Homework 1

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Problem 1

Let's begin with the purified state, $|\psi_{\rm CM}\rangle$ (where "C" stands for "contestant" and "M" stands for "Monty")

$$|\psi_{\text{CM}}\rangle = \frac{1}{\sqrt{3}} (|1\rangle |1\rangle + |2\rangle |2\rangle + |3\rangle |3\rangle)$$

The contestant's state represents their state of belief about which door the car is behind. Monty's state represents his state of belief about which door he will open to reveal a goat. The contestant's selection of door 1 induces the transformation

$$\begin{aligned} |\psi_{\text{CM}}\rangle &\to \frac{1}{\sqrt{3}} \left[|1\rangle \left(\frac{|2\rangle + |3\rangle}{\sqrt{2}} \right) + |2\rangle |3\rangle + |3\rangle |2\rangle \right] \\ &= \frac{1}{\sqrt{6}} |1\rangle |2\rangle + \frac{1}{\sqrt{6}} |1\rangle |3\rangle + \frac{1}{\sqrt{3}} |2\rangle |3\rangle + \frac{1}{\sqrt{3}} |3\rangle |2\rangle \\ &= \left(\frac{1}{\sqrt{6}} |1\rangle + \frac{1}{\sqrt{3}} |2\rangle \right) |2\rangle + \left(\frac{1}{\sqrt{6}} |1\rangle + \frac{1}{\sqrt{3}} |2\rangle \right) |3\rangle \end{aligned}$$

Now, a projective measurment on Monty's state (i.e., Monty choosing to open door 2 or 3) will collapse the state one of

$$\left(\sqrt{\frac{1}{3}}|1\rangle + \sqrt{\frac{2}{3}}|2\rangle\right)|2\rangle$$
$$\left(\sqrt{\frac{1}{3}}|1\rangle + \sqrt{\frac{2}{3}}|2\rangle\right)|3\rangle$$

with equal probability. In either case, the contestant's part of the state becomes

$$|\psi_{\rm C}\rangle = \sqrt{\frac{1}{3}} |1\rangle + \sqrt{\frac{2}{3}} |2\rangle$$

indicating that with probability 2/3 the car is behind door 2 and the contestant should switch.

Problem 2

$$x \approx x_0 + \lambda x_1 + \lambda^2 x_2 + \cdots$$

= 12.002383785691716

(a)

$$x = (x_0 + \lambda x_1)^3$$

= $x_0^3 + 3\lambda x_0^2 x_1 + 3\lambda^2 x_0 x_1^2 + \lambda^3 x_1^3$
= $x_0^3 + \lambda$

Matching terms proportional to λ gives

$$\lambda = 3\lambda x_0^2 x_1 \implies 3x_0^2 x_1 = 1 \implies x_1 = \frac{1}{3x_0^2}$$

The current approximation for x is therefore

$$x \approx x_0 + \lambda x_1 = 12 + \frac{1.03}{3 \times 12^2} = 12.002384\overline{259}$$

(b) Keeping terms only proportional to λ^2 we have

$$(x_0 + \lambda x_1 + \lambda^2 x_2)^3 \to 3x_0^2 x_2 \lambda^2 + 3x_0 x_1^2 \lambda^2$$

= $(3x_0^2 x_2 + 3x_0 x_1^2) \lambda^2$

matching terms proportional to λ^2 gives

$$3x_0^2x_2 + 3x_0x_1^2 = 0 \implies x_2 = -\frac{x_0x_1^2}{x_0^2} = -\frac{x_1^2}{x_0} = -\frac{1}{9x_0^5}$$

The current approximation for x is therefore

$$x \approx x_0 + \lambda x_1 + \lambda^2 x_2 = 12 + \frac{1.03}{3 \times 12^2} - \frac{1.03^2}{9 \times 12^5} = 12.00238473298$$

Problem 3

 Δ_4 is a sum over all sets of 5 nonnegative indicies that add to 3:

$$\Delta_4 = (01110\cdot) + (10011\cdot) + (10101\cdot) + (11001\cdot) + (00120\cdot) + (00210\cdot) + (01020\cdot) + (01200\cdot) + (01200\cdot) + (02100\cdot) + (02010\cdot) + (10002\cdot) + (20001\cdot) + (00030\cdot) + (00300\cdot) + (03000\cdot)$$

