Physics 633 Homework 1

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1) Starting with the series

$$x(\lambda) = x_0 + x_1\lambda + x_2\lambda^2 + ... \tag{1}$$

we will attempt to find an approximate solution to

$$x^3 = 12^3 + \lambda \tag{2}$$

a) Setting $\lambda = 0$ and $x_0 = 12$, to first order we have

$$\begin{aligned} x(\lambda) &= x_0 + x_1\lambda \\ x^3 &= 12^3 + \lambda \\ (x_0 + x_1\lambda)^3 &= 12^3 + \lambda \\ x_0^3 + 3x_0^2x_1\lambda + 3x_0x_1^2\lambda^2 + x_1^3\lambda^3 &= 12^3 + \lambda \\ \implies x_1 &= \frac{1}{3x_0^2} \end{aligned} \tag{3}$$

The approximate value of x, to first order, is

$$\begin{aligned} x(\lambda) &= x_0 + \frac{1}{3x_0^2}\lambda \\ x(1.03) &= 12 + \frac{1.03}{432} \\ x(1.03) &\approx 12.00238426 \end{aligned} \tag{4}$$

b) Now setting $x(\lambda) = x_0 + x_1\lambda + x_2\lambda^2$, we have

$$\begin{aligned} x(\lambda) &= x_0 + x_1\lambda + x_2\lambda^2 \\ x^3 &= 12^3 + \lambda \\ (x_0 + x_1\lambda + x_2\lambda^2)^3 &= 12^3 + \lambda \\ \implies 3x_0x_1^2\lambda^2 + 3x_0^2x_2\lambda^2 &= 0 \\ x_1^2 + x_0x_2 &= 0 \\ x_2 &= -\frac{x_1^2}{x_0} \\ x_2 &= -\frac{1}{9x_0^5} \end{aligned} \tag{5}$$

The approximate value of x, to second order, is

$$\begin{aligned}
x(\lambda) &= x_0 + \frac{1}{3x_0^2}\lambda - \frac{1}{9x_0^5}\lambda^2 \\
x(1.03) &= 12 + \frac{1.03}{432} + \frac{1.03^2}{2239488} \\
x(1.03) &\approx 12.00238379
\end{aligned} \tag{6}$$

Which is pretty darn good, considering it's about as many decimals as Mathematica will give you if you don't ask for more.

2) We start the expression for Δ_n in equation (53) in the reading.

$$\Delta_n = \sum_{\substack{k1,\ldots,k_{n+1} \\ (k_1+\ldots+k_{n+1}=n-1)}} S_{k_1} V S_{k_2} V \ldots V S_{k_{n+1}} \tag{7}$$

and plug in $n = 4$ to get

$$\begin{aligned}
\Delta_4 = &S_0VS_0VS_0VS_0VS_3 + S_0VS_0VS_0VS_1VS_2 + S_0VS_0VS_0VS_2VS_1 + S_0VS_0VS_0VS_3VS_0 \\
&+ S_0VS_0VS_1VS_0VS_2 + S_0VS_0VS_1VS_1VS_1 + S_0VS_0VS_1VS_2VS_0 + S_0VS_0VS_2VS_0VS_1 \\
&+ S_0VS_0VS_2VS_1VS_0 + S_0VS_0VS_3VS_0VS_0 + S_0VS_1VS_0VS_0VS_2 + S_0VS_1VS_0VS_1VS_1 \\
&+ S_0VS_1VS_0VS_2VS_0 + S_0VS_1VS_1VS_0VS_1 + S_0VS_1VS_1VS_1VS_0 + S_0VS_1VS_2VS_0VS_0 \\
&+ S_0VS_2VS_0VS_0VS_1 + S_0VS_2VS_0VS_1VS_0 + S_0VS_2VS_1VS_0VS_0 + S_0VS_3VS_0VS_0VS_0 \\
&+ S_1VS_0VS_0VS_0VS_2 + S_1VS_0VS_0VS_1VS_1 + S_1VS_0VS_0VS_2VS_0 + S_1VS_0VS_1VS_0VS_1 \\
&+ S_1VS_0VS_1VS_1VS_0 + S_1VS_0VS_2VS_0VS_0 + S_1VS_1VS_0VS_0VS_1 + S_1VS_1VS_0VS_1VS_0 \\
&+ S_1VS_1VS_1VS_0VS_0 + S_1VS_2VS_0VS_0VS_0 + S_2VS_0VS_0VS_0VS_1 + S_2VS_0VS_0VS_1VS_0 \\
&+ S_2VS_0VS_1VS_0VS_0 + S_2VS_1VS_0VS_0VS_0 + S_3VS_0VS_0VS_0VS_0
\end{aligned} \tag{8}$$

