Tues 15 May 07

$\boxed{\text{QM Ch 13: H atom}}$ #2 p. 363 (1)

So far we have, for $V(r)$, $\psi = R_{E\ell}(r)\,Y_\ell^m(\theta,\varphi)$

where $R_{E\ell}(r) = \dfrac{U_{E\ell}(r)}{r}$ and $U_{E\ell} \xrightarrow[r\to 0]{} r^{\ell+1}$, $U_{E\ell} \xrightarrow[r\to\infty]{} e^{-\rho}$, $\rho = \sqrt{2mW}\,\dfrac{r}{\hbar}$

① $$\left\{\frac{d^2}{dr^2} + \frac{2m}{\hbar^2}\left[E + \underbrace{\frac{e^2}{r}}_{\text{Coulomb } V(r)} - \frac{\ell(\ell+1)\hbar^2}{2mr^2}\right]\right\} U_{E\ell} = 0 \qquad (13.1.2)$$

(13.1.7)

Now let $r R(r) = U_{E\ell}(r) \overset{②}{=} e^{-\rho(r)}\, v_{E\ell}(r)$ and try to find v.

Sub ② into ① and get (13.1.8) $\quad \dfrac{d\rho}{dr} = c = \dfrac{\sqrt{2mW}}{\hbar}$

ⓐ $$\frac{dU}{dr} = \frac{dU}{d\rho}\frac{d\rho}{dr} = c\frac{d}{d\rho}\left(e^{-\rho}v\right) = c e^{-\rho}\left(\frac{\partial v}{\partial\rho} - v\right)$$

$$\frac{d^2U}{dr^2} = \frac{d}{dr}\left(\frac{dU}{dr}\right) = \frac{d\rho}{dr}\frac{d}{d\rho}\left[c e^{-\rho}\left(\frac{\partial v}{\partial\rho} - v\right)\right] = c^2 e^{-\rho}\left[-\left(-v + \frac{\partial v}{\partial\rho}\right) + \left(-\frac{\partial v}{\partial\rho} + \frac{\partial^2 v}{\partial\rho^2}\right)\right]$$
$$= c^2 e^{-\rho}\left[v - \frac{2\partial v}{\partial\rho} + \frac{\partial^2 v}{\partial\rho^2}\right] = \frac{2mW}{\hbar^2}\underbrace{e^{-\rho}v}_{U}\left[1 - \frac{2}{v}\frac{\partial v}{\partial\rho} + \frac{1}{v}\frac{\partial^2 v}{\partial\rho^2}\right]$$

(13.1.2) → $$\frac{2mW}{\hbar^2}U\left[1 - \frac{2}{v}\frac{\partial v}{\partial\rho} + \frac{1}{v}\frac{\partial^2 v}{\partial\rho^2}\right] + \frac{2m}{\hbar^2}\left[-W + \frac{e^2}{\rho}\frac{\sqrt{2mW}}{\hbar} - \frac{\ell(\ell+1)\hbar^2}{2m\rho^2}\frac{2mW}{\hbar^2}\right]U = 0$$

$W = -E$ $$\frac{1}{v}\left[-2\frac{\partial v}{\partial\rho} + \frac{\partial^2 v}{\partial\rho^2}\right] + \frac{e^2}{\rho}\underbrace{\sqrt{\frac{2m}{W\hbar^2}}}_{\lambda} - \frac{\ell(\ell+1)}{\rho^2} = 0$$

(13.1.8) $$\frac{d^2v}{d\rho^2} - 2\frac{dv}{d\rho} + \left[\frac{e^2\lambda}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right] = 0 \quad \text{where } \lambda = \sqrt{\frac{2m}{\hbar^2 W}}$$

Try a series solution for $v = \rho^{\ell+1}\sum_{k=0}^{\infty} C_k\rho^k$

and get recursion relation $\dfrac{C_{k+1}}{C_k}$ (13.1.11)

#13.1.1 Derive 13.1.11 from 13.1.8, and 13.1.14 from 13.1.10
367

$\frac{C_{k+1}}{C_k}$ $\quad$ $\frac{d^2v}{d\rho^2}$ ...