Where only terms in which the first and last indicies do not cancel under trace have been kept. Some further simplification is given by

$$(10002\cdot) \to (3000)$$

$$(2001\cdot) \to (3000)$$

$$(00030\cdot), (03000\cdot), (00300\cdot) \to -(3000)$$

$$(00120\cdot) \to -(0011\cdot1) \to -(10011\cdot)$$

$$(00210\cdot) \to -(001\cdot11) \to -(11001\cdot)$$

$$(01020\cdot) \to -(0101\cdot1) \to -(10101\cdot)$$

$$(01200\cdot) \to -(011\cdot10) \to -(10011\cdot)$$

$$(02100\cdot) \to -(01\cdot110) \to -(11001\cdot)$$

$$(02010\cdot) \to -(01\cdot101) \to -(10101\cdot)$$

Giving

$$\Delta_4 = (01110 \cdot) - (10011 \cdot) - (11001 \cdot) - (10101 \cdot) - (3000)$$

= -(0111) - (2001) - (2100) - (2010) - (3000)

Now let's handle the trace of each term individually

$$Tr[-(0111)] = Tr \left[P_0 V \sum_{\alpha \neq 0} \frac{|\alpha\rangle\langle\alpha|}{E_{0\alpha}} V \sum_{\beta \neq 0} \frac{|\beta\rangle\langle\beta|}{E_{0\beta}} V \sum_{\gamma \neq 0} \frac{|\gamma\rangle\langle\gamma|}{E_{0\gamma}} V \right]$$

$$= Tr \left[P_0 V \sum_{\alpha \neq 0} \frac{|\alpha\rangle\langle\alpha|}{E_{0\alpha}} V \sum_{\beta \neq 0} \frac{|\beta\rangle\langle\beta|}{E_{0\beta}} V \sum_{\gamma \neq 0} \frac{|\gamma\rangle\langle\gamma|}{E_{0\gamma}} V P_0 \right]$$

$$= Tr \left[P_0 \sum_{\alpha,\beta,\gamma \neq 0} \frac{V_{0\alpha}V_{\alpha\beta}V_{\beta\gamma}V_{\gamma0}}{E_{0\alpha}E_{0\beta}E_{0\gamma}} \right]$$

$$= \sum_{\alpha,\beta,\alpha \neq 0} \frac{V_{0\alpha}V_{\alpha\beta}V_{\beta\gamma}V_{\gamma0}}{E_{0\alpha}E_{0\beta}E_{0\gamma}}$$

$$-\operatorname{Tr}[(2010)] = -\operatorname{Tr}\left[\sum_{\alpha\neq 0} \frac{|\alpha\rangle\langle\alpha|}{E_{0\alpha}^2} V P_0 V \sum_{\beta\neq 0} \frac{|\beta\rangle\langle\beta|}{E_{0\beta}} V P_0 V\right]$$

$$= -\operatorname{Tr}\left[P_0 V \sum_{\alpha\neq 0} \frac{|\alpha\rangle\langle\alpha|}{E_{0\alpha}^2} V P_0 V \sum_{\beta\neq 0} \frac{|\beta\rangle\langle\beta|}{E_{0\beta}} V P_0\right]$$

$$= -\operatorname{Tr}\left[P_0 \sum_{\alpha,\beta\neq 0} \frac{V_{0\alpha} V_{\alpha 0} V_{0\beta} V_{\beta 0}}{E_{0\alpha}^2 E_{0\beta}}\right]$$

$$= -\sum_{\alpha,\beta\neq 0} \frac{\left|V_{0\alpha}\right|^2 \left|V_{0\beta}\right|^2}{E_{0\alpha}^2 E_{0\beta}}$$

$$-\operatorname{Tr}[(2001)] = -\operatorname{Tr}\left[\sum_{\alpha\neq0} \frac{|\alpha\rangle\langle\alpha|}{E_{0\alpha}^2} V P_0 V P_0 V \sum_{\beta\neq0} \frac{|\beta\rangle\langle\beta|}{E_{0\beta}} V\right]$$

$$= -\operatorname{Tr}\left[P_0 V \sum_{\beta\neq0} \frac{|\beta\rangle\langle\beta|}{E_{0\beta}} V \sum_{\alpha\neq0} \frac{|\alpha\rangle\langle\alpha|}{E_{0\alpha}^2} V P_0 V P_0\right]$$

$$= -\operatorname{Tr}\left[P_0 \sum_{\alpha,\beta\neq0} \frac{V_{0\beta} V_{\beta\alpha} V_{\alpha0}}{E_{0\alpha}^2 E_{0\beta}} V_{00}\right]$$

