Evaluate an upper bound for the ground state of the electron in a hydrogen atom, using the trial wave functions:

a)$\psi_\alpha(r) = e^{-\frac{r}{\alpha}}$

b)$\psi_\alpha(r) = e^{-\frac{r^2}{\alpha^2}}$

Treat $\alpha$ as the variational parameter. Interpret your results.
[1] [2]

1) for hydrogen (radial part):

$$\frac{\langle\tilde{0}|H|\tilde{0}\rangle}{\langle\tilde{0}|\tilde{0}\rangle} \geq E_0, \quad H\psi = -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{1}{\sin\Theta}\left(\frac{\partial}{\partial r}(r^2\frac{\partial\psi}{\partial r})\sin\Theta\right) - \frac{e^2}{4\pi\varepsilon_0 r}\psi$$

a)

$$\psi_\alpha(r) = e^{-\frac{r}{\alpha}}, \quad \frac{\partial\psi}{\partial r} = -\frac{1}{\alpha}e^{-\frac{r}{\alpha}}$$

$$\langle\tilde{0}|\tilde{0}\rangle = \int_0^\infty e^{-\frac{2r}{\alpha}}r^2\,dr\int_0^\pi \sin\Theta\,d\Theta\int_0^{2\pi}d\phi = 4\pi\frac{\alpha^3}{4}$$

$$-\frac{1}{\alpha}\frac{\partial}{\partial r}\left(r^2e^{-\frac{r}{\alpha}}\right) = -\frac{2r}{\alpha}e^{-\frac{r}{\alpha}} + \frac{r^2}{\alpha^2}e^{-\frac{r}{\alpha}}$$

$$H\psi_\alpha = -\frac{\hbar^2}{2m}\left(-\frac{2}{\alpha r}e^{-\frac{r}{\alpha}} + \frac{1}{\alpha^2}e^{-\frac{r}{\alpha}}\right) - \frac{e^2}{4\pi\varepsilon_0 r}e^{-\frac{r}{\alpha}}$$

$$\langle\tilde{0}|H|\tilde{0}\rangle = \int_0^\infty e^{-\frac{r}{\alpha}}\left[-\frac{\hbar^2}{2m}\left(-\frac{2}{\alpha r}e^{-\frac{r}{\alpha}} + \frac{1}{\alpha^2}e^{-\frac{r}{\alpha}}\right) - \frac{e^2}{4\pi\varepsilon_0 r}e^{-\frac{r}{\alpha}}\right]r^2\,dr\int_0^\pi \sin\Theta\,d\Theta\int_0^{2\pi}d\phi$$

$$\frac{\langle\tilde{0}|H|\tilde{0}\rangle}{\langle\tilde{0}|\tilde{0}\rangle} = \frac{\hbar^2}{2\alpha^2 m} - \frac{e^2}{4\pi\varepsilon_0\alpha} = \langle H\rangle_\alpha$$

$$\frac{\partial\langle H\rangle_\alpha}{\partial\alpha} = -\frac{\hbar^2}{\alpha^3 m} + \frac{e^2}{4\pi\varepsilon_0\alpha^2} = 0$$

$$\alpha = \frac{4\pi\varepsilon_0\hbar^2}{e^2 m} \quad \text{which yields} \quad E_0 = -\frac{e^4 m}{32\varepsilon_0^2\hbar^2\pi^2}$$

b)

$$\psi_\alpha(r) = e^{-\frac{r^2}{\alpha^2}}, \quad \frac{\partial\psi}{\partial r} = -\frac{2r}{\alpha^2}e^{-\frac{r^2}{\alpha^2}}$$

$$\langle\tilde{0}|\tilde{0}\rangle = 4\pi\int_0^\infty e^{-\frac{2r^2}{\alpha^2}}r^2\,dr = 4\pi\frac{\alpha^3}{8}\sqrt{\frac{\pi}{2}}$$

$$-\frac{2}{\alpha^2}\frac{\partial}{\partial r}\left(r^3e^{-\frac{r^2}{\alpha^2}}\right) = -\frac{2}{\alpha^2}\left(3r^2e^{-\frac{r^2}{\alpha^2}} - 2r^4\frac{1}{\alpha^2}e^{-\frac{r^2}{\alpha^2}}\right)$$

