Problem 1 | | Problem Set 6

For $\hat{H} = \hat{H}^0 + \lambda \hat{H}'$, & $|\psi\rangle$ satisfying $\hat{H}|\psi\rangle = E|\psi\rangle$, we assume: $E = E^0 + \lambda E'$, & then the Feynman-Hellman theorem:

$$\frac{\partial E}{\partial \lambda} = \langle \psi | \frac{\partial \hat{H}}{\partial \lambda} | \psi \rangle \longrightarrow E' = \langle \psi | \hat{H}' | \psi \rangle$$

& if $|\psi\rangle = |\psi^0\rangle + \lambda|\psi'\rangle$, $E' \cong \langle \psi^0 | \hat{H}' | \psi^0 \rangle + O(\lambda)$.

Problem 2 (7.43)

From $u'' = \left(\frac{l(l+1)}{r^2} - \frac{2}{ar} + \frac{1}{n^2a^2}\right)u$, we have:

$$u r^s u'' = \left(l(l+1) r^{s-2} - \frac{2}{a} r^{s-1} + \frac{1}{n^2a^2} r^s\right) u^2$$

Integrating gives: $\int_0^\infty u r^s u'' dr = l(l+1)\langle r^{s-2}\rangle - \frac{2}{a}\langle r^{s-1}\rangle + \frac{1}{n^2a^2}\langle r^s\rangle$ (o)

Using integration by parts (assuming $u \xrightarrow[r\to\infty]{r\to 0} 0$)

$$\int_0^\infty u r^s u'' dr = -\int_0^\infty (ur^s)' u' dr = -\int_0^\infty (s r^{s-1} u u' + u' r^s u') dr \quad (*)$$

now we'll establish relations to use in (*)

1. $\int_0^\infty (u r^s u') dr = -\int_0^\infty (ur^s)' u dr = -\int_0^\infty u' r^s u dr - \int_0^\infty u \cdot s r^{s-1} u dr$

combine

or

$$2\int_0^\infty u r^s u' dr = -s\langle r^{s-1}\rangle \Rightarrow \int_0^\infty u r^s u' dr = -\tfrac{1}{2} s \langle r^{s-1}\rangle \quad (+)$$

2. $\int_0^\infty u'' r^{s+1} u' dr = -\int_0^\infty u' (r^{s+1} u')' dr = -\int_0^\infty u' r^{s+1} u'' dr - (s+1)\int_0^\infty u' r^s u' dr$

combine

so $\int_0^\infty u' r^s u' dr = -\frac{2}{s+1}\int_0^\infty u'' r^{s+1} u' dr$

$$= -\frac{2}{s+1}\left[\int_0^\infty \left(\frac{l(l+1)}{r^2} - \frac{2}{ar} + \frac{1}{n^2a^2}\right) u r^{s+1} u' dr\right.$$

$$= -\frac{2}{s+1}\left[l(l+1)\int_0^\infty u r^{s-1} u' dr - \frac{2}{a}\int_0^\infty u r^s u' dr + \frac{1}{n^2a^2}\int_0^\infty u r^{s+1} u' dr\right]$$

$$= -\frac{2}{s+1}\left[l(l+1)\left(-\tfrac{1}{2}(s-1)\langle r^{s-2}\rangle\right) - \frac{2}{a}\left(-\tfrac{1}{2}s\langle r^{s-1}\rangle\right) + \frac{1}{n^2a^2}\left(-\tfrac{1}{2}(s+1)\langle r^s\rangle\right)\right]$$

using (+) on all 3 terms

$$= \frac{2}{s+1}\left[\tfrac{1}{2} l(l+1)(s-1)\langle r^{s-2}\rangle - \frac{s}{a}\langle r^{s-1}\rangle + \frac{(s+1)}{2n^2a^2}\langle r^s\rangle\right]$$