$$= -V_{00} \sum_{\alpha,\beta\neq0} \frac{V_{0\beta} V_{\beta\alpha} V_{\alpha0}}{E_{0\alpha}^2 E_{0\beta}}$$

$$= -V_{00} \sum_{\alpha,\beta\neq0} \frac{V_{0\alpha} V_{\alpha\beta} V_{\beta0}}{E_{0\alpha} E_{0\beta}^2}$$

$$-\operatorname{Tr}[(2100)] = -\operatorname{Tr}\left[\sum_{\alpha \neq 0} \frac{|\alpha\rangle\langle\alpha|}{E_{0\alpha}^2} V \sum_{\beta \neq 0} \frac{|\beta\rangle\langle\beta|}{E_{0\beta}} V P_0 V P_0 V\right]$$

$$= -\operatorname{Tr}\left[P_0 V \sum_{\alpha \neq 0} \frac{|\alpha\rangle\langle\alpha|}{E_{0\alpha}^2} V \sum_{\beta \neq 0} \frac{|\beta\rangle\langle\beta|}{E_{0\beta}} V P_0 V P_0\right]$$

$$= -\operatorname{Tr}\left[P_0 \sum_{\alpha,\beta \neq 0} \frac{V_{0\alpha} V_{\alpha\beta} V_{\beta0}}{E_{0\alpha}^2 E_{0\beta}} V_{00}\right]$$

$$= -V_{00} \sum_{\alpha,\beta \neq 0} \frac{V_{0\alpha} V_{\alpha\beta} V_{\beta0}}{E_{0\alpha}^2 E_{0\beta}}$$

$$-\operatorname{Tr}[(3000)] = \operatorname{Tr}\left[\sum_{\alpha \neq 0} \frac{|\alpha\rangle\langle\alpha|}{E_{0\alpha}^3} V P_0 V P_0 V P_0 V\right]$$

$$= \operatorname{Tr}\left[P_0 V \sum_{\alpha \neq 0} \frac{|\alpha\rangle\langle\alpha|}{E_{0\alpha}^3} V P_0 V P_0 V P_0\right]$$

$$= \operatorname{Tr}\left[P_0 \sum_{\alpha \neq 0} \frac{V_{0\alpha} V_{\alpha 0}}{E_{0\alpha}^3} V_{00} V_{00}\right]$$

$$= V_{00}^2 \sum_{\alpha \neq 0} \frac{|V_{0\alpha}|^2}{E_{0\alpha}^3}$$

Putting it all together we have

$$\operatorname{Tr}[\Delta_{4}] = \sum_{\alpha,\beta,\gamma\neq0} \frac{V_{0\alpha}V_{\alpha\beta}V_{\beta\gamma}V_{\gamma0}}{E_{0\alpha}E_{0\beta}E_{0\gamma}} - \sum_{\alpha,\beta\neq0} \frac{\left|V_{0\alpha}\right|^{2}\left|V_{0\beta}\right|^{2}}{E_{0\alpha}^{2}E_{0\beta}} - V_{00} \sum_{\alpha,\beta\neq0} \left[\frac{V_{0\alpha}V_{\alpha\beta}V_{\beta0}}{E_{0\alpha}E_{0\beta}^{2}} + \frac{V_{0\alpha}V_{\alpha\beta}V_{\beta0}}{E_{0\alpha}^{2}E_{0\beta}}\right] + V_{00}^{2} \sum_{\alpha\neq0} \frac{\left|V_{0\alpha}\right|^{2}}{E_{0\alpha}^{3}}$$

In the case that $Tr[\Delta_1] = Tr[\Delta_2] = Tr[\Delta_3] = 0$ this reduces to just the first term:

$$Tr[\Delta_4] = \sum_{\alpha,\beta,\gamma\neq 0} \frac{V_{0\alpha}V_{\alpha\beta}V_{\beta\gamma}V_{\gamma0}}{E_{0\alpha}E_{0\beta}E_{0\gamma}}$$

