Dana jest funkcja postaci $\Phi = Ne^{-\alpha r^2}$, gdzie r – odległość, $N \in \mathbb{R}$ – stała normalizacyjna, $\alpha \in \mathbb{R}$ – parametr wariacyjny. Znajdźmy optymalną wartość α oraz przybliżenie do energii stanu podstawowego atomu wodoru (z nieruchomym jądrem). Element objętości w układzie sferycznym: $dV = r^2 \sin(\theta) dr d\theta d\phi$.

Laplasjan: $\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin(\theta)}\frac{\partial}{\partial \theta}\left(\sin(\theta)\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2 \sin^2(\theta)}\frac{\partial^2}{\partial \phi^2}$

$\int_0^\infty dx \;\; x \;\; exp\left[-x^2\right] = 1/2$

$\int_0^\infty dx \;\; x^2 \;\; exp\left[-x^2\right] = \sqrt{\pi}/4$

$\int_0^\infty dx \;\; x^4 \;\; exp\left[-x^2\right] = 3\sqrt{\pi}/8$

$$\varepsilon = \frac{\langle\Phi|\hat{H}|\Phi\rangle}{\langle\Phi|\Phi\rangle}, \qquad \hat{H} = \hat{T} + \hat{V} = -\frac{\Delta}{2} - \frac{1}{r}$$

$$\langle\Phi|\Phi\rangle = \int_V d^3 r N^2 exp\left[-2\alpha r^2\right] = \int_0^\pi d\theta \sin(\theta) \int_0^{2\pi} d\phi \int_0^\infty dr \;\; r^2 N^2 exp\left[-2\alpha r^2\right] =$$
$$= 4N^2\pi \int_0^\infty dr \;\; r^2 exp\left[-2\alpha r^2\right]$$

Po podstawieniu $x = \sqrt{2\alpha} r$, $dx = \sqrt{2\alpha} dr$:

$$\langle\Phi|\Phi\rangle = 4N^2\pi \int_0^\infty dx \, (2\alpha)^{-3/2} \, x^2 exp\left[-x^2\right] =$$
$$= N^2 \left(\frac{\pi}{2\alpha}\right)^{3/2}$$

Jakkolwiek nie jest to potrzebne do rozwiązania zadania, możemy łatwo wyznaczyć stałą normalizacyjną:

$$\langle\Phi|\Phi\rangle = 1 \qquad \Rightarrow \qquad N = \pm\left(\frac{2\alpha}{\pi}\right)^{3/4}$$

Pozostałe całki:

$$\langle\Phi|\hat{V}|\Phi\rangle = -4N^2\pi\int_0^\infty dr\ \ r\ \ exp\left[-2\alpha r^2\right] =$$

$$= -4N^2\pi\int_0^\infty dx\ \ \frac{1}{2\alpha}x\ \ exp\left[-x^2\right] = -\frac{N^2\pi}{\alpha}$$

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\Phi\right) = Nexp\left[-\alpha r^2\right]\left(4\alpha^2 r^4 - 6\alpha r^2\right)$$

$$\langle\Phi|\hat{T}|\Phi\rangle = -\,2N^2\pi\int_0^\infty dr\ \ exp\left[-2\alpha r^2\right]\left(4\alpha^2 r^4 - 6\alpha r^2\right) =$$

$$= -\,(2\alpha)^{-5/2}\,8N^2\pi\alpha^2\int_0^\infty dx\ \ x^4\ \ exp\left[-x^2\right] +$$

$$+\,(2\alpha)^{-3/2}\,12N^2\pi\alpha\int_0^\infty dx\ \ x^2\ \ exp\left[-x^2\right] =$$

$$= -\,\frac{3(\pi)^{3/2}N^2}{2^{5/2}\sqrt{\alpha}} + \frac{3(\pi)^{3/2}N^2}{2^{3/2}\sqrt{\alpha}} = \frac{3(\pi)^{3/2}N^2}{2^{5/2}\sqrt{\alpha}}$$

$$\frac{\langle\Phi|\hat{T}|\Phi\rangle}{\langle\Phi|\Phi\rangle} = \frac{3}{2}\alpha, \qquad \frac{\langle\Phi|\hat{V}|\Phi\rangle}{\langle\Phi|\Phi\rangle} = -\frac{2^{3/2}\sqrt{\alpha}}{\sqrt{\pi}}, \qquad \varepsilon(a) = \frac{3}{2}\alpha - \frac{2^{3/2}\sqrt{\alpha}}{\sqrt{\pi}}$$

Pozostaje wyznaczyć minimum:

$$\frac{\partial\varepsilon}{\partial a} = 0 = \frac{3}{2} - \frac{\sqrt{2}}{\sqrt{\alpha}\sqrt{\pi}}$$

$$\sqrt{\alpha} = \frac{\sqrt{8}}{3\sqrt{\pi}}$$

$$\alpha_{min} = \frac{8}{9\pi} \approx 0.282942$$

$$\varepsilon_{min} = \frac{4}{3\pi} - \frac{8}{3\pi} = -\frac{4}{3\pi} \approx -0.424413 \ \ [a.u]$$