Similiary to part a):

$$H\psi_\alpha = \frac{\hbar^2}{\alpha^2 m}3e^{-\frac{r^2}{\alpha^2}} - \frac{\hbar^2}{\alpha^2 m}2r^2\frac{1}{\alpha^2}e^{-\frac{r^2}{\alpha^2}} - \frac{e^2}{4r\pi\varepsilon_0}e^{-\frac{r^2}{\alpha^2}}$$

$$\frac{\langle\tilde{0}|H|\tilde{0}\rangle}{\langle\tilde{0}|\tilde{0}\rangle} = \frac{3\hbar^2}{2m\alpha^2} - \frac{e^2}{\sqrt{2\pi}\varepsilon_0\pi\alpha} = \langle H\rangle_\alpha$$

$$\frac{\partial\langle H\rangle_\alpha}{\partial\alpha} = -\frac{3\hbar^2}{\alpha^3 m} + \frac{e^2}{\sqrt{2\pi}\pi\alpha^2\varepsilon_0} = 0$$

$$\alpha = \frac{3\sqrt{2}\varepsilon_0\hbar^2\pi^{\frac{3}{2}}}{e^2 m} \quad \text{and} \quad E_0 = -\frac{e^4 m}{12\varepsilon_0^2\hbar^2\pi^3} \qquad \left[\frac{c^4kgm^2}{F^2J^2S^2} = \frac{c^4kgm^2J^2}{c^4J^2S^2} = 1\right]$$

[1] In this work candidacy formula worksheet was used.

[2] Almost all calculations were omitted as trivial. Only final results were given.

Both values of $E_0$ have same dimension and just differ by factor $\frac{8}{3\pi} \approx 0.85$

Real wavefunctions of the hydrogen ground state are $\sim e^{-\frac{r}{\alpha}}$, so 1 a) gives more exact value. It also has lower bound. Although 1 b) gives quite good value of $E_0$ which proves the power of variational method.

2) a) Use the trial wave function $\psi_\alpha(r) = e^{-\frac{r^2}{\alpha^2}}$ to obtain an upper bound for the ground- state energy for the one-dimensional Schr dinger equation with linear potential $V(x) = C|x|$, where $C > 0$.

b) Compare your solution with the exact solution and the WKB solution discussed in Sec. 2.5 of Sakurai's book. (Note that the main focus of the discussion on the WKB solution is on the odd-parity solutions of this problem.)

$$\psi_\alpha(x) = e^{-\frac{x^2}{\alpha^2}}, \quad V(x) = C|x|, \quad C > 0; \quad V(x) = \begin{cases} Cx, & \text{x>0} \\ -Cx, & \text{x<0} \end{cases}$$

$$\langle\tilde{0}|H|\tilde{0}\rangle = \int\limits_{-\infty}^{\infty} e^{-\frac{x^2}{\alpha^2}} \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + C|x|\right) e^{-\frac{x^2}{\alpha^2}}\, dx$$

$$\langle\tilde{0}|H|\tilde{0}\rangle = -\frac{\hbar^2}{2m}\frac{1}{\alpha}\sqrt{\frac{\pi}{2}} + \frac{\sqrt{2\pi}\hbar\sqrt[3]{2}}{\sqrt{2}2m\alpha} + \frac{C\alpha^2}{2}, \quad \langle\tilde{0}|\tilde{0}\rangle = \alpha\sqrt{\frac{\pi}{2}}$$

$$\frac{\langle\tilde{0}|H|\tilde{0}\rangle}{\langle\tilde{0}|\tilde{0}\rangle} = \frac{\hbar^2}{2m\alpha^2} + \frac{\alpha C}{\sqrt{2\pi}} = \langle H\rangle_\alpha; \quad \frac{\partial\langle H\rangle_\alpha}{\partial\alpha} = -\frac{\hbar^2}{\alpha^3 m} + \frac{C}{\sqrt{2\pi}} = 0$$

$$\alpha = \sqrt[3]{\frac{\hbar^2\sqrt{2\pi}}{mC}}; \quad E_0 = \frac{\hbar^{\frac{2}{3}}c^{\frac{2}{3}}}{m^{\frac{1}{3}}}\frac{3}{2^{\frac{4}{3}}\pi^{\frac{1}{3}}} \quad \text{the dimension is 1 (energy)} \Rightarrow \approx 0.813\frac{\hbar^{\frac{2}{3}}c^{\frac{2}{3}}}{m^{\frac{1}{3}}}$$

The exact solution (from Sakurai):

$$E_0 \approx 0.809\frac{\hbar^{\frac{2}{3}}c^{\frac{2}{3}}}{m^{\frac{1}{3}}}$$

$\approx 1\%$ difference, which means our initial guess was very good. Also $E_{variational} > E_{exact}$, which is physically true.

WKB solution (from Sakurai): In WKB approximation ground state will be the first exited state in the full line problem.

In the book

$$E_n = \left(\frac{(3(n-\frac{1}{n})\pi)^{\frac{2}{3}}}{2}\right)\left(mg^2\hbar^2\right)^{\frac{1}{3}}$$

$$\text{for} \quad n = 0 \quad E_0 = 0.885\left(mg^2\hbar^2\right)^{\frac{1}{3}}$$

$$\text{for} \quad n = 1 \quad E_1 = 1.842\left(mg^2\hbar^2\right)^{\frac{1}{3}}$$