$\boxed{\text{Problem 31.2}}$ We use the normalized Gaussian orbitals

$$\langle \vec{r} \,|\, n\ell m \rangle = N_{n\ell m}\, r^{n-1} e^{-\alpha r^2} Y_\ell^m(\Omega) = \psi_{n\ell m}(r,\Omega) \text{ . So}$$

$$\psi_{100}(r,\Omega) = N_{100}\, e^{-\alpha r^2} Y_0^0 = \frac{N_{100}}{\sqrt{4\pi}} e^{-\alpha r^2}$$

$$\psi_{200}(r,\Omega) = N_{200}\, r e^{-\alpha r^2} Y_0^0 = \frac{N_{200}}{\sqrt{4\pi}} r e^{-\alpha r^2}$$

As in Prob. 31.1,

$$\langle 100 | 100 \rangle = 1 \quad \Rightarrow \quad \boxed{|N_{100}|^2 = 8\alpha \sqrt{\frac{2\alpha}{\pi}}}$$

$$\langle 200 | 200 \rangle = 1$$

$$\Rightarrow \frac{|N_{200}|^2}{4\pi} \int d\Omega \int_0^\infty dr\, r^2\, r^2 e^{-2\alpha r^2} = |N_{200}|^2 \int_0^\infty dr\, r^4 e^{-2\alpha r^2}$$

using the Gaussian integral formulas given in the last prob.

$$= |N_{200}|^2 \cdot \frac{3}{32\alpha^2} \sqrt{\frac{\pi}{2\alpha}} = 1$$

$$\Rightarrow \boxed{|N_{200}|^2 = \frac{32\alpha^2}{3} \sqrt{\frac{2\alpha}{\pi}}}$$

For the variation parameter α, we will use the value

$$\boxed{\alpha = \frac{8}{9\pi} \frac{Z^2 e^4 m^2}{\hbar^4}}$$

(for a hydrogen-like atom with a single orbiting electron and nuclear charge Ze)

(as obtained from the last problem), which minimizes $\langle 100 | H | 100 \rangle$.

Now do configuration interaction (CI) expansion to get a state wave function of the form

$$\psi_0(\vec{r}) = C_1 \psi_{100}(\vec{r}) + C_2 \psi_{200}(\vec{r})$$

which will give an improved estimate of the ground state energy eigenvalue calculated by

$$\langle \psi_0 | H | \psi_0 \rangle$$

$\boxed{\text{P31.2}}$ cont'd

We would be tempted to choose $\psi_{100}(\vec{r})$ and $\psi_{200}(\vec{r})$ as basis states and set up the Hamiltonian matrix

$$H' = \begin{pmatrix} \langle 100|H|100\rangle & \langle 100|H|200\rangle \\ \langle 200|H|100\rangle & \langle 200|H|200\rangle \end{pmatrix},$$

and then diagonalize H' to obtain an improved ground state energy eigenvalue. However, since the states $|100\rangle$ and $|200\rangle$ (with Gaussian orbitals) are not orthogonal to each other, it would be better to use Schmidt orthogonalization to ~~form~~ obtain two states

$$|1\rangle \equiv |100\rangle \quad \text{and} \quad |2'\rangle \equiv \overset{\text{some constant}}{C}\{|200\rangle - \langle 100|200\rangle|100\rangle\}$$

$$\equiv C\{|2\rangle - \langle 1|2\rangle|1\rangle\}$$

where we have denoted $|2\rangle \equiv |200\rangle$

such that $|1\rangle$ and $|2'\rangle$ are orthogonal to each other.

Indeed, $\langle 1|2'\rangle = C\{\langle 1|2\rangle - \langle 1|2\rangle\underbrace{\langle 1|1\rangle}_{1}\} = 0$

Requiring $|2'\rangle$ to be normalized also, we have

$$\langle 2'|2'\rangle = 1 = |C|^2\left(\langle 2| - \langle 2|1\rangle\langle 1|\right)\left(|2\rangle - \langle 1|2\rangle|1\rangle\right)$$

$$= |C|^2\left\{\underbrace{\langle 2|2\rangle}_{1} - \langle 2|1\rangle\langle 1|2\rangle - \langle 2|1\rangle\langle 1|2\rangle + \langle 2|1\rangle\langle 1|2\rangle\cdot\underbrace{\langle 1|1\rangle}_{1}\right\}$$

$$= |C|^2\{1 - |\langle 1|2\rangle|^2\}$$

Choosing C to be real, we have

$$C = \frac{1}{1 - \langle 1|2\rangle|^2}$$

$\boxed{P31.2}$ cont'd Thus

$$|2'\rangle = \frac{|200\rangle - |100\rangle\langle 100|200\rangle}{\sqrt{1 - |\langle 100|200\rangle|^2}}$$