Plug $v=\sum_{k=0}^{\infty} C_k \rho^{l+1+k}$ into $\frac{d^2v}{d\rho^2}-2\frac{dv}{d\rho}+\left[\frac{e^2\lambda}{\rho}-\frac{l(l+1)}{\rho^2}\right]v=0$ (2)

$$\frac{dv}{d\rho}=\sum C_k(l+1+k)\rho^{l+k}$$

$$\frac{d^2v}{d\rho^2}=\sum C_k(l+1+k)(l+k)\rho^{l+k-1}$$

$$v\left[\frac{e^2\lambda}{\rho}-\frac{l(l+1)}{\rho^2}\right]=\sum C_k e^2\lambda\rho^{l+k}-\sum C_k\, l(l+1)\rho^{l+k-1}$$

(13.1.8) becomes:

$$(3)\quad \sum C_k\left[(l+1+k)(l+k)-l(l+1)\right]\rho^{l+k-1}+\sum C_k\left[e^2\lambda-(l+k+1)\right]\rho^{l+k}=0$$

Now define $m=k-1$, $m+1=k$, rewrite (3):

$$0=\sum_{\substack{m=-1\\(k=0)}}^{\infty} C_{m+1}\{(l+m+2)(l+m+1)-l(l+1)\}\rho^{l+m}+\sum_{k=0}^{\infty}C_k\{e^2\lambda-2(l+k+1)\}\rho^{l+k}$$

We can rename this m to k and gather terms of ρ^{l+k} together:

$k=0$ or $m=-1$ term

$$0=C_0\underbrace{\{(l+1)l-l(l+1)\}}_{0}\rho^{l-1}+\sum_{k=0}\rho^{l+k}\left[C_{k+1}\{(l+k+2)(l+k+1)-l(l+1)\}+C_k\{e^2\lambda\right.$$

$$0=\sum\rho^{l+k}\left[C_{k+1}\{(l+k+2)(l+k+1)-l(l+1)\}+C_k\{e^2\lambda-2(l+k+1)\}\right]$$

$$\frac{C_{k+1}}{C_k}=\frac{2(l+k+1)-e^2\lambda}{(l+k+2)(l+k+1)-l(l+1)}$$

Energy Levels of H-atom:

We found that $\frac{C_{k+1}}{C_k} = \frac{-e^2\lambda + 2(k+l+1)}{(k+l+2)(k+l+1) - l(l+1)} \xrightarrow[k\to\infty]{} \frac{2}{k}$

describes $v_{El} = \rho^{l+1} \sum_{k=0}^{\infty} C_k \rho^k \to \rho^m e^{2\rho}$ $\square$

$u \underset{\rho\to\infty}{\sim} ve^{-\rho} \sim \rho^m e^{-\rho} e^{2\rho} \sim \rho^m e^{\rho}$ must terminate at some k.

Need $-e^2\lambda + 2(k+l+1) = 0$ at some k

(13.1.9) $\lambda^2 = \frac{2m}{\hbar^2 W}$: $\underline{\text{SOLVE for } W = E(m, \hbar, e, k, l)}$

$\lambda^2 = \left[2(l+k+1)/e^2\right]^2 = \frac{2m}{\hbar^2 W} = \frac{4(l+k+1)^2}{e^4}$

(13.1.14) $\underline{W = \frac{2me^4}{4\hbar^2(l+k+1)^2}} = \frac{me^4}{2\hbar^2(l+k+1)^2}$

Write this in terms of the principal quantum number

$n = k + l + 1$

$\underline{E_n = -W = \frac{-me^4}{2\hbar^2 n^2}}$

$k = 0, 1, \ldots$

At each n, the allowed values of l are (13.1.7):

$l = n-1, n-2, \ldots, 0$

$\rho = \sqrt{2mW}\,\frac{r}{\hbar} = rme^2/\hbar^2 n$

$W = me^4/2\hbar^2 n^2$

* **13.1.3.** Starting from the recursion relation, find ψ_{210}.

$$\psi_{Elm}(\vec{r}) = R_{El}(r)\,Y_l^m(\theta,\varphi) = \frac{U_{El}(r)}{r}\,Y_l^m(\theta,\varphi)$$

$$U_{El}(\rho) = V_{nl}(\rho)\,e^{-\rho} \quad \text{where } \boxed{\rho = \frac{r}{na_0}} \text{ from (13.1.23)+(13.1.24)}$$

$$V_{nl}(\rho) = \sum_{k=0}^{\infty} C_k\,\rho^{l+k+1} \qquad n = k+l+1$$

$$\frac{C_{k+1}}{C_k} = \frac{[-2n] + 2(k+l+1)}{(k+l+2)(k+l+1) - l(l+1)}$$

[From (13.1.11) with $\lambda = \sqrt{\frac{2m}{\hbar^2 W}} = \sqrt{\frac{2m}{\hbar^2}\left[\frac{2\hbar^2 n^2}{me^4}\right]} = \sqrt{4n^2/e^4} = \frac{2n}{e^2}$
(13.1.9) (13.1.16)

So $e^2\lambda = e^2\frac{2n}{e^2} = 2n$ ✓ $= 2n$]

ψ_{210} : $n = 2$ $l = 1$ $m = 0$

$$\frac{C_1}{C_0} = \frac{-2n + 2n}{(n+1)n - l(l+1)} = 0$$

Therefore all $C_k = 0$ except C_0. Just leave C_0 as an unknown constant for now.