Taking the trace of (8) and cancelling terms with S_0 acting on $S_{1,2,3}$, we have

$$\begin{aligned}
\mathrm{tr}(\Delta_4) = &\mathrm{tr}(S_0VS_0VS_0VS_3VS_0) + \mathrm{tr}(S_0VS_0VS_1VS_2VS_0) + \mathrm{tr}(S_0VS_0VS_2VS_1VS_0) \\
&+ \mathrm{tr}(S_0VS_0VS_3VS_0VS_0) + \mathrm{tr}(S_0VS_1VS_0VS_2VS_0) + \mathrm{tr}(S_0VS_1VS_1VS_1VS_0) \\
&+ \mathrm{tr}(S_0VS_1VS_2VS_0VS_0) + \mathrm{tr}(S_0VS_2VS_0VS_1VS_0) + \mathrm{tr}(S_0VS_2VS_1VS_0VS_0) \\
&+ \mathrm{tr}(S_0VS_3VS_0VS_0VS_0) + \mathrm{tr}(S_1VS_0VS_0VS_0VS_2) + \mathrm{tr}(S_1VS_0VS_0VS_1VS_1) \\
&+ \mathrm{tr}(S_1VS_0VS_1VS_0VS_1) + \mathrm{tr}(S_1VS_1VS_0VS_0VS_1) + \mathrm{tr}(S_2VS_0VS_0VS_0VS_1)
\end{aligned} \tag{9}$$

Now, using the fact that $S_1S_1 = S_2$ and $S_1S_2 = S_2S_1 = S_3$ and $S_0^2 = -S_0$, and the fact that the trace is invariant under cyclic permutations of its argument, we have

$$\begin{aligned}
\mathrm{tr}(\Delta_4) &= \mathrm{tr}(S_0VS_0VS_1VS_2VS_0) + \mathrm{tr}(S_0VS_0VS_2VS_1VS_0) + \mathrm{tr}(S_0VS_0VS_3VS_0VS_0) \\
&\quad + \mathrm{tr}(S_0VS_1VS_1VS_1VS_0) + \mathrm{tr}(S_0VS_2VS_0VS_1VS_0) \\
\mathrm{tr}(\Delta_4) &= -\mathrm{tr}(S_0VS_0VS_1VS_2V) - \mathrm{tr}(S_0VS_0VS_2VS_1V) + \mathrm{tr}(S_0VS_0VS_3VS_0VS_0) \\
&\quad + \mathrm{tr}(S_0VS_1VS_1VS_1VS_0) - \mathrm{tr}(S_0VS_2VS_0VS_1V)
\end{aligned} \tag{10}$$

Now inserting $S_k = \sum_{\alpha\neq 0} \frac{|\alpha\rangle\langle\alpha|}{E_{0\alpha}^k}$, we have

