[10 points] Question 1: Two non-interacting electrons are placed in the same potential. One electron will be in the single-particle stationary state ψ_1 while the other is in state ψ_2.

List out all four allowed normalized stationary states at this energy. Electrons are, of course, indistinguishable spin-1/2 fermions.

Fermions are in total states that are antisymmetric under exchange. This can be a spatially symmetric state with a spin antisymmetric state or a spatially antisymmetric state with a spin symmetric state.

For two spin-$\frac{1}{2}$, the $|0\ 0\rangle$ singlet is spin antisymmetric while the three $|1\ m\rangle$ triplet states are spin symmetric.

$$\frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2)+\psi_2(x_1)\psi_1(x_2)\right)|0\ 0\rangle$$

$$\frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2)-\psi_2(x_1)\psi_1(x_2)\right)|1\ -1\rangle$$

$$\frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2)-\psi_2(x_1)\psi_1(x_2)\right)|1\ 0\rangle$$

$$\frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2)-\psi_2(x_1)\psi_1(x_2)\right)|1\ +1\rangle$$

[15 points] Question 2: The excited states of helium come in two types: orthohelium and parahelium. Parahelium states have higher energy than the equivalent orthohelium states.

Write a paragraph describing the difference between the orthohelium and parahelium states. Explain the following in your answer: Why are the parahelium states at higher energies?

The $1s2s$ states occur with one electron in the single-particle ground state ($n = 1$, $l = 0$) and the other in a single particle $n = 2$, $l = 0$ state. What are the degeneracies of orthohelium $1s2s$ state and of the parahelium $1s2s$ state? (Note: these degeneracies come solely from spin because both electrons are in $l = 0$ states.)

Parahelium states are spatially symmetric and spin antisymmetric (singlet). Orthohelium states are spatially antisymmetric and spin symmetric (triplet).

Particles in a symmetric combination are (on average) closer together than those in an antisymmetric combination. (This is due to exchange forces.) Closer electrons increases the Coulomb repulsion energy (and also weakens screening). Therefore Parahelium states have higher energy.

Parahelium $1s2s$ → degeneracy = 1 (singlet)

Orthohelium $1s2s$ → degeneracy = 3 (triplet)

[20 points] Question #3: In this problem we will use natural units, so that $\hbar = m = \omega = 1$. Our unperturbed system is a simple harmonic oscillator. This system is perturbed by adding a delta function barrier of strength α at position $x = 1$:

$$V(x) = \frac{1}{2}x^2 + \alpha\delta(x-1), \qquad \text{so } V'(x) = \alpha\delta(x-1)$$

(a) Determine the first-order correction to the ground state energy.

(b) Determine the first nonzero term in the second-order correction to the ground state energy.

$$\psi_0^0(x) = \left(\frac{1}{\pi}\right)^{1/4} e^{-\frac{1}{2}x^2} \text{ with } E_0^0 = \frac{1}{2}$$

$$\psi_1^0(x) = \left(\frac{1}{\pi}\right)^{1/4} \sqrt{2}xe^{-\frac{1}{2}x^2} \text{ with } E_1^0 = \frac{3}{2}$$

a) $E_0' = \langle \psi_0^0 | \hat{H}' | \psi_0^0 \rangle$

$= \int \left(\left(\frac{1}{\pi}\right)^{1/4} e^{-\frac{1}{2}x^2}\right)^* \alpha\,\delta(x-1) \left(\frac{1}{\pi}\right)^{1/4} e^{-\frac{1}{2}x^2} dx = \frac{\alpha}{\sqrt{\pi}} e^{-1}$

$$\boxed{E_0' = \frac{\alpha}{\sqrt{\pi}} e^{-1}}$$

b) $E_0^2 = \sum_{m \neq 0} \frac{|\langle \psi_m^0 | \hat{H}' | \psi_0^0 \rangle|^2}{E_0^0 - E_m^0}$ $\quad m=1$ is 1^{st} term

$\langle \psi_1^0 | \hat{H}' | \psi_0^0 \rangle = \int \left(\left(\frac{1}{\pi}\right)^{1/4} \sqrt{2}\, x e^{-\frac{1}{2}x^2}\right)^* \alpha\,\delta(x-1) \left(\left(\frac{1}{\pi}\right)^{1/4} e^{-\frac{1}{2}x^2}\right) dx$

$= \sqrt{2}\,\frac{\alpha}{\sqrt{\pi}} e^{-1}$

$$\frac{\left|\sqrt{2}\,\frac{\alpha}{\sqrt{\pi}} e^{-1}\right|^2}{\frac{1}{2} - \frac{3}{2}} = -\frac{2\alpha^2}{\pi} e^{-2}$$

$$\boxed{E_0^2 = -\frac{2\alpha^2}{\pi} e^{-2}}$$

$$E_0 = \frac{1}{2} + \frac{\alpha}{\sqrt{\pi}} e^{-1} - \frac{2\alpha^2}{\pi} e^{-2} + \cdots$$

[20 points] Question #4: We'll again consider a particle constrained to a circle, using polar coordinates and $0 \le \phi < 2\pi$. One way to list the pair of degenerate first excited states is

$$\psi_a^0(\phi) = \sqrt{\frac{1}{2\pi}}\, e^{+i\phi} \qquad \text{and} \qquad \psi_b^0(\phi) = \sqrt{\frac{1}{2\pi}}\, e^{-i\phi}$$

We then add a perturbation that is a constant upward potential shift V_0 over the region $0 \le \phi \le \frac{\pi}{2}$. Therefore:

$$V'(\phi) = \begin{cases} V_0 & 0 \le \phi \le \frac{\pi}{2} \\ 0 & \frac{\pi}{2} < \phi < 2\pi \end{cases}$$

Construct the W matrix and determine the two first-order energy corrections $E_\pm^1$.