$$V_{21}(\rho) = C_0\,\rho^{1+0+1} = C_0\,\rho^{1+1} = C_0\,\rho^2 = C_0\,\frac{r^2}{4a_0^2}$$

$$U_{21}(r) = \frac{C_0 r^2}{4a_0^2}\,e^{-r/2a_0}, \quad R_{21} = \frac{U_{21}}{r} = \frac{C_0 r}{4a_0^2}\,e^{-r/2a_0} \rightarrow$$

$$\psi_{210} = R_{21} Y_1^0 = \frac{C_0 r}{4a_0^2} e^{-r/2a_0} Y_1^0$$

Normalizing ψ_{210}: The normalization condition on $U_{21}(r)$ is

$$1 = \int_0^\infty |U_{21}(r)|^2 \, dr = \int \frac{C_0^2 r^4}{16 a_0^4} e^{-2r/2a_0} \, dr$$

$$= \frac{C_0^2}{16 a_0^4} \int_0^\infty r^4 e^{-r/a_0} \, dr = \frac{C_0^2}{4 \cdot 4 a_0^4} 4 \cdot 6 \, a_0^5 = \frac{6}{4} C_0^2 a_0$$

Special integral: $\int_0^\infty r^4 e^{-r/a_0} \, dr = (4!) a_0^5$ (Dwight 860.07)

Find $C_0^2 = \frac{2}{3a_0} \rightarrow C_0 = \sqrt{\frac{2}{3a_0}}$ $\qquad = \sqrt{\frac{2}{3a_0}}$

Finally $\psi_{210}(r, \theta, \varphi) = \frac{\sqrt{\frac{2}{3a_0}}}{4a_0^2} \, r e^{-r/2a_0} \, Y_1^0(\theta, \varphi)$

$$\frac{\sqrt{\frac{2}{3a_0}}}{4a_0^2} = \frac{1}{a_0} \sqrt{\frac{2}{3 \cdot 16 \, a_0^3}} = \frac{1}{a_0} \sqrt{\frac{1}{3 \cdot 8 a_0^3}}$$

Spherical harmonics

$Y_1^0(\theta, \varphi) = \sqrt{\frac{3}{4\pi}} \cos\theta \qquad$ (12, 5, 39) p. 346

$$\psi_{210} = \frac{r}{a_0} e^{-r/2a_0} \sqrt{\frac{1}{3 \cdot 8 a_0^3}} \sqrt{\frac{3}{4\pi}} \cos\theta = \frac{r}{a_0} e^{-r/2a_0} \cos\theta \sqrt{\frac{1}{32 a_0^3}}$$

$$\psi_{210}(r, \theta, \varphi) = \sqrt{\frac{1}{32\pi a_0^2}} \left(\frac{r}{a_0}\right) e^{-r/2a_0} \cos\theta$$

QM Spring - Tues wk 8 E/7

Ch 14 # 14.3.2, 3.4(i) 4.1 (Ehrenfest), 5.1.(i)

14.3.2 / 395 (i) Show that the eigenvectors of $\vec{\sigma}\cdot\hat{n}$ are given by (14.3.28)

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma} \text{ and } \hat{n}\cdot\vec{S} = \frac{\hbar}{2}\begin{bmatrix}\cos\theta & \sin\theta e^{-i\varphi} \\ \sin\theta e^{i\varphi} & -\cos\theta\end{bmatrix} \quad (14.3.27) / 390$$

So $\hat{n}\cdot\vec{\sigma} = \vec{\sigma}\cdot\hat{n} = \begin{bmatrix}\cos\theta & \sin\theta e^{-i\varphi} \\ \sin\theta e^{i\varphi} & -\cos\theta\end{bmatrix}$. To find the eigenvalues λ, solve $\begin{vmatrix}\cos\theta-\lambda & \sin\theta e^{-i\varphi} \\ \sin\theta e^{i\varphi} & -\cos\theta-\lambda\end{vmatrix} = 0$

$$0 = (\cos\theta-\lambda)(-\cos\theta-\lambda) - \sin\theta e^{i\varphi}(\sin\theta e^{-i\varphi})$$
$$= -\cos^2\theta + \lambda\cos\theta - \lambda\cos\theta + \lambda^2 - \sin^2\theta = \lambda^2 - 1 = (\lambda+1)(\lambda-1)$$

Eigenvalues are $\lambda = 1$, $\lambda = -1$.