Problem 2 (continued)

putting the results from (1) + (2) into the RHS of (*) gives:

$$\int_0^\infty u r^s u'' dr = -s\left(-\tfrac{1}{2}(s-1)\langle r^{s-2}\rangle\right) - \frac{\ell(\ell+1)(s-1)}{s+1}\langle r^{s-2}\rangle + \frac{2s}{a(s+1)}\langle r^{s-1}\rangle - \frac{1}{n^2a^2}\langle r^s\rangle$$

|| from (0)

$$\ell(\ell+1)\langle r^{s-2}\rangle - \frac{2}{a}\langle r^{s-1}\rangle + \frac{1}{n^2a^2}\langle r^s\rangle = \tfrac{1}{2}s(s-1)\langle r^{s-2}\rangle - \frac{\ell(\ell+1)(s-1)}{s+1}\langle r^{s-2}\rangle + \frac{2s}{a(s+1)}\langle r^{s-1}\rangle - \frac{1}{n^2a^2}\langle r^s\rangle$$

collecting terms:

$$\langle r^s\rangle\left[\frac{2}{n^2a^2}\right] + \langle r^{s-1}\rangle\left[-\frac{2}{a} - \frac{2s}{a(s+1)}\right] + \langle r^{s-2}\rangle\left[\ell(\ell+1) - \tfrac{1}{2}s(s-1) + \frac{\ell(\ell+1)(s-1)}{s+1}\right] = 0$$

multiplying by $\frac{1}{2}a^2(s+1)$ gives:

$$\langle r^s\rangle\frac{s+1}{n^2} - \langle r^{s-1}\rangle a[s+1+s] + \langle r^{s-2}\rangle\tfrac{1}{2}a^2\Big[\underbrace{\ell(\ell+1)(s+1) - \tfrac{1}{2}s(s-1)(s+1) + \ell(\ell+1)(s-1)}\Big] = 0$$

$$s\left[2\ell(\ell+1) - \tfrac{1}{2}(s^2-1)\right] = \tfrac{1}{2}s\left[4\ell^2+4\ell+1-s^2\right]$$

$$= \tfrac{1}{2}s\left[(2\ell+1)^2 - s^2\right]$$

so, finally,

$$\langle r^s\rangle\frac{s+1}{n^2} - \langle r^{s-1}\rangle(2s+1)a + \langle r^{s-2}\rangle\frac{a^2s}{4}\left[(2\ell+1)^2 - s^2\right] = 0 \quad (D)$$

Problem 3 (7.44)

a For $s=0$, (D) gives: $\frac{1}{n^2} - a\langle r^{-1}\rangle = 0 \Rightarrow \langle \frac{1}{r}\rangle = \frac{1}{an^2}$ ✓ (7.56)

" $s=1$ $\quad \langle r\rangle\frac{2}{n^2} - 3a + \langle r^{-1}\rangle\frac{a^2}{4}\left[(2\ell+1)^2 - 1\right] = 0$

so that

$$\langle r\rangle = \frac{n^2}{2}\left[3a - \frac{a}{4n^2}\Big(\underbrace{(2\ell+1)^2-1}_{=4\ell(\ell+1)}\Big)\right] = \frac{3an^2}{2} - \frac{a}{2}\ell(\ell+1)$$

For $s=2$, $\quad \langle r^2\rangle\frac{3}{n^2} - \langle r\rangle(5a) + \tfrac{1}{2}a^2\left[(2\ell+1)^2 - 4\right] = 0$

$$\langle r^2\rangle = \frac{n^2}{3}\left[5a\left(\frac{3an^2}{2} - \frac{a}{2}\ell(\ell+1)\right) - \tfrac{1}{2}a^2\left((2\ell+1)^2-4\right)\right]$$

$$= \frac{5a^2n^4}{2} - \frac{5a^2}{6}n^2\ell(\ell+1) - \frac{n^2a^2}{6}\left((2\ell+1)^2-4\right)$$

$$= \frac{5a^2n^4}{2} - \frac{n^2a^2}{6}\Big(\underbrace{5\ell(\ell+1) + (2\ell+1)^2 - 4}_{=-3+9\ell(\ell+1)}\Big) = \frac{5a^2n^4}{2} - \frac{n^2a^2}{2}\left(3\ell(\ell+1) - 1\right)$$

