c) yes
(d) yes
$[\hat{L}_x^2, \hat{L}^2] = \hat{L}_x[\hat{L}_x, \hat{L}^2] + [\hat{L}_x, \hat{L}^2]\hat{L}_x = 0$

5.18

$[\hat{L}_x^2, \hat{L}_y] = \hat{L}_x[\hat{L}_x, \hat{L}_y] + [\hat{L}_x, \hat{L}_y]\hat{L}_x$
$= i\hbar(\hat{L}_x\hat{L}_z + \hat{L}_z\hat{L}_x)$

5.19

coordinate conversion
$(x, y, z) -> (r, \theta, \phi)$
$r = \sqrt{x^2 + y^2 + z^2}$
$\theta = cos^{-1}(\frac{z}{r})$
$\phi = tan^{-1}(\frac{y}{x})$
(a) given$(1, 2, 0)$
$r = \sqrt{5}$
$\theta = \frac{\pi}{2}$
$\phi = tan^{-1}2$
(b) given $(-1, 0, 3)$
$r = \sqrt{10}$
$\theta = cos^{-1}(\frac{3}{\sqrt{10}})$
$\phi = tan^{-1}0 = \pi$
(c) given $(3, 1, -2)$
$r = \sqrt{14}$
$\theta = cos^{-1}(\frac{-2}{\sqrt{14}})$
$\phi = tan^{-1}(\frac{1}{3})$
(d) given $(-1, -1, -1)$
$r = \sqrt{3}$
$\theta = cos^{-1}(\frac{-1}{\sqrt{3}})$
$\phi = tan^{-1}(1) = \frac{5}{4}\pi$

5.20

Coordinate conversion:
$x = rsin\theta cos\phi$

$y = rsin\theta sin\phi$
$z = rcos\theta$
(a) given $r = 1, \theta = \pi/2, \phi = \pi$
$x = -1, y = 0, z = 0$
(b) given $r = 2, \theta = \pi/4, \phi = 0$
$x = \sqrt{2}, y = 0, \sqrt{2}$

5.21
(a) sphere
(b) cone
(c) plane perpendicular to xy plane

5.22
the volume is:
$V = \int_0^{2\pi} \int_0^{\pi} \int_0^{r} r^2 sin\theta dr d\theta d\phi = \frac{4}{3}\pi r^3$

5.23
the shape of $\overrightarrow{L}$ is a cone
So the eigenvalue of $c = \overrightarrow{L}_z = m\hbar$
the eigenvalue of $b = \overrightarrow{L}^2 = l(l+1)\hbar^2$
$cos\theta = \frac{c}{\sqrt{b}} = \frac{m}{\sqrt{l(l+1)}}$
given $l = 2$
$m = -2, -1, 0, 1, 2$
then $cos\theta = \frac{-2}{\sqrt{6}}, \frac{-1}{\sqrt{6}}, 0, \frac{1}{\sqrt{6}}, \frac{2}{\sqrt{6}}$

5.24
Given $cos\theta = \frac{c}{\sqrt{b}} = \frac{m}{\sqrt{l(l+1)}}$
when $m = -l, -l+1, \ldots, l-1, l$
when $m = l$, $cos^2\theta = \frac{l}{l+1}$
when $l- >$ inf then $cos\theta - > 1, \theta = 0$

5.28
$\hat{L}^2 Y_2^0 = 2 * (2+1) Y_2^0$

5.29
$\hat{L}_z^3 Y_l^m = (m\hbar)^3 Y_l^m$

5.30

$\hat{L}_x^2 + \hat{L}_y^2 = \hat{L}^2 - \hat{L}_z^2$
So the eigenvalue is $l(l+1)\hbar^2 - m^2\hbar^2$

5.31
(a) given $l = 2$, $m = -2, -1, 0, 1, 2$
the measured value $m\hbar = -2\hbar, -\hbar, 0, \hbar, 2\hbar$
(b) given $l = 3$
the measured value $m\hbar = -3\hbar, -2\hbar, -\hbar, 0, \hbar, 2\hbar, 3\hbar$

5.32
similar to $\hat{L}_z$, $[\hat{L}^2, \hat{L}_y] = 0$
the eigenvalue is also $-\hbar, 0, \hbar$

5.33
the other parameters are not important since it is time term
Given Y_2^1
the measurement of $\hat{L}^2 = l(l+1)\hbar = 6\hbar$
the measurement of $\hat{L}_z = m\hbar = \hbar$

5.35
$\hat{L}_- Y_1^1 = Y_1^0$
$\hat{L}_-^2 Y_1^1 = Y_1^{-1}$
$\hat{L}_-^3 Y_1^1 = 0$

5.37
(a) true
(b) false
(c) true
(d) true
(e) true
(f) false
it is possible to find an eigenfunction, but not a set of eigenfunction