We show that $|100\rangle$ and $|200\rangle$ are not orthogonal as follows:

$$\langle 100|200\rangle = N_{100}^{*} N_{200} \int_0^\infty dr\, r^2\, r e^{-2\alpha r^2} = \frac{N_{100}^{*} N_{200}}{8\alpha^2} \neq 0$$

$|1\rangle$ and $|2'\rangle$ now form an improved set of basis states and we will diagonalize the Hamiltonian matrix

$$H = \begin{pmatrix} \langle 1|H|1\rangle & \langle 1|H|2'\rangle \\ \langle 2'|H|1\rangle & \langle 2'|H|2'\rangle \end{pmatrix}$$

to obtain an improved ground state energy. We will next calculate the above matrix elements. Since all states involve only $l=0$, ~~we~~ the Hamiltonian operator is given by

$$H = \frac{-\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{Ze^2}{r}.$$

It has already been shown in the last problem that

$$\boxed{\langle 1|H|1\rangle = \frac{-4mZ^2e^4}{3\pi\hbar^2}},$$

and from the above

$$\langle 100|200\rangle = \frac{N_{200}^{*} N_{100}}{8\alpha^2} = \frac{N_{200}N_{100}}{8\alpha^2} = \sqrt{\frac{32}{3}}\cdot\alpha\left(\frac{2\alpha}{\pi}\right)^{1/4}\cdot\sqrt{8\alpha}\left(\frac{2\alpha}{\pi}\right)^{1/4}\cdot\frac{1}{8\alpha^2} = \sqrt{\frac{8}{3\pi}}$$

$\boxed{\text{P.31.2}}$ cont'd . So

$$|2'\rangle = \frac{|200\rangle - \sqrt{8/3\pi}\,|100\rangle}{\sqrt{1 - 8/3\pi}} \quad \text{, and}$$

$$\langle 1|H|2'\rangle = \langle 2'|H|1\rangle^* \quad \text{since } H \text{ is hermitian.}$$

$$\langle 1|H|2'\rangle = \frac{1}{\sqrt{1-\frac{8}{3\pi}}}\left[\overset{\langle 100|H|200\rangle}{\cancel{\langle 100|200\rangle}} - \sqrt{\frac{8}{3\pi}}\langle 100|H|100\rangle\right]$$

We have already found $\langle 100|H|100\rangle = \langle 1|H|1\rangle = -\dfrac{4mZ^2e^4}{3\pi\hbar^2}$

$$\langle 100|H|200\rangle = \overbrace{8\alpha^2\sqrt{\frac{8}{3\pi}}}^{N_{100}N_{200}}\int_0^\infty dr\, r^2 e^{-\alpha r^2}\left\{\frac{-\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{Ze^2}{r}\right\} r e^{-\alpha r^2}$$

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

So

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

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

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

$$= 2re^{-\alpha r^2}\left[-2\alpha r^2 + \left(1-2\alpha r^2\right)\left(1-\alpha r^2\right)\right]$$

$$= 2re^{-\alpha r^2}\left[-2\alpha r^2 + 1 - 2\alpha r^2 - \alpha r^2 + 2\alpha^2 r^4\right]$$

$$= 2re^{-\alpha r^2}\left[1 - 5\alpha r^2 + 2\alpha^2 r^4\right]$$

$$\therefore \langle 100|H|200\rangle = 8\alpha^2\sqrt{\frac{8}{3\pi}}\left[\int_0^\infty dr\left(\frac{-\hbar^2}{m}\right) r e^{-2\alpha r^2}\left(1 - 5\alpha r^2 + 2\alpha^2 r^4\right) - Ze^2\int_0^\infty dr\, r^2 e^{-2\alpha r^2}\right],$$

