Answers: Exam #2

1. $$E = \frac{\int_0^\infty e^{-\alpha r^2} H e^{-\alpha r^2} r^2 dr}{\int_0^\infty e^{-2\alpha r^2} r^2 dr} = \frac{3}{2}\alpha - \frac{2\alpha^{1/2}}{\sqrt{\pi/2}}$$

The minimum occurs for $\alpha \approx 0.28$

$E(\alpha = 0.28) = -0.425$ a.u.

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2. The minimum is shifted by 0.1 a.u. by the electric field.

$$E = E_{HO} - 10^{-4}\left[\frac{|\langle 0|x + x^3|1\rangle|^2}{\omega} + \frac{|\langle 0|x^3|3\rangle|^2}{3\omega}\right]$$

I have ω rather than $\hbar\omega$ in the denominator due to the use of atomic units.

$$E = E_{HO} - 10^{-4}\left[\frac{(1/\sqrt{2} + 3/\sqrt{8})^2}{\omega} + \frac{(\sqrt{6}/\sqrt{8})^2}{3\omega}\right] = E_{HO} - \frac{29}{16}10^{-4}\frac{1}{\omega}$$

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3. $\epsilon_- = h_e + J_{ee} - J_{ep}$, $\epsilon_+ = h_p - 2J_{ep}$

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4. $\psi(^3P) = \frac{1}{\sqrt{2}}(p_+p_0 - p_0p_+)\alpha\alpha$

$\psi(^1D) = \frac{1}{2}(p_+p_0 + p_0p_+)(\alpha\beta - \beta\alpha)$

$E(^3P) = 2h + J - K$, $E(^1D) = 2h + J + K$

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5. $$E = \frac{3}{2}\hbar\omega + q^4\frac{\left|\langle 0|\frac{2x_1x_2}{R_{12}^3} + \frac{2x_2x_3}{R_{23}^3} + \frac{2x_1x_3}{R_{13}^3}|i\rangle\right|^2}{E_0 - E_i}$$

$$E = \frac{3}{2}\hbar\omega - \frac{2q^4\hbar}{m^2\omega^3}\left[\frac{1}{R_{12}^6} + \frac{1}{R_{23}^6} + \frac{1}{R_{13}^6}\right]$$

Note that the ground state is $|000\rangle$ and the excited states are $|110\rangle$, $|101\rangle$, and $|011\rangle$. There is no 3-body contribution at this level.