$$\begin{aligned}
\mathrm{tr}(\Delta_4) &= -\sum_{\alpha,\beta\neq 0} \frac{V_{00}V_{0\alpha}V_{\alpha\beta}V_{\beta 0}}{E_{0\alpha}E_{0\beta}^2} - \sum_{\alpha,\beta\neq 0} \frac{V_{00}V_{0\alpha}V_{\alpha\beta}V_{\beta 0}}{E_{0\alpha}^2 E_{0\beta}} + \sum_{\alpha\neq 0} \frac{V_{00}V_{0\alpha}V_{\alpha 0}V_{00}}{E_{0\alpha}^3} \\
&\quad + \sum_{\alpha,\beta,\gamma\neq 0} \frac{V_{0\alpha}V_{\alpha\beta}V_{\beta\gamma}V_{0\gamma}}{E_{0\alpha}E_{0\beta}E_{0\gamma}} - \sum_{\alpha,\beta\neq 0} \frac{V_{00}V_{0\alpha}V_{\alpha 0}V_{0\beta}V_{\beta 0}}{E_{0\alpha}^2 E_{0\beta}} \\
\mathrm{tr}(\Delta_4) &= \sum_{\alpha,\beta,\gamma\neq 0} \frac{V_{0\alpha}V_{\alpha\beta}V_{\beta\gamma}V_{0\gamma}}{E_{0\alpha}E_{0\beta}E_{0\gamma}} - V_{00} \sum_{\alpha,\beta\neq 0} \frac{|V_{0\alpha}|^2 |V_{0\beta}|^2}{E_{0\alpha}^2 E_{0\beta}} \\
&\quad - V_{00} \sum_{\alpha,\beta\neq 0} \left[\frac{V_{0\alpha}V_{\alpha\beta}V_{\beta 0}}{E_{0\alpha}E_{0\beta}^2} + \frac{V_{0\alpha}V_{\alpha\beta}V_{\beta 0}}{E_{0\alpha}^2 E_{0\beta}} \right] + V_{00}^2 \sum_{\alpha\neq 0} \frac{|V_{0\alpha}|^2}{E_{0\alpha}^3}
\end{aligned} \tag{11}$$

as desired.

3) We consider a particle in the potential $V(\mathbf{r}) = \lambda r^n$ and compute the commutator $[\mathbf{r}\cdot\mathbf{p}, H]$, where $H = \mathbf{p}^2/2m + V(\mathbf{r})$.

$$\begin{aligned}
[\mathbf{r}\cdot\mathbf{p}, H] &= \mathbf{r}\cdot[\mathbf{p}, H] + [\mathbf{r}, H]\cdot\mathbf{p} \\
[\mathbf{r}\cdot\mathbf{p}, H] &= \mathbf{r}\cdot[\mathbf{p}, \lambda r^n] + \left[\mathbf{r}, \frac{\mathbf{p}^2}{2m}\right]\cdot\mathbf{p} \\
[\mathbf{r}\cdot\mathbf{p}, H] &= \lambda\mathbf{r}\cdot[\mathbf{p}, r^n] + \frac{1}{2m}\left[\mathbf{r}, \mathbf{p}^2\right]\cdot\mathbf{p} \\
[\mathbf{r}\cdot\mathbf{p}, H] &= -i\hbar\lambda\mathbf{r}\cdot(nr^{n-1}\hat{\mathbf{r}}) + \frac{1}{2m}\left[\mathbf{r}, \mathbf{p}^2\right]\cdot\mathbf{p} \\
[\mathbf{r}\cdot\mathbf{p}, H] &= -i\hbar\left(n\lambda r^n + \frac{1}{2m}\left[\mathbf{r}, \mathbf{p}^2\right]\cdot\nabla\right) \\
[\mathbf{r}\cdot\mathbf{p}, H] &= -i\hbar\left(n\lambda r^n + \frac{1}{2m}\sum_i \left[r_i, \mathbf{p}^2\right]\frac{\partial}{\partial r_i}\right) \\
[\mathbf{r}\cdot\mathbf{p}, H] &= -i\hbar\left(n\lambda r^n - \frac{\hbar^2}{2m}\sum_i \left[r_i, \nabla^2\right]\frac{\partial}{\partial r_i}\right) \\
[\mathbf{r}\cdot\mathbf{p}, H] &= -i\hbar\left(n\lambda r^n - \frac{\hbar^2}{2m}\sum_i \left(-2\frac{\partial}{\partial r_i}\frac{\partial}{\partial r_i}\right)\right) \\
[\mathbf{r}\cdot\mathbf{p}, H] &= -i\hbar\left(n\lambda r^n + 2\frac{\hbar^2}{2m}\nabla^2\right) \\
[\mathbf{r}\cdot\mathbf{p}, H] &= -i\hbar\left(n\lambda r^n - 2\frac{\mathbf{p}^2}{2m}\right) \\
[\mathbf{r}\cdot\mathbf{p}, H] &= -i\hbar\left(nV(\mathbf{r}) - 2T\right)
\end{aligned} \tag{12}$$