$\lambda = +1$ Eigenvector $\begin{bmatrix}a\\b\end{bmatrix}$ satisfies $\begin{bmatrix}\cos\theta-1 & \sin\theta e^{-i\varphi} \\ \sin\theta e^{i\varphi} & -\cos\theta-1\end{bmatrix}\begin{bmatrix}a\\b\end{bmatrix} = 0$

$$a\cos\theta - a + b\sin\theta e^{-i\varphi} = 0 \rightarrow b = a\frac{(\cos\theta-1)}{\sin\theta e^{-i\varphi}}$$
$$a\sin\theta e^{i\varphi} - b\cos\theta - b = 0 \qquad \frac{b}{a} = \frac{-2\sin^2\frac{\theta}{2}}{-2\sin\frac{\theta}{2}\cos\frac{\theta}{2}} e^{i\varphi} = \frac{\sin\frac{\theta}{2}e^{i\varphi}}{\cos\frac{\theta}{2}}$$

[Dwight 404.12 & 403.02] $\longrightarrow$

If we let $b = \sin\frac{\theta}{2}e^{i\varphi/2}$ then $a = \cos\frac{\theta}{2}e^{-i\varphi/2}$

$$|\lambda=1\rangle = |\hat{n}+\rangle = \begin{bmatrix}\cos\frac{\theta}{2}e^{-i\varphi/2} \\ \sin\frac{\theta}{2}e^{i\varphi/2}\end{bmatrix} \quad ✓ \ (14.3.28a)$$

QM #14.3.2 continued...

($\lambda=-1$) Eigenvector $\begin{bmatrix} a \\ b \end{bmatrix}$ satisfies $\begin{bmatrix} \cos\theta+1 & \sin\theta e^{-i\varphi} \\ \sin\theta e^{i\varphi} & -\cos\theta+1 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = 0$

$$a(\cos\theta+1) + b\sin\theta e^{-i\varphi} = 0 \rightarrow \frac{b}{a} = \frac{(\cos\theta+1)e^{i\varphi}}{-\sin\theta} = \frac{2\cos^2\frac{\theta}{2}e^{i\varphi/2}}{-2\sin\frac{\theta}{2}\cos\frac{\theta}{2}e^{-i\varphi/2}}$$
$$a\sin\theta e^{i\varphi} + b(1-\cos\theta) = 0$$

DWIGHT 404,22

$$a = -\sin\frac{\theta}{2}e^{-i\varphi/2} \rightarrow |\lambda=-1\rangle = |\hat{n}-\rangle = \begin{bmatrix} -\sin\frac{\theta}{2}e^{-i\varphi/2} \\ \cos\frac{\theta}{2}e^{i\varphi/2} \end{bmatrix}$$
$$b = \cos\frac{\theta}{2}e^{i\varphi/2}$$

(14.3.28b) ✓

Check normalization of $|\hat{n}+\rangle$ and $|\hat{n}-\rangle$:

$\langle\hat{n}+|\hat{n}+\rangle = \cos^2\frac{\theta}{2}e^0 + \sin^2\frac{\theta}{2}e^0 = 1$ ✓ already normalized

$\langle\hat{n}-|\hat{n}-\rangle = \sin^2\frac{\theta}{2}e^0 + \cos^2\frac{\theta}{2}e^0 = 1$ ✓ already normalized

These are not the only way to write the eigenvectors of the $\vec{S}$ or $\vec{\vec{T}}$ matrix, but they are consistent and convenient.

(ii) Verify (14.3.29) $\langle\hat{n}\pm|\vec{S}|\hat{n}\pm\rangle = \pm\frac{\hbar}{2}(\hat{i}\sin\theta\cos\varphi + \hat{j}\sin\theta\sin\varphi + \hat{k}\cos\theta)$
391
$= \pm\frac{\hbar}{2}\hat{n}$

Need to calculate $\langle\hat{n}\pm|S_x|\hat{n}\pm\rangle$, $\langle\hat{n}\pm|S_y|\hat{n}\pm\rangle$, $\langle\hat{n}\pm|S_z|\hat{n}\pm\rangle$

where the components of the spin matrix are $S_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $S_y = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$, $S_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

and we just found $|\hat{n}+\rangle$ and $|\hat{n}-\rangle$ above in (i)...

14.3.2 (ii)

$$\langle n+|S_x|n+\rangle = \left[\cos\tfrac{\theta}{2}e^{i\frac{\varphi}{2}},\ \sin\tfrac{\theta}{2}e^{-i\frac{\varphi}{2}}\right]\frac{\hbar}{2}\begin{bmatrix}0&1\\1&0\end{bmatrix}\begin{bmatrix}\cos\frac{\theta}{2}e^{-\frac{i\varphi}{2}}\\ \sin\frac{\theta}{2}e^{+i\varphi/2}\end{bmatrix}$$

$$=\left[\ \text{''}\qquad \text{''}\ \right]\frac{\hbar}{2}\begin{bmatrix}\sin\frac{\theta}{2}e^{i\varphi/2}\\ \cos\frac{\theta}{2}e^{-i\varphi/2}\end{bmatrix}$$