P31.2 cont'd

$$\langle 100|H|200\rangle = 8\alpha^2\sqrt{\frac{8}{3\pi}}\left[-\frac{\hbar^2}{m}\left\{\int_0^\infty dr.\, r\, e^{-2\alpha r^2} - 5\alpha\int_0^\infty dr.\, r^3 e^{-2\alpha r^2} + 2\alpha^2\int_0^\infty dr\, r^5 e^{-2\alpha r^2}\right\} - Ze^2\int_0^\infty dr.\, r^2 e^{-2\alpha r^2}\right]$$

using the Gaussian integrals formulas again

$$= 8\alpha^2\sqrt{\frac{8}{3\pi}}\left[-\frac{\hbar^2}{m}\left\{\frac{1}{4\alpha} - 5\alpha\cdot\frac{1}{8\alpha^2} + 2\alpha^2\cdot\frac{1}{8\alpha^3}\right\} - Ze^2\cdot\frac{1}{8\alpha}\sqrt{\frac{\pi}{2\alpha}}\right]$$

$$= 8\alpha^2\sqrt{\frac{8}{3\pi}}\left[-\frac{\hbar^2}{m}\left\{\frac{1}{4\alpha} - \frac{5}{8\alpha} + \frac{1}{4\alpha}\right\} - \frac{Ze^2}{8\alpha}\sqrt{\frac{\pi}{2\alpha}}\right]$$

$$= 8\alpha^2\sqrt{\frac{8}{3\pi}}\left[-\frac{\hbar^2}{m}\left(-\frac{1}{8\alpha}\right) - \left(\frac{1}{8\alpha}\right)Ze^2\sqrt{\frac{\pi}{2\alpha}}\right]$$

$$= \alpha\sqrt{\frac{8}{3\pi}}\left[\frac{\hbar^2}{m} - Ze^2\sqrt{\frac{\pi}{2\alpha}}\right]$$

use previous result $\alpha = \dfrac{8Z^2e^4m^2}{9\pi\hbar^4}$

Then

$$\langle 100|H|200\rangle = \left(\frac{8Z^2e^4m^2}{9\pi\hbar^4}\right)\sqrt{\frac{8}{3\pi}}\left[\frac{\hbar^2}{m} - Ze^2\left(\frac{3\pi\hbar^2}{4Ze^2m}\right)\right]$$

$$= \left(\frac{8Z^2e^4m^2}{9\pi\hbar^4}\right)\sqrt{\frac{8}{3\pi}}\left[\frac{\hbar^2}{m} - \left(\frac{3\pi}{4}\right)\frac{\hbar^2}{m}\right]$$

$$= \left(\frac{8Z^2e^4m}{9\pi\hbar^2}\right)\sqrt{\frac{8}{3\pi}}\left(1 - \frac{3\pi}{4}\right) = \langle 200|H|100\rangle$$ (Since H is hermitian and the matrix element is real)

$\therefore$ $\langle 1|H|2'\rangle$ is real and

$$\langle 1|H|2'\rangle = \langle 2'|H|1\rangle \quad ;$$

and from the above result for $\langle 1|H|2'\rangle$, we have and $\langle 100|H|100\rangle$

$\boxed{\text{P31.2}}$ cont'd

$$\langle 1|H|2'\rangle = \frac{1}{\sqrt{1-\frac{8}{3\pi}}}\left[\langle 100|H|200\rangle - \sqrt{\frac{8}{3\pi}}\langle 100|H|100\rangle\right]$$

$$= \frac{1}{\sqrt{1-8/3\pi}}\left\{\left(\frac{8Z^2e^4m}{9\pi\hbar^2}\right)\sqrt{\frac{8}{3\pi}}\left(1-\frac{3\pi}{4}\right)+\sqrt{\frac{8}{3\pi}}\left(\frac{4mZ^2e^4}{3\pi\hbar^2}\right)\right\}$$

$$= \left(\frac{1}{\sqrt{1-8/3\pi}}\right)\left(\frac{4Z^2e^4m}{3\pi\hbar^2}\right)\sqrt{\frac{8}{3\pi}}\left[\frac{2}{3}\left(1-\frac{3\pi}{4}\right)+1\right]$$

$$= \frac{4}{3}\left(\frac{Z^2e^4m}{\pi\hbar^2}\right)\sqrt{\frac{8/3\pi}{1-8/3\pi}}\left(\frac{2}{3}-\frac{\pi}{2}+1\right)$$

$$= \frac{4}{3}\left(\frac{Z^2e^4m}{\pi\hbar^2}\right)\sqrt{\frac{1}{\left(\frac{3\pi}{8}-1\right)}}\left(\frac{5}{3}-\frac{\pi}{2}\right) = 0.3029\left(\frac{Z^2e^4m}{\pi\hbar^2}\right)$$