For $s=3$: $\quad \langle r^3\rangle\frac{4}{n^2} - \langle r^2\rangle\cdot 7a + \langle r\rangle\frac{3a^2}{4}\left[(2\ell+1)^2 - 9\right] = 0$

$$\langle r^3\rangle = \frac{n^2}{4}\left[7a\left(\frac{5a^2n^4}{2} - \frac{n^2a^2}{2}(3\ell(\ell+1)-1)\right) - \frac{3a^2}{4}\left[(2\ell+1)^2 - 9\right]\left(\frac{3an^2}{2} - \frac{a}{2}\ell(\ell+1)\right)\right]$$

$$= \frac{n^2a^3}{8}\left[3\ell^4 + 6\ell^3 - 3\ell^2(1+10n^2) - 6\ell(1+5n^2) + 5n^2(5+7n^2)\right]$$

Problem 3 (continued)

b. For $s=-1$, (B) is: $\langle r^{-2}\rangle a - \langle r^{-3}\rangle \frac{a^2}{4}\underbrace{\left[(2l+1)^2-1\right]}_{=4l(l+1)} = 0$

so

$$\langle r^{-3}\rangle = \frac{\langle r^{-2}\rangle}{a\,l(l+1)}.$$

c. using $\langle r^{-2}\rangle = \frac{1}{(l+\frac{1}{2})n^3a^2}$, we get $\langle r^{-3}\rangle = \frac{1}{n^3a^3}\cdot\frac{1}{l(l+\frac{1}{2})(l+1)}$.

Problem 4

Our target is a state w/ $J=\frac{1}{2}$, $M=-\frac{1}{2}$ made up out of states w/ $l=1$. The states that could contribute are: $|n\,1\,-1\rangle|\uparrow\rangle$ & $|n\,1\,0\rangle|\downarrow\rangle$, so

$$|J=\tfrac{1}{2}\;M=-\tfrac{1}{2}\rangle = A\,|n\,1\,-1\rangle|\uparrow\rangle + B|n\,1\,0\rangle|\downarrow\rangle.$$

Looking at the $1\times\frac{1}{2}$ Clebsch-Gordan table, the coefficient $B=\frac{1}{\sqrt{3}}$ & $A=-\sqrt{\frac{2}{3}}$, so

$$|\tfrac{1}{2}\,\tfrac{1}{2}\rangle = \frac{1}{\sqrt{3}}\left(-\sqrt{2}\,|n\,1\,-1\rangle|\uparrow\rangle + |n\,1\,0\rangle|\downarrow\rangle\right)$$

Problem 5 (7.25)

The components of $\langle nl'm'|\vec{V}|nlm\rangle$ are:

$$\langle nl'm'|V_x|nlm\rangle = \frac{1}{\sqrt{2}}\left[C^{l1l'}_{m-1m'} - C^{l1l'}_{m1m'}\right]\langle nl'\|V\|nl\rangle$$

$$\langle nl'm'|V_y|nlm\rangle = \frac{i}{\sqrt{2}}\left[C^{l1l'}_{m-1m'} + C^{l1l'}_{m1m'}\right]\langle nl'\|V\|nl\rangle$$

$$\langle nl'm'|V_z|nlm\rangle = C^{l1l'}_{m0m'}\langle nl'\|V\|nl\rangle$$

so we can write: $\langle nl'm'|\vec{V}|nlm\rangle = \underbrace{\begin{pmatrix}\frac{1}{\sqrt{2}}\left[C^{l1l'}_{m-1m'} - C^{l1l'}_{m1m'}\right]\\ \frac{i}{\sqrt{2}}\left[C^{l1l'}_{m-1m'} + C^{l1l'}_{m1m'}\right]\\ C^{l1l'}_{m0m'}\end{pmatrix}}_{=\vec{u}}\underbrace{\langle nl'\|V\|nl\rangle}_{\text{just some number}}$

but the same is true for $\vec{W}$: $\langle nl'm'|\vec{W}|nlm\rangle = \vec{u}\underbrace{\langle nl'm'\|W\|nlm\rangle}_{\text{some number}}$

then: $\langle nl'm'|\vec{V}|nlm\rangle = \vec{u}\langle nl'm'\|V\|nlm\rangle$

$$= \langle nl'm'|\vec{W}|nlm\rangle\cdot\underbrace{\left[\frac{\langle nl'm'\|V\|nlm\rangle}{\langle nl'm'\|W\|nlm\rangle}\right]}_{=\alpha}$$

so $\langle nl'm'|\vec{V}|nlm\rangle = \alpha\langle nl'm'|\vec{W}|nlm\rangle$

could be zero.