$$=\frac{\hbar}{2}\left(\cos\tfrac{\theta}{2}\sin\tfrac{\theta}{2}e^{i\varphi}+\sin\tfrac{\theta}{2}\cos\tfrac{\theta}{2}e^{-i\varphi}\right)=\frac{\hbar}{2}\cos\frac{\theta}{2}\underline{\sin\frac{\theta}{2}}\left(e^{i\varphi}+e^{-i\varphi}\right)$$

$$\underline{\langle n_+|S_x|n_+\rangle}=\frac{\hbar}{2}\left(\tfrac{1}{2}\sin\theta\right)\left(2\cos\varphi\right)=\underline{\frac{\hbar}{2}\sin\theta\cos\varphi}$$

$$\langle n-|S_x|n-\rangle=\left[-\sin\tfrac{\theta}{2}e^{i\varphi/2},\ \cos\tfrac{\theta}{2}e^{-i\varphi/2}\right]\frac{\hbar}{2}\begin{bmatrix}0&1\\1&0\end{bmatrix}\begin{bmatrix}-\sin\frac{\theta}{2}e^{-i\varphi/2}\\ \cos\frac{\theta}{2}e^{i\varphi/2}\end{bmatrix}$$

$$=\left[\ \text{''}\qquad \text{''}\ \right]\frac{\hbar}{2}\begin{bmatrix}\cos\frac{\theta}{2}e^{i\varphi/2}\\ -\sin\frac{\theta}{2}e^{-i\varphi/2}\end{bmatrix}$$

$$=\frac{\hbar}{2}\left(-\sin\tfrac{\theta}{2}\cos\tfrac{\theta}{2}e^{i\varphi}-\cos\tfrac{\theta}{2}\sin\tfrac{\theta}{2}e^{-i\varphi}\right)=-\frac{\hbar}{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2}\left(e^{i\varphi}+e^{-i\varphi}\right)$$

$$\underline{\langle n-|S_x|n-\rangle}=-\frac{\hbar}{2}\left(\tfrac{1}{2}\sin\theta\right)\left(2\cos\varphi\right)=\underline{-\frac{\hbar}{2}\sin\theta\cos\varphi}=-\langle n+|S_x|n+\rangle$$

$$\langle n+|S_y|n+\rangle=\left[\cos\tfrac{\theta}{2}e^{i\varphi/2},\ \sin\tfrac{\theta}{2}e^{-i\varphi/2}\right]\frac{\hbar}{2}\begin{bmatrix}0&-i\\i&0\end{bmatrix}\begin{bmatrix}\cos\frac{\theta}{2}e^{-i\varphi/2}\\ \sin\frac{\theta}{2}e^{i\varphi/2}\end{bmatrix}$$

$$=\left[\qquad\qquad\right]\frac{\hbar}{2}\begin{bmatrix}-i\sin\frac{\theta}{2}e^{i\varphi/2}\\ i\cos\frac{\theta}{2}e^{-i\varphi/2}\end{bmatrix}$$

$$=\frac{\hbar}{2}\left(-i\sin\tfrac{\theta}{2}\cos\tfrac{\theta}{2}e^{i\varphi}+i\sin\tfrac{\theta}{2}\cos\tfrac{\theta}{2}e^{-i\varphi}\right)=-\frac{i\hbar}{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2}\left(e^{i\varphi}-e^{-i\varphi}\right)$$

$$\underline{\langle n+|S_y|n+\rangle}=\frac{\hbar}{2i}\left(e^{i\varphi}-e^{-i\varphi}\right)\left(\tfrac{1}{2}\sin\theta\right)=\underline{\frac{\hbar}{2}\sin\theta\sin\varphi}\qquad\left[\frac{e^{i\varphi}-e^{-i\varphi}}{2i}=\sin\varphi\right]$$

$$\langle n-|S_y|n-\rangle = \left[-\sin\tfrac{\theta}{2}e^{i\varphi/2},\ \cos\tfrac{\theta}{2}e^{-i\varphi/2}\right]\frac{\hbar}{2}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}\begin{bmatrix}-\sin\frac{\theta}{2}e^{-i\varphi/2}\\ \cos\frac{\theta}{2}e^{i\varphi/2}\end{bmatrix}$$

$$= \left[\qquad\qquad\right]\frac{\hbar}{2}\begin{bmatrix}-i\cos\frac{\theta}{2}e^{i\varphi/2}\\ -i\sin\frac{\theta}{2}e^{-i\varphi/2}\end{bmatrix}$$

$$= \frac{\hbar}{2}\left(i\sin\tfrac{\theta}{2}\cos\tfrac{\theta}{2}e^{i\varphi} - i\sin\tfrac{\theta}{2}\cos\tfrac{\theta}{2}e^{-i\varphi}\right)$$

