Variational Calculation Algebra

Our dimensionless Schrodinger equation is now:

$$\frac{\partial^2 \psi}{\partial s^2} - \delta(s)\, \psi(s) = \epsilon\, \psi(s)$$

We assume a variational wave function:

$$\psi(s) = \frac{1}{(\pi\, \alpha)^{1/4}}\, e^{-\frac{s^2}{2\alpha}}$$

It's normalized:

$$\int \psi(s)^2\, ds = \frac{1}{(\pi\, \alpha)^{1/2}} \int_{-\infty}^{\infty} e^{-\frac{s^2}{\alpha}}\, ds = \frac{1}{(\pi\, \alpha)^{1/2}}\, (\pi\, \alpha)^{1/2} = 1$$

To calculate the kinetic energy we need to take the second derivative:

$$\frac{\partial \psi}{\partial s} = \frac{1}{(\pi\, \alpha)^{1/4}} \left(-\frac{s}{\alpha}\right) e^{-\frac{s^2}{2\alpha}} = -\frac{s}{\pi^{1/4}\, \alpha^{5/4}}\, e^{-\frac{s^2}{2\alpha}}$$

$$\frac{\partial^2 \psi}{\partial s^2} = -\frac{1}{\pi^{1/4}} \left(\frac{1}{\alpha^{5/4}} - \frac{s^2}{\alpha^{9/4}}\right) e^{-\frac{s^2}{2\alpha}}$$

So that the expectation value of the kinetic energy term (actually, the negative of the kinetic energy) is:

$$\left(\psi, \frac{\partial^2 \psi}{\partial s^2}\right) = \frac{1}{(\pi\, \alpha)^{1/4}} \int_{-\infty}^{\infty} e^{-\frac{s^2}{2\alpha}} \times -\frac{1}{\pi^{1/4}} \left(\frac{1}{\alpha^{5/4}} - \frac{s^2}{\alpha^{9/4}}\right) e^{-\frac{s^2}{2\alpha}}\, ds$$

$$= -\frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \left(\frac{1}{\alpha^{3/2}} - \frac{s^2}{\alpha^{5/2}}\right) e^{-\frac{s^2}{\alpha}}\, ds$$

$$= -\frac{1}{\sqrt{\pi}} \left(\frac{1}{\alpha^{3/2}} \sqrt{\pi\, \alpha} - \frac{1}{\alpha^{5/2}}\, \frac{1}{2} \sqrt{\pi}\, \alpha^{3/2}\right)$$

$$= -\frac{1}{2\,\alpha}$$

The potential energy is trivially:

$$(\psi, \delta(s)\, \psi) = \frac{1}{\sqrt{\pi\, \alpha}}\, e^{-\frac{s^2}{\alpha}} \Big|_{s=0} = \frac{1}{\sqrt{\pi\, \alpha}}$$

So our variational quantity is:

$$J\, (\alpha) = \frac{1}{2\,\alpha} - \frac{1}{\sqrt{\pi\, \alpha}}$$

Our variation yields:

$$\frac{\partial J}{\partial \alpha} = -\frac{1}{2\,\alpha^2} - \frac{1}{\sqrt{\pi}} \left(-\frac{1}{2}\right) \frac{1}{\alpha^{3/2}} = 0$$

So that

$$\frac{1}{\sqrt{\alpha}} = \frac{1}{\sqrt{\pi}} \longrightarrow \alpha = \pi$$

The variational energy is therefore:

$$J(\pi) = -\frac{1}{2\,\pi} + \frac{1}{\sqrt{\pi \times \pi}} = \frac{1}{2\,\pi}$$