Let $|\psi\rangle$ be an energy eigenstate with eigenvalue E. Then we have

$$
\begin{aligned}
\langle\psi|\,[\mathbf{r}\cdot\mathbf{p}, H]\,|\psi\rangle &= \langle\psi|\,(\mathbf{r}\cdot\mathbf{p})H\,|\psi\rangle - \langle\psi|\,H(\mathbf{r}\cdot\mathbf{p})\,|\psi\rangle \\
\langle\psi|\,[\mathbf{r}\cdot\mathbf{p}, H]\,|\psi\rangle &= E\,\langle\psi|\,\mathbf{r}\cdot\mathbf{p}\,|\psi\rangle - E\,\langle\psi|\,\mathbf{r}\cdot\mathbf{p}\,|\psi\rangle \\
\langle\psi|\,[\mathbf{r}\cdot\mathbf{p}, H]\,|\psi\rangle &= 0 \\
\implies 0 &= -i\hbar\,\langle\psi|\,(nV(\mathbf{r}) - 2T)\,|\psi\rangle \\
0 &= n\big\langle V(\mathbf{r})\big\rangle - 2\big\langle T\big\rangle \\
n\big\langle V\big\rangle &= 2\big\langle T\big\rangle
\end{aligned}
\tag{13}
$$

4) For the hydrogen atom, $V(\mathbf{r}) = -\hbar c\alpha/r$.

a) From (13), we have

$$
\begin{aligned}
\big\langle H\big\rangle &= \big\langle T\big\rangle + \big\langle V\big\rangle \\
\big\langle H\big\rangle &= \frac{1}{2}\big\langle V\big\rangle \\
{}_n = E - \frac{\alpha^2 c^2 \mu}{2n^2} &= -\frac{1}{2}\left\langle \frac{\hbar c\alpha}{r}\right\rangle \\
\implies \left\langle \frac{1}{r}\right\rangle &= \frac{\mu\alpha c}{\hbar n^2} \\
\left\langle \frac{1}{r}\right\rangle &= \frac{1}{a_0 n^2}
\end{aligned}
\tag{14}
$$

b) Starting with the Hamiltonian for the hydrogen atom,

$$
H = \frac{p_r^2}{2m_e} + \frac{\hbar^2 L(L+1)}{2m_e r^2} - \frac{\hbar c\alpha}{r}
\tag{15}
$$

we have, by the Hellmann–Feynman theorem,

$$
\begin{aligned}
\left\langle \frac{\partial H}{\partial\alpha}\right\rangle &= \frac{\partial E}{\partial\alpha} \\
-\hbar c\left\langle \frac{1}{r}\right\rangle &= -\frac{\alpha c^2\mu}{n^2} \\
\left\langle \frac{1}{r}\right\rangle &= \frac{\alpha c\mu}{\hbar n^2} \\
\left\langle \frac{1}{r}\right\rangle &= \frac{1}{a_0 n^2}
\end{aligned}
\tag{16}
$$

c) We apply the Hellmann–Feynman theorem again with $\lambda = \ell$ and using the fact that, at fixed angular momentum, $\frac{\partial n}{\partial \ell} = 1$.

$$
\begin{aligned}
\left\langle \frac{\partial H}{\partial \ell} \right\rangle &= \frac{\partial E}{\partial \ell} \\
\frac{\hbar^2(2\ell+1)}{2m_e}\left\langle \frac{1}{r^2} \right\rangle &= \frac{\partial E}{\partial n}\frac{\partial n}{\partial \ell} \\
\left\langle \frac{1}{r^2} \right\rangle &= \frac{m_e}{\hbar^2(\ell+1/2)}\frac{\alpha^2 c^2 m_e}{n^3} \\
\left\langle \frac{1}{r^2} \right\rangle &= \frac{\alpha^2 c^2 m_e^2}{\hbar^2(\ell+1/2)n^3} \\
\left\langle \frac{1}{r^2} \right\rangle &= \frac{1}{a_0^2(\ell+1/2)n^3}
\end{aligned} \tag{17}
$$

d) For any operator, A, acting on an energy eigenstate, $\langle [H, A] \rangle = 0$ by the algebra in equation (13). Below we compute $\langle [H, p_r] \rangle$.