$$= -\frac{\hbar}{2i}\left(e^{i\varphi}-e^{-i\varphi}\right)\sin\tfrac{\theta}{2}\cos\tfrac{\theta}{2}) = -\hbar\sin\varphi\,\tfrac{1}{2}\sin\theta$$

$$\underline{\langle n-|S_y|n-\rangle = -\tfrac{\hbar}{2}\sin\varphi\sin\theta} = -\langle n+|S_y|n+\rangle$$

$$\underline{\langle n+|S_z|n+\rangle} = \left[\cos\tfrac{\theta}{2}e^{i\varphi/2},\ \sin\tfrac{\theta}{2}e^{-i\varphi/2}\right]\frac{\hbar}{2}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\begin{bmatrix}\cos\frac{\theta}{2}e^{-i\varphi/2}\\ \sin\frac{\theta}{2}e^{i\varphi/2}\end{bmatrix}$$

$$= \left[\qquad\qquad\right]\frac{\hbar}{2}\begin{bmatrix}\cos\frac{\theta}{2}e^{-i\varphi/2}\\ -\sin\frac{\theta}{2}e^{i\varphi/2}\end{bmatrix}$$

$$= \frac{\hbar}{2}\left(\cos^2\tfrac{\theta}{2}e^0 - \sin^2\tfrac{\theta}{2}e^0\right) = \underline{\tfrac{\hbar}{2}\cos\theta} \quad (\text{DWIGHT } 403.22)$$

$$\langle n-|S_z|n-\rangle = \left[-\sin\tfrac{\theta}{2}e^{i\varphi/2},\ \cos\tfrac{\theta}{2}e^{-i\varphi/2}\right]\frac{\hbar}{2}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\begin{bmatrix}-\sin\frac{\theta}{2}e^{-i\varphi/2}\\ \cos\frac{\theta}{2}e^{i\varphi/2}\end{bmatrix}$$

$$= \frac{\hbar}{2}\left[\qquad\qquad\right]\begin{bmatrix}-\sin\frac{\theta}{2}e^{-i\varphi/2}\\ -\cos\frac{\theta}{2}e^{i\varphi/2}\end{bmatrix}$$

$$= \frac{\hbar}{2}\left(+\sin^2\tfrac{\theta}{2}e^0 - \cos^2\tfrac{\theta}{2}e^0\right) = \underline{-\tfrac{\hbar}{2}\cos\theta}$$

$$= \underline{-\langle n+|S_z|n+\rangle}$$

In Summary, $\langle n\pm|S_x|n\pm\rangle = \pm\frac{\hbar}{2}\sin\theta\cos\varphi$

$$\langle n\pm|S_y|n\pm\rangle = \pm\frac{\hbar}{2}\sin\theta\sin\varphi$$

$$\langle n\pm|S_z|n\pm\rangle = \pm\frac{\hbar}{2}\cos\theta$$

(14.3.29) $\langle \hat{n}\pm|\vec{S}|\hat{n}\pm\rangle = \pm\frac{\hbar}{2}(\hat{i}\sin\theta\cos\varphi + \hat{j}\sin\theta\sin\varphi + \hat{k}\cos\theta) = \pm\frac{\hbar}{2}\hat{n}$

391

These are equivalent ✓

#14.3.4 Derive (14.3.39) $(A\cdot\vec\sigma)(B\cdot\vec\sigma) = A\cdot B\,\overleftrightarrow{I} + i(A\times B)\cdot\overleftrightarrow{\sigma}$

395 where A & B are vectors or operators that commute with $\vec\sigma$:
$[A,\sigma]=0 \quad [B,\sigma]=0$ from $[\sigma_x,\sigma_y]=2i\sigma_z$ (14.3.38)
$[\sigma_i,\sigma_j]=2i\sum_k \sigma_k\,\epsilon_{ijk}$

Two ways:

① Write $\sigma_i\sigma_j$ in terms of $[\sigma_i,\sigma_j]_+ = \sigma_i\sigma_j + \sigma_j\sigma_i$
and $[\sigma_i,\sigma_j] = \sigma_i\sigma_j - \sigma_j\sigma_i$

ADD: $[\sigma_i,\sigma_j]_+ + [\sigma_i,\sigma_j] = 2\sigma_i\sigma_j \rightarrow \sigma_i\sigma_j = \dfrac{[\sigma_i,\sigma_j]_+ + [\sigma_i,\sigma_j]}{2}$

SUBTRACT: $[\sigma_i,\sigma_j]_+ - [\sigma_i,\sigma_j] = 2\sigma_j\sigma_i \rightarrow \sigma_j\sigma_i = \dfrac{[\sigma_i,\sigma_j]_+ - [\sigma_i,\sigma_j]}{2}$

How does this help?