$$= \langle 2'|H|1\rangle$$

Now calculate $\langle 2'|H|2'\rangle$

$$\langle 2'|H|2'\rangle = \frac{1}{(1-8/3\pi)}\left[\left(\langle 200| - \sqrt{\frac{8}{3\pi}}\langle 100|\right)H\left(|200\rangle - \sqrt{\frac{8}{3\pi}}|100\rangle\right)\right]$$

$$= \frac{1}{(1-8/3\pi)}\left[\langle 200|H|200\rangle - 2\sqrt{\frac{8}{3\pi}}\underbrace{\langle 100|H|200\rangle}_{\text{calculated already}} + \frac{8}{3\pi}\underbrace{\langle 100|H|100\rangle}_{\text{calculated already}}\right]$$

$$\langle 200|H|200\rangle = N_{200}^2\int_0^\infty dr\, r^2 re^{-\alpha r^2}\underbrace{\left\{\frac{-\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)-\frac{Ze^2}{r}\right\}\left(re^{-\alpha r^2}\right)}_{\parallel \text{ (from above) } -\frac{\hbar^2}{mr}e^{-\alpha r^2}(1-5\alpha r^2+2\alpha^2r^4)-Ze^2e^{-\alpha r^2}}$$

using result for N_{200}^2 above

$$= \frac{32\alpha^2}{3}\sqrt{\frac{2\alpha}{\pi}}\left[\frac{-\hbar^2}{m}\int_0^\infty dr\, r^2e^{-2\alpha r^2}\left(1-5\alpha r^2+2\alpha^2r^4\right)-Ze^2\int_0^\infty dr\, r^3e^{-2\alpha r^2}\right]$$

$\boxed{P31.2}$ cont'd

$$\langle 200|H|200\rangle = \left(\frac{32\alpha^2}{3}\right)\sqrt{\frac{2\alpha}{\pi}}\left[-\frac{\hbar^2}{m}\left\{\int_0^\infty dr\, r^2 e^{-2\alpha r^2} - 5\alpha\int_0^\infty dr\, r^4 e^{-2\alpha r^2} + 2\alpha^2\int_0^\infty dr\, r^6 e^{-2\alpha r^2}\right\} - Ze^2\int_0^\infty dr\, r^3 e^{-2\alpha r^2}\right]$$

$$= \left(\frac{32\alpha^2}{3}\right)\sqrt{\frac{2\alpha}{\pi}}\left[-\frac{\hbar^2}{m}\left(\frac{1}{8\alpha}\sqrt{\frac{\pi}{2\alpha}} - \frac{5\alpha.3}{32\alpha^2}\sqrt{\frac{\pi}{2\alpha}} + \frac{2\alpha^2.15}{128\alpha^3}\sqrt{\frac{\pi}{2\alpha}}\right) - \frac{Ze^2}{8\alpha^2}\right]$$

$$= \left(\frac{32\alpha^2}{3}\right)\sqrt{\frac{2\alpha}{\pi}}\left[\frac{-\hbar^2}{m}\cdot\frac{1}{8\alpha}\sqrt{\frac{\pi}{2\alpha}}\left(1 - \frac{15}{4} + \frac{15}{8}\right) - \frac{Ze^2}{8\alpha^2}\right]$$

$$= \left(\frac{32\alpha^2}{3}\right)\sqrt{\frac{2\alpha}{\pi}}\left[\frac{\hbar^2}{m}\cdot\frac{7}{64\alpha}\sqrt{\frac{\pi}{2\alpha}} - \frac{Ze^2}{8\alpha^2}\right] = \left(\frac{32\alpha^2}{3}\right)\sqrt{\frac{2\alpha}{\pi}}\left(\frac{1}{8\alpha}\right)\left[\frac{\hbar^2}{m}\cdot\frac{7}{8}\sqrt{\frac{\pi}{2\alpha}} - \frac{Ze^2}{\alpha}\right]$$

$$= \left(\frac{4\alpha}{3}\right)\sqrt{\frac{2\alpha}{\pi}}\left[\frac{\hbar^2}{m}\left(\frac{7}{8}\right)\sqrt{\frac{\pi}{2\alpha}} - \frac{Ze^2}{\alpha}\right] \qquad \left(\text{use } \alpha = \frac{8}{9\pi}\frac{Z^2e^4m^2}{\hbar^4} \text{ from above}\right)$$