Problem 4

$$\begin{split} [\vec{r} \cdot \vec{p}, H] &= \left[\vec{r} \cdot \vec{p}, \frac{p^2}{2m} \right] + [\vec{r} \cdot \vec{p}, V(r)] \\ &= \frac{1}{2m} [\vec{r}, p^2] \cdot \vec{p} + \vec{r} \cdot [\vec{p}, V(r)] \\ &= \frac{1}{2m} (2i\hbar \vec{p}) \cdot \vec{p} - i\hbar \vec{r} \cdot \nabla V(r) \\ &= i\hbar \left(\frac{p^2}{m} - \vec{r} \cdot \nabla V(r) \right) \\ &= i\hbar \left(2T - \vec{r} \cdot \nabla V \right) \end{split}$$

Now,

$$\langle [\vec{r} \cdot \vec{p}, H] \rangle = 0 \implies 2 \langle T \rangle = \langle \vec{r} \cdot \nabla V \rangle$$

but

$$\langle \vec{r} \cdot \nabla V \rangle = \langle \vec{r} \cdot n \lambda r^{n-1} \hat{r} \rangle = \langle n \lambda r^n \rangle = n \langle V \rangle$$

SO

$$2\left\langle T\right\rangle =n\left\langle V\right\rangle$$

Problem 5

(a) For the hydrogen atom we have n = -1, so

$$\langle T \rangle = -\frac{1}{2} \langle v \rangle \implies E_n = \langle T \rangle_n + \langle V \rangle_n = \frac{1}{2} \langle V \rangle_n$$

$$\implies -\frac{\alpha^2 \mu c^2}{2n^2} = \frac{\hbar c \alpha}{2} \langle r^{-1} \rangle$$

$$\implies \langle r^{-1} \rangle = \frac{\alpha \mu c}{\hbar n^2} = \frac{1}{a_0 n^2}$$

(b) Given
$$H = \frac{p_r^2}{2m_e} + \frac{\hbar^2 L(L+1)}{2m_e r^2} - \frac{\hbar c\alpha}{r}$$
, $E_n = -\frac{\alpha^2 \mu c^2}{2n^2}$,

$$\partial_{\alpha}E = -\frac{\alpha\mu c^{2}}{n^{2}}$$

$$\langle \partial_{\alpha}H \rangle = \left\langle -\frac{\hbar c}{r} \right\rangle = -\hbar c \left\langle r^{-1} \right\rangle$$

$$\partial_{\alpha}E = \langle \partial_{\alpha}H \rangle \implies \left\langle r^{-1} \right\rangle = \frac{\alpha\mu c}{\hbar n^{2}} = \frac{1}{a_{0}n^{2}}$$

(c)
$$\partial_L E = \partial_L \left(-\frac{\alpha^2 \mu c^2}{2(L+k)^2} \right) = \frac{\alpha^2 \mu c^2}{(L+k)^3} = \frac{\alpha^2 \mu c^2}{n^3}$$

$$\langle \partial_L H \rangle = \left\langle \partial_L \left(\frac{p_r^2}{2\mu} + \frac{\hbar^2 L(L+1)}{2\mu r^2} - \frac{\hbar c\alpha}{r} \right) \right\rangle = \frac{\hbar^2 (L+1/2)}{\mu} \left\langle r^{-2} \right\rangle$$

$$\partial_L E = \left\langle \partial_L H \right\rangle \implies \left\langle r^{-2} \right\rangle = \frac{\alpha^2 \mu^2 c^2}{\hbar^2 (L+1/2) n^3} = \frac{1}{a_0^2 (L+1/2) n^3}$$

(d) $[H, p_r] = \frac{\hbar^2 L(L+1)}{2\mu} [r^{-2}, p_r] - \hbar \alpha c [r^{-1}, p_r]$ $= -\frac{i\hbar^3 L(L+1)}{\mu} r^{-3} + i\hbar^2 \alpha c r^{-2}$

Since the expectation value of any operator with the Hamiltonian vanishes with respect to any of the Hamiltonian's eigenstates,

$$\langle [H, p_r] \rangle = 0 \implies i\hbar^2 \alpha c \left\langle r^{-2} \right\rangle = \frac{i\hbar^3 L(L+1)}{\mu} \left\langle r^{-3} \right\rangle$$

$$\implies \left\langle r^{-3} \right\rangle = \frac{\alpha \mu c}{\hbar L(L+1)} \left\langle r^{-2} \right\rangle = \frac{1}{a_0 L(L+1)} \left\langle r^{-2} \right\rangle$$

Substituting in the value for $\langle r^{-2} \rangle$ gives

$$\langle r^{-3} \rangle = \frac{1}{L(L+1/2)(L+1)a_0^3 n^3}$$