(ii) Use (14.3.42) $M = \sum m_\alpha \sigma_\alpha$
and (14.3.43) $m_\beta = \frac{1}{2}\,\mathrm{Tr}(M\sigma_\beta)$

Well, let's start with $(A\times B)_i$ = ith component of $A\times B$

For example, Cartesian
$$A\times B = \begin{vmatrix} \hat i & \hat j & \hat k \\ A_x & A_y & A_z \\ B_x & B_y & B_z \end{vmatrix} = \hat i(A_yB_z - A_zB_y) - \hat j(A_xB_z - A_zB_x) + \hat k(A_xB_y - A_yB_x)$$

① $(A\times B)_i = A_yB_z - A_zB_y = \sum_j\sum_k A_jB_k\,\epsilon_{ijk}$
$= A_yB_z(+) + A_zB_y(-)$

Note that the permutation symbol
$\epsilon_{ijk} = \epsilon_{123} = \epsilon_{xyz} = \epsilon_{yzx} = \epsilon_{zxy} = +1$.
If any index is reversed or switched, for example, $\epsilon = -1$:
$\epsilon_{ikj} = \epsilon_{132} = \epsilon_{xzy} = \epsilon_{yxz} = \epsilon_{zyx} = -1$

(14.3.4) continued... Show $(\bar{A}\cdot\bar{\sigma})(\bar{B}\cdot\bar{\sigma}) = \bar{A}\cdot\bar{B}I + i(\bar{A}\times\bar{B})\cdot\bar{\sigma}$

$(\bar{A}\cdot\bar{\sigma}) = \sum_i A_i\sigma_i$ and $\bar{B}\cdot\bar{\sigma} = \sum_j B_j\sigma_j$ so

$(\bar{A}\cdot\bar{\sigma})(\bar{B}\cdot\bar{\sigma}) = \sum_i\sum_j A_i\sigma_i B_j\sigma_j = \sum_i\sum_j A_iB_i\sigma_i\sigma_j$

Ah, we found earlier that $\sigma_i\sigma_j = \frac{1}{2}[\sigma_i,\sigma_j] + \frac{1}{2}[\sigma_i,\sigma_j]$

$= \frac{1}{2}(2\delta_{ij}I) + \frac{1}{2}(2i\sigma_z)$

(14.3.37) p.392 (14.3.38) p.393

So $\sigma_i\sigma_j = \delta_{ij}I + i\sigma_z = I\delta_{ij} + \sum_k i\sigma_k\epsilon_{ijk}$

to match term in $\bar{A}\times\bar{B}$

Then $(\bar{A}\cdot\bar{\sigma})(\bar{B}\cdot\bar{\sigma}) = \sum_i\sum_j A_iB_i\left[I\delta_{ij} + \sum_k i\sigma_k\epsilon_{ijk}\right]$

$= \sum_i\sum_j A_iB_i\delta_{ij}I + i\underbrace{\sum_i\sum_j\sum_k A_iB_j\sigma_k\epsilon_{ijk}}$ (2)

Compare last term to $(\bar{A}\times\bar{B})_i = \sum_j\sum_k A_jB_k\epsilon_{ijk}$ (1)

$(\bar{A}\times\bar{B})_k = \sum_i\sum_j A_iB_j\epsilon_{kij}$ (1)'

$\epsilon_{kij} = \epsilon_{ijk}$ (Same order)

So $i\sum_i\sum_j\sum_k A_iB_j\sigma_k\epsilon_{ijk} = i\sum_k(\bar{A}\times\bar{B})_k\sigma_k$

$= i(\bar{A}\times\bar{B})\cdot\bar{\sigma}$

And term (2) $= \sum_i\sum_j A_iB_iI\delta_{ij} = (\bar{A}\cdot\bar{B})I$

Finally $(\bar{A}\cdot\bar{\sigma})(\bar{B}\cdot\bar{\sigma}) = (\bar{A}\cdot\bar{B})I + i(\bar{A}\times\bar{B})\cdot\bar{\sigma}$ ✓

14.H.1 (Ehrenfest) Show that if $H = -\gamma \mathbf{L}\cdot\mathbf{B}$ and $\mathbf{B}$ is POSITION INDEPENDENT, then $\frac{d\langle L\rangle}{dt} = \langle \bar{\mu}\times\mathbf{B}\rangle = \langle\mu\rangle\times\mathbf{B}$

We know from classical mechanics that ($\gamma\bar{L} = \bar{\mu}$)

Torque = rate of change of angular momentum = magnetic moment × magnetic field

$$\vec{\tau} = \frac{d\bar{L}}{dt} = \bar{\mu}\times\bar{B} \qquad [L_i, L_j] = i\hbar L_k = i\hbar \sum_k L_k \epsilon_{ijk}$$

Ehrenfest's Thm: Angular momentum operator L_i expectation value evolves as $\frac{d\langle L_i\rangle}{dt} = \frac{-i}{\hbar}\langle [L_i, H]\rangle$

