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

In[14]:= `$Assumptions = {a > 0, b > 0}`

Out[14]= {a > 0, b > 0}

pick trial wavefunction for gnd state

In[44]:= $\texttt{psi} = \dfrac{a}{1 + b\,s^2}$;

find normalization

In[45]:= $\texttt{Integrate}\left[\texttt{psi}^2, \{s, -\infty, \infty\}\right]$

Out[45]= $\dfrac{a^2\,\pi}{2\,\sqrt{b}}$

In[16]:= `Solve[% == 1, a]`

Out[16]= $\left\{\left\{a \to -b^{1/4}\,\sqrt{\dfrac{2}{\pi}}\right\}, \left\{a \to b^{1/4}\,\sqrt{\dfrac{2}{\pi}}\right\}\right\}$

correctly normalized wavefunction

In[46]:= $\texttt{psi} = \dfrac{a}{1 + b\,s^2}\ \texttt{/.}\ a \to b^{1/4}\,\sqrt{\dfrac{2}{\pi}}$;

expectation value of kinetic energy

In[18]:= $\texttt{Integrate}\left[\dfrac{-1}{2}\,\texttt{psi}\,\texttt{D[psi, \{s, 2\}]}, \{s, -\infty, \infty\}\right]$

Out[18]= $\dfrac{b}{4}$

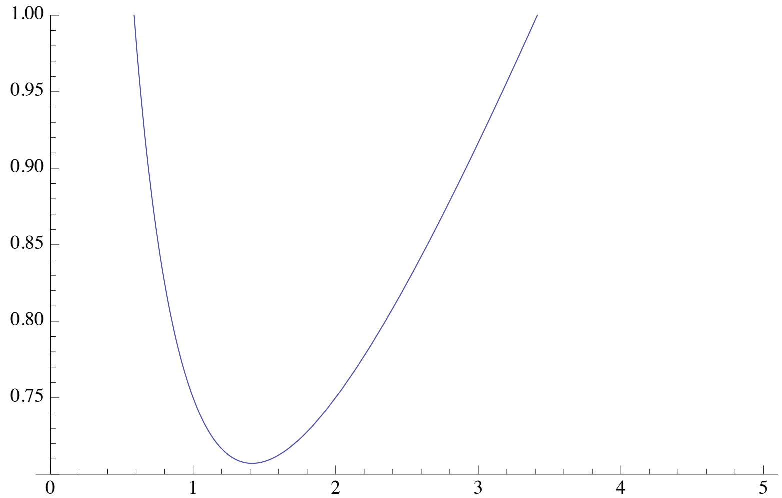
expectation value of potential energy

In[19]:= $\texttt{Integrate}\left[\dfrac{1}{2}\,\texttt{psi}\,s^2\,\texttt{psi}, \{s, -\infty, \infty\}\right]$

Out[19]= $\dfrac{1}{2\,b}$

In[22]:= `Plot[b/4 + 1/(2 b), {b, 0, 5}, PlotRange → {.7, 