$$= \frac{4}{3}\cdot\frac{8}{9\pi}\frac{Z^2e^4m^2}{\hbar^4}\sqrt{\frac{2}{\pi}}\cdot\frac{\sqrt{8}}{3\sqrt{\pi}}\frac{Ze^2m}{\hbar^2}\left[\left(\frac{7}{8}\right)\frac{\hbar^2}{m}\sqrt{\frac{\pi}{2}}\,\frac{3\sqrt{\pi}}{\sqrt{8}}\cdot\frac{\hbar^2}{Ze^2m} - \frac{Ze^2(9\pi)}{8}\cdot\frac{\hbar^4}{Z^2e^4m^2}\right]$$

$$= \frac{4.8}{3.9}\frac{\sqrt{2.8}}{3}\frac{1}{\pi^2}\left(\frac{Z^2e^4m^2}{\hbar^2}\right)\left(\frac{Ze^2m}{\hbar^2}\right)\underbrace{\left[\left(\frac{7}{8}\right)\frac{(3\pi)}{\sqrt{2.8}}\frac{\hbar^4}{Ze^2m^2} - \frac{9\pi}{8}\cdot\frac{\hbar^4}{Ze^2m^2}\right]}_{-\frac{15\pi}{32}\frac{\hbar^4}{Ze^2m^2}}$$

$$= \left(\frac{32}{27}\right)\left(\frac{4}{3}\right)\left(\frac{1}{\pi^2}\right)\left(\frac{Z^2e^4m}{\hbar^2}\right)\left(\frac{Ze^2m^2}{\hbar^4}\right)\left(-\frac{15\pi}{32}\cdot\frac{\hbar^4}{Ze^2m^2}\right)$$

$$= -\frac{20}{27}\cdot\frac{Z^2e^4m}{\pi\hbar^2}.$$

$$\langle 200|H|200\rangle = -\frac{20}{27}\cdot\frac{Z^2e^4m}{\pi\hbar^2}$$

$\boxed{P31.2}$ cont'd. So,

$$\langle 2'|H|2'\rangle = \left(\frac{1}{1-8/3\pi}\right)\left(\frac{Z^2e^4m}{\pi\hbar^2}\right)$$

$$\times\left\{-\frac{20}{27} - 2\sqrt{\frac{8}{3\pi}}\cdot\frac{8}{9}\sqrt{\frac{8}{3\pi}}\left(1-\frac{3\pi}{4}\right) + \frac{8}{3\pi}\left(-\frac{4}{3}\right)\right\}$$

$$= \left(\frac{Z^2e^4m}{\pi\hbar^2}\right)\left(\frac{1}{1-8/3\pi}\right)\left\{-\frac{20}{27} - \frac{128}{27\pi} + \frac{32}{9} - \frac{32}{9\pi}\right\}$$

$$= \left(\frac{Z^2e^4m}{\pi\hbar^2}\right)\left(\frac{1}{1-8/3\pi}\right)\left(\frac{76}{27} - \frac{224}{27\pi}\right) = \frac{Z^2e^4m}{\pi\hbar^2}\left(\frac{4}{27}\right)\frac{\left(19-\frac{56}{\pi}\right)}{\left(1-\frac{8}{3\pi}\right)}$$

$$= 1.1511\left(\frac{Z^2e^4m}{\pi\hbar^2}\right)$$

Collecting results for the required matrix elements we have

$$\boxed{\begin{aligned}
\langle 1|H|1\rangle &= -\frac{4}{3}\left(\frac{Z^2e^4m}{\pi\hbar^2}\right) = -1.3333\left(\frac{Z^2e^4m}{\pi\hbar^2}\right) \\
\langle 1|H|2'\rangle = \langle 2'|H|1\rangle &= \frac{4}{3}\left(\frac{5}{3}-\frac{\pi}{2}\right)\frac{1}{\sqrt{\frac{3\pi}{8}-1}}\cdot\left(\frac{Z^2e^4m}{\pi\hbar^2}\right) = 0.3029\left(\frac{Z^2e^4m}{\pi\hbar^2}\right) \\
\langle 2'|H|2'\rangle &= \left(\frac{4}{27}\right)\left(\frac{19-\frac{56}{\pi}}{1-\frac{8}{3\pi}}\right)\left(\frac{Z^2e^4m}{\pi\hbar^2}\right) = 1.1511\left(\frac{Z^2e^4m}{\pi\hbar^2}\right)
\end{aligned}}$$

$$\therefore\ H = \mathcal{E}_0\begin{pmatrix} \underset{a}{-1.3333} & \underset{b}{0.3029} \\ \underset{b}{0.3029} & \underset{c}{1.1511} \end{pmatrix}, \quad \text{where } \mathcal{E}_0 = \frac{Z^2e^4m}{\pi\hbar^2}$$