Here, $H = -\gamma \mathbf{L}\cdot\mathbf{B} = -\gamma(L_x B_x + L_y B_y + L_z B_z) = -\gamma\sum L_i B_i = -\gamma\sum L_j B_j$
$= -\gamma \sum L_k B_k$

$$[L_i, H] = [L_i, -\gamma\sum_j L_j B_j] = -\gamma[L_i, \sum_j L_j B_j]$$

pick j to distinguish from i. Could also have $j=i$.

$$= -\gamma[\sum_j L_i, L_j B_j] = -\gamma\{\sum_j B_j [L_i, L_j]\}$$

B components are just numbers,

$$= -\gamma\{\sum_j B_j \; i\hbar \sum_k \epsilon_{ijk} L_k\}$$

$$[L_i, H] = -i\hbar\gamma \sum_j\sum_k \epsilon_{ijk} B_j L_k =$$

$$\frac{d\langle L_i\rangle}{dt} = \frac{-i}{\hbar}\langle -i\hbar\gamma\sum_j\sum_k \epsilon_{ijk} B_j L_k\rangle = -\gamma\sum_j\sum_k \epsilon_{ijk} B_j\langle L_k\rangle$$
$$= -\gamma \quad (\bar{B}\times\langle\bar{L}\rangle)_i$$
$$= -(\bar{B}\times\langle\gamma\bar{L}\rangle)_i = -(\bar{B}\times\langle\bar{\mu}\rangle)_i$$
$$= +(\langle\bar{\mu}\rangle\times\bar{B})_i$$

So $\frac{d\langle\bar{L}\rangle}{dt} = \langle\bar{\mu}\rangle\times\bar{B}$!

$$H = -\gamma \mathbf{L}\cdot\mathbf{B} \quad , \quad [L_i, L_j] = i\hbar L_z \quad , \quad \gamma L = \mu$$

#14.4.1 Alternate method - instead of using ϵ_{ijk}, you could figure out each component of $\frac{d}{dt}\langle \bar{L}\rangle = \langle\bar{\mu}\rangle \times \bar{B}$ using Ehrenfest $\frac{d}{dt}\langle L_i\rangle = -\frac{i}{\hbar}\langle [L_i, H]\rangle$

$$H = -\gamma \mathbf{L}\cdot\mathbf{B} = -\gamma(L_x B_x + L_y B_y + L_z B_z)$$

$$[L_x, H] = -\gamma\left\{[L_x, L_x B_x] + [L_x, L_y B_y] + [L_x, L_z B_z]\right\}$$

$$= -\gamma \left\{B_x[L_x, L_x] + B_y[L_x, L_y] + B_z[L_x, L_z]\right\}$$

$$= -\gamma \left\{ 0 + B_y(i\hbar L_z) + B_z(-i\hbar L_y)\right\}$$

$$= i\hbar\left(-B_y \gamma L_z + B_z \gamma L_y\right)$$

$$\langle [L_x, H]\rangle = i\hbar\left(-B_y\langle\mu_z\rangle + B_z\langle\mu_y\rangle\right)$$

$$\frac{d}{dt}\langle L_x\rangle = -\frac{i}{\hbar}\langle [L_x, H]\rangle = -\frac{i}{\hbar}\, i\hbar\left(-B_y\langle\mu_z\rangle + B_z\langle\mu_y\rangle\right)$$

$$= 1\left(-B_y\langle\mu_z\rangle + B_z\langle\mu_y\rangle\right)$$

$$\underline{\frac{d}{dt}\langle L_x\rangle = \left(\langle\bar{\mu}\rangle \times \bar{B}\right)_x}$$

and so forth for L_y and L_z ...

#14.5.1 ① Why is the coupling of the proton's intrinsic
p. 410 moment to B an order $\frac{m}{M}$ correction to ?

$$H = H_{Coulomb} - \left(\frac{-eB}{2mc}\right) L_z - \left(\frac{-eB}{mc}\right) S_z \quad \frac{(14.5.4)}{409}$$

Proton spin = electron spin = $\frac{\hbar}{2}$. The z component is:

$\mu_{z(p)} = \gamma_p S_z(p) = 5.6 \frac{e}{2Mc}\left(\frac{\hbar}{2}\right)$ where M = proton mass

$\mu_z(e) = \gamma_e S_z(e) = \frac{e}{mc}\left(\frac{\hbar}{2}\right)$ where m = electron mass.

$$\frac{\mu_z(p)}{\mu_z(e)} = \frac{5.6}{2}\frac{m}{M} \approx \frac{m}{M}$$

The energy of a spinning particle in a magnetic field $E = \bar{\mu} \cdot \bar{B}$. Since $\frac{\mu(p)}{\mu(e)} \approx \frac{m}{M}$, the proton coupling is weak.