Problem 8 - Variational Theorem for Hydrogen's GS

In[19]:= $u_1[\rho\_, b\_] := \rho\, e^{-b \rho}$

$u_2[\rho\_, b\_] := \dfrac{\rho}{b^2 + \rho^2}$

$u_3[\rho\_, b\_] := \rho^2\, e^{-b \rho}$

In[23]:= $\text{Energy}_1[b\_] = \text{Integrate}\left[u_1[\rho, b]\left(-\partial_{\{\rho,2\}} u_1[\rho, b] - \dfrac{2\, u_1[\rho, b]}{\rho}\right), \{\rho, 0, \infty\}, \text{Assumptions} \to b > 0 \,\&\&\, b \in \mathbb{R}\right] \Big/ \text{Integrate}[u_1[\rho, b]\, u_1[\rho, b], \{\rho, 0, \infty\}, \text{Assumptions} \to b > 0 \,\&\&\, b \in \mathbb{R}]$

Out[23]= $(-2 + b)\, b$

In[24]:= $\text{Energy}_2[b\_] = \text{Integrate}\left[u_2[\rho, b]\left(-\partial_{\{\rho,2\}} u_2[\rho, b] - \dfrac{2\, u_2[\rho, b]}{\rho}\right), \{\rho, 0, \infty\}, \text{Assumptions} \to b > 0 \,\&\&\, b \in \mathbb{R}\right] \Big/ \text{Integrate}[u_2[\rho, b]\, u_2[\rho, b], \{\rho, 0, \infty\}, \text{Assumptions} \to b > 0 \,\&\&\, b \in \mathbb{R}]$

Out[24]= $\dfrac{-8\, b + \pi}{2\, b^2\, \pi}$

In[26]:= $\text{Energy}_3[b\_] = \text{Integrate}\left[u_3[\rho, b]\left(-\partial_{\{\rho,2\}} u_3[\rho, b] - \dfrac{2\, u_3[\rho, b]}{\rho}\right), \{\rho, 0, \infty\}, \text{Assumptions} \to b > 0 \,\&\&\, b \in \mathbb{R}\right] \Big/ \text{Integrate}[u_3[\rho, b]\, u_3[\rho, b], \{\rho, 0, \infty\}, \text{Assumptions} \to b > 0 \,\&\&\, b \in \mathbb{R}]$

Out[26]= $\dfrac{1}{3}(-3 + b)\, b$

In[27]:= $\text{Minimize}[\text{Energy}_1[b], b]$

Out[27]= $\{-1, \{b \to 1\}\}$

In[31]:= $\text{Minimize}[\text{Energy}_2[b], b]$

Out[31]= $\left\{-\dfrac{8}{\pi^2}, \left\{b \to \dfrac{\pi}{4}\right\}\right\}$

In[ ]:= $\text{Minimize}[\text{Energy}_3[b], b]$

In[29]:= $\left\{-\dfrac{3}{4}, \left\{b \to \dfrac{3}{2}\right\}\right\}$

In[47]:= $\sqrt{\left(\dfrac{\int_0^\infty u_1[\rho, 1]\, \rho^2\, u_1[\rho, 1]\, d\rho}{\int_0^\infty u_1[\rho, 1]\, u_1[\rho, 1]\, d\rho}\right)}$

Out[47]= $\sqrt{3}$

In[48]:= $$\sqrt{\left(\frac{\int_0^\infty u_2\left[\rho, \frac{\pi}{4}\right] \rho^2\, u_2\left[\rho, \frac{\pi}{4}\right] \, d\rho}{\int_0^\infty u_2\left[\rho, \frac{\pi}{4}\right]\; u_2\left[\rho, \frac{\pi}{4}\right] \, d\rho}\right)}$$

... Integrate: Integral of $\frac{\rho^4}{\left(\frac{\pi^2}{16}+\rho^2\right)^2}$ does not converge on {0, ∞}.

Out[48]= $$\sqrt{\int_0^\infty \frac{\rho^4}{\left(\frac{\pi^2}{16}+\rho^2\right)^2} \, d\rho}$$

In[49]:= $$\sqrt{\frac{\int_0^\infty u_3\left[\rho, \frac{3}{2}\right] \rho^2\, u_3\left[\rho, \frac{3}{2}\right] \, d\rho}{\int_0^\infty u_3\left[\rho, \frac{3}{2}\right]\; u_3\left[\rho, \frac{3}{2}\right] \, d\rho}}$$

Out[49]= $$\sqrt{\frac{10}{3}}$$