variational principle for SHO, $H = \hbar \omega \left( -\frac{1}{2} \frac{d^2}{ds^2} + \frac{1}{2} s^2 \right)$

\begin{verbatim}
In[14]:= $Assumptions = \{ a > 0, b > 0 \}
Out[14]= \{ a > 0, b > 0 \}

pick trial wavefunction for gnd state

In[44]:= \( \psi = \frac{a}{1 + b s^2} \);

find normalization

In[45]:= Integrate[\( \psi^2 \), \{ s, -\infty, \infty \}] 
Out[45]= \( \frac{a^2 \pi}{2 \sqrt{b}} \)

In[16]:= Solve[\( a = 1, a \)] 
Out[16]= \{ \{ a \to -b^{1/4} \sqrt{\frac{2}{\pi}} \}, \{ a \to b^{1/4} \sqrt{\frac{2}{\pi}} \} \}

correctly normalized wavefunction

In[46]:= \( \psi = \frac{a}{1 + b s^2} /. \{ a \to -b^{1/4} \sqrt{\frac{2}{\pi}} \}; \)

expectation value of kinetic energy

In[18]:= Integrate[\( -\frac{1}{2} \psi D[\psi, \{ s, 2 \}] \), \{ s, -\infty, \infty \}] 
Out[18]= \( \frac{b}{4} \)

expectation value of potential energy

In[19]:= Integrate[\( \frac{1}{2} \psi s^2 \psi \), \{ s, -\infty, \infty \}] 
Out[19]= \( \frac{1}{2 b} \)
minimum value is at \( b = \sqrt{2} \)

\[
\text{In}[21]:= \quad \frac{b}{4} + \frac{1}{2 \ b} \quad / \quad b \to \sqrt{2}.
\]

\text{Out}[21]= 0.707107

therefore the upper bound on the energy is 0.707 \( \hbar \omega \), not too impressive. Probably could have done better with a wavefunction that fell off faster at large \( s \)

Now try \( V = V_0 (x/\alpha)^4 \) with a Gaussian trial function

\[
\text{In}[23]:= \quad \text{Integrate} \left[ \exp \left( -2 \ b \ s^2 \right) \right], \{s, -\infty, \infty\}
\]

\text{Out}[23]= \frac{\sqrt{\frac{\pi}{2}}}{\sqrt{b}}

properly normalized wavefunction

\[
\text{In}[24]:= \quad \text{psi} = (2 \ b / \pi)^{1/4} \exp \left[-b \ s^2\right]
\]

\text{Out}[24]= \frac{1}{2} \ b^{1/4} \ \exp \left[-b \ s^2\right]

\[
\text{In}[25]:= \quad \text{Integrate} \left[ -\frac{1}{2} \ \text{psi} \ \frac{\partial}{\partial \ s} \ \text{psi}, \{s, 2\}\right], \{s, -\infty, \infty\}
\]

\text{Out}[25]= \frac{b}{2}

\[
\text{In}[26]:= \quad \text{Integrate} \left[ q \ \text{psi}^4 \ \text{psi}, \{s, -\infty, \infty\}\right]
\]

\text{Out}[26]= \frac{3 \ q}{16 \ b^2}
Actual energy is \(0.668 \, q^{1/3}\). Here is a plot of the correct wavefunction (in dots) as compared to the trial wavefunction (red). Our trial wavefunction was pretty good.

Now get the first excited state of the oscillator—pick an odd trial function.

\[
\psi = \frac{a \, s}{1 + b \, s^4}
\]
In[38]:= Integrate\[\frac{-1}{2} \psi D[\psi, \{s, 2\}], \{s, -\infty, \infty\}\]

Out[38]= \[\frac{5 \sqrt{b}}{4}\]

In[39]:= Integrate\[\frac{1}{2} \psi s^2 \psi, \{s, -\infty, \infty\}\]

Out[39]= \[\frac{1}{2 \sqrt{b}}\]

In[42]:= Plot\[\frac{5 \sqrt{b}}{4} + \frac{1}{2 \sqrt{b}}, \{b, 0, .5\}\]

Out[42]=

In[43]:= \[\frac{5 \sqrt{b}}{4} + \frac{1}{2 \sqrt{b}} \] / . b \rightarrow 0.4

Out[43]= 1.58114

The correct value is 1.5 so this is pretty close!