Note: $\displaystyle\int_0^{\pi/2} e^{\pm i2\phi}\, d\phi = \pm i$

$$W_{aa} = \langle \psi_a^0 | \hat{H}' | \psi_a^0 \rangle = \int_0^{\frac{\pi}{2}} \left(\left(\tfrac{1}{2\pi}\right)^{1/2} e^{i\phi}\right)^* V_0 \left(\left(\tfrac{1}{2\pi}\right)^{1/2} e^{i\phi}\right) d\phi$$

$$= \int_0^{\frac{\pi}{2}} \frac{1}{2\pi} V_0\, d\phi = \frac{1}{2\pi} V_0 \frac{\pi}{2} = \frac{V_0}{4}$$

W_{bb} is the same

$$W_{ab} = \langle \psi_a^0 | \hat{H}' | \psi_b^0 \rangle = \int_0^{\frac{\pi}{2}} \left(\frac{1}{\sqrt{2\pi}} e^{i\phi}\right)^* V_0 \left(\frac{1}{\sqrt{2\pi}} e^{-i\phi}\right) d\phi$$

$$= \frac{V_0}{2\pi} \int_0^{\frac{\pi}{2}} e^{-2i\phi}\, d\phi = \frac{-iV_0}{2\pi} \qquad W_{ba} = W_{ab}^* = \frac{iV_0}{2\pi}$$

$$W = \begin{pmatrix} \frac{V_0}{4} & \frac{-iV_0}{2\pi} \\ \frac{iV_0}{2\pi} & \frac{V_0}{4} \end{pmatrix}$$

$$E_{\pm}' = \frac{1}{2}\left[W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab}|^2}\right]$$

$$= \frac{1}{2}\left[\frac{V_0}{4} + \frac{V_0}{4} \pm \sqrt{0^2 + 4\left|\frac{-iV_0}{2\pi}\right|^2}\right]$$

$$= \frac{V_0}{4} \pm \frac{V_0}{2\pi}$$

$$\boxed{E_-' = \frac{V_0}{4} - \frac{V_0}{2\pi} \qquad E_+' = \frac{V_0}{4} + \frac{V_0}{2\pi}}$$

[20 points] Question #5: You are using the variational principle to estimate the bound state energy for a delta function well: $V(x) = -\alpha\delta(x)$. (α will be a positive constant with dimensions of energy·length.) Your trial wave function will be

$$\psi(x) = \begin{cases} \sqrt{\frac{2}{a}}\cos\left(\frac{\pi x}{a}\right) & -\frac{a}{2} \le x \le \frac{a}{2} \\ 0 & |x| > \frac{a}{2} \end{cases}$$

(a) Determine $\langle T \rangle$.

(b) Determine $\langle V \rangle$.

(c) Find the value of a that will minimize $\langle H \rangle$.

Reminder: $\hat{T} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$.

This wave function is normalized: $\int_{-a/2}^{a/2} \frac{2}{a}\cos^2\left(\frac{\pi x}{a}\right) dx = 1$

a) $\frac{d^2}{dx^2}\psi = -\sqrt{\frac{2}{a}}\frac{\pi^2}{a^2}\cos\left(\frac{\pi x}{a}\right)$ so $\hat{T}\psi = \frac{\hbar^2\pi^2}{2ma^2}\psi$

$\langle T \rangle = \int \psi^* \left(\frac{\hbar^2\pi^2}{2ma^2}\psi\right) dx = \frac{\hbar^2\pi^2}{2ma^2}$

$$\boxed{\langle T \rangle = \frac{\hbar^2\pi^2}{2ma^2}}$$

b) $\langle V \rangle = \int \psi^* \, -\alpha\delta(x) \, \psi \, dx = -\alpha|\psi(0)|^2 = -\frac{2\alpha}{a}$

$$\boxed{\langle V \rangle = \frac{-2\alpha}{a}}$$

c) $\frac{d}{da}\left(\frac{\hbar^2\pi^2}{2ma^2} - \frac{2\alpha}{a}\right) = -\frac{\hbar^2\pi^2}{ma^3} + \frac{2\alpha}{a^2} = 0$

$\frac{\hbar^2\pi^2}{m} = 2\alpha a$

$$\boxed{a_{min} = \frac{\hbar^2\pi^2}{2m\alpha}}$$

Note: $\langle H \rangle_{min} = \frac{2m\alpha^2}{\hbar^2\pi^2} - \frac{4m\alpha^2}{\hbar^2\pi^2} = -\frac{2m\alpha^2}{\hbar^2\pi^2} \ge E_{g.s.}$

[15 points] Question #6: You are estimating the ground state energy of the Li^+ ion (two electrons orbiting a nucleus with three protons). You use the variational principle, modeling each electron's wave function as hydrogen-like where the effective nuclear charge β is the variational parameter. This gives an energy expectation value of

$$\langle H \rangle = (13.6 \text{ eV}) \left[2\beta^2 - 12\beta + \frac{5}{4}\beta \right].$$

What is your bound on the ground state energy?

$$\frac{d\langle H \rangle}{d\beta} = (13.6 \text{ eV})\left[4\beta - 12 + \tfrac{5}{4}\right] = 0$$

$$\beta = \frac{12 - 5/4}{4} = \frac{43}{16} = 2.6875$$

$$\langle H_{min} \rangle = (13.6 \text{ eV})\left[2(2.6875)^2 - 10.75(2.6875)\right]$$

$$\approx -14.44 \cdot (13.6 \text{ eV})$$

$$\boxed{\langle H \rangle_{min} \approx -196 \text{ eV} \geq E_{g.s.}}$$