$\boxed{P31.2}$ cont'd

We ~~hav~~ want to diagonalize

$$\frac{1}{\mathcal{E}_0} \cdot H = \begin{pmatrix} a & b \\ b & c \end{pmatrix}$$

set $\begin{vmatrix} a-\mathcal{E} & b \\ b & c-\mathcal{E} \end{vmatrix} = 0$

that is, $(a-\mathcal{E})(c-\mathcal{E}) - b^2 = 0$

$$\mathcal{E}^2 - \mathcal{E}(a+c) - (b^2 - ac) = 0$$

$$\mathcal{E}_\pm = \left(\frac{a+c}{2}\right) \pm \frac{1}{2}\sqrt{(a+c)^2 + 4(b^2 - ac)}$$

$$= \left(\frac{a+c}{2}\right) \pm \frac{1}{2}\sqrt{(a-c)^2 + 4b^2}$$

$$= \frac{(1.1511 - 1.3333)}{2} \pm \frac{1}{2}\sqrt{(-1.3333 - 1.1511)^2 + 4(0.3029)^2}$$

$$= -0.0911 \pm 1.2786 = \begin{cases} 1.1875 \\ -1.3697 \end{cases}$$

We discard the positive root since we know that bound state energies must be negative.

$\therefore$ The improved ground state energy for a hydrogen-like atom is given by

$$\boxed{\mathcal{E}_{100} = -1.3697 \frac{Z^2 e^4 m}{\pi \hbar^2}}$$

P31.2 cont'd

or,

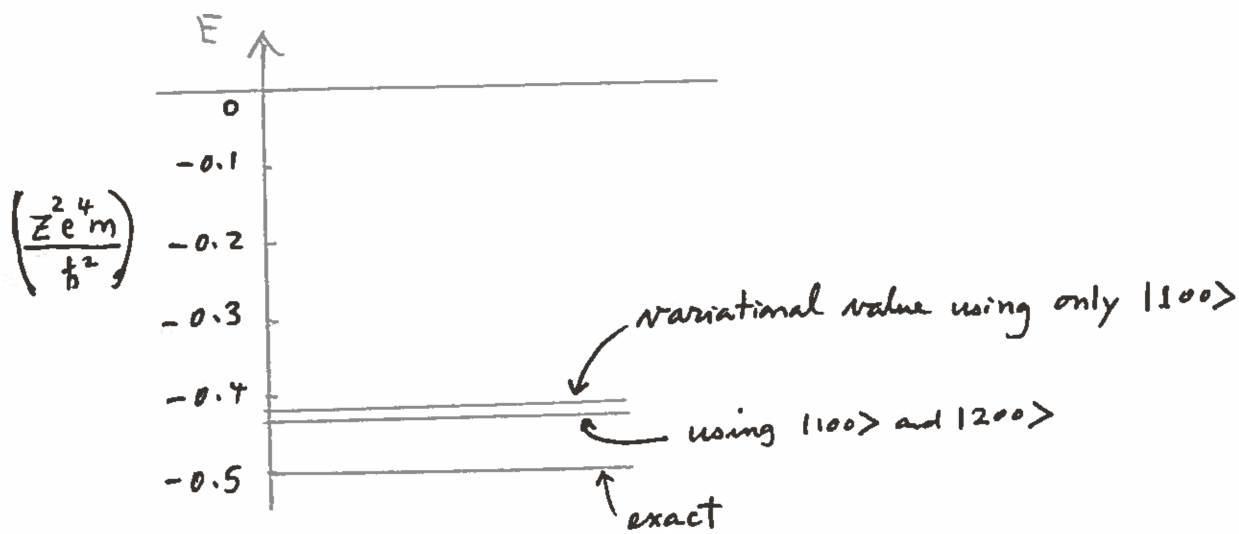
$$\boxed{\mathcal{E}_{100} = -0.4360 \frac{Z^2 e^4 m}{\hbar^2}}$$

From P.31.1 (the last problem), using just the $|100\rangle$ state

$$E_{100}^{variational} = -0.4244 \frac{Z^2 e^4 m}{\hbar^2}$$

while the exact energy is

$$E_{100} = -0.5 \frac{Z^2 e^4 m}{\hbar^2}$$



error of $E_{100}^{variational}$ = 15.12%

error of $\mathcal{E}_{100}$ (using CI) = 12.8%

Seems like a lot of work for relatively little improvement, but that's life!