$$
\begin{aligned}
\langle [H, p_r] \rangle &= \frac{\hbar^2 \ell(\ell+1)}{2m_e}\left\langle [\frac{1}{r^2}, p_r] \right\rangle - \hbar c\alpha \left\langle [\frac{1}{r}, p_r] \right\rangle \\
0 &= \frac{\hbar^2 \ell(\ell+1)}{2m_e}\left\langle \frac{-2i\hbar}{r^3} \right\rangle - \hbar c\alpha \left\langle \frac{-i\hbar}{r^2} \right\rangle \\
0 &= \frac{\hbar^2 \ell(\ell+1)}{m_e}\left\langle \frac{1}{r^3} \right\rangle - \hbar c\alpha \left\langle \frac{1}{r^2} \right\rangle \\
\frac{\hbar^2 \ell(\ell+1)}{m_e}\left\langle \frac{1}{r^3} \right\rangle &= \frac{\hbar c\alpha}{a_0^2(\ell+1/2)n^3} \\
\left\langle \frac{1}{r^3} \right\rangle &= \frac{c\alpha m_e}{\hbar a_0^2 \ell(\ell+1)(\ell+1/2)n^3} \\
\left\langle \frac{1}{r^3} \right\rangle &= \frac{1}{\ell(\ell+1)(\ell+1/2)a_0^3 n^3}
\end{aligned} \tag{18}
$$

5) The $n = 3$ states are

$$
\begin{aligned}
&|3\ 0\ 0\rangle \\
&|3\ 1\ 0\rangle\,,\ |3\ 1\ \pm 1\rangle \\
&|3\ 2\ 0\rangle\,,\ |3\ 2\ \pm 1\rangle\,,\ |3\ 2\ \pm 2\rangle
\end{aligned} \tag{19}
$$

Since the integral $\int d\Omega \cos(\theta) Y_0^0(\Omega)^* Y_l^m(\Omega)$ vanishes for all l and m except $l = 1$ and $m = 0$, we need only calculate the term carrying $|3\ 1\ 0\rangle$.

$$
\begin{aligned}
\delta E_2 &\approx e^2\mathscr{E}^2\left(\frac{|z_{01}|^2}{E_{01}}+\frac{|z_{02}|^2}{E_{02}}\right)\\
z_{02} &= \frac{\sqrt{2}}{81\pi a_0^3}\int_0^\infty dr\int d\Omega\left[6-\frac{r}{a_0}\right]\frac{r}{a_0}e^{-r/a_0}e^{-r/3a_0}r^3\cos^2(\theta)\\
z_{02} &= \frac{3^3 a_0}{2^6\sqrt{2}}\\
\delta E_2 &\approx -\frac{2^{20}}{3^{11}}\pi\epsilon_0 a_0^3\mathscr{E}^2+e^2\mathscr{E}^2\frac{|z_{02}|^2}{E_{02}}\\
\delta E_2 &\approx -\frac{2^{20}}{3^{11}}\pi\epsilon_0 a_0^3\mathscr{E}^2-\frac{3^8}{2^{13}}\pi\epsilon_0 a_0^3\mathscr{E}^2\\
\delta E_2 &\approx -\left(\frac{2^{33}+3^{19}}{3^{11}2^{13}}\right)\pi\epsilon_0 a_0^3\mathscr{E}^2\\
\delta E_2 &\approx -6.72\pi\epsilon_0 a_0^3\mathscr{E}^2
\end{aligned}
\tag{20}
$$

Which is about $6.72/9 \approx 74.67\%$ of the value in equation (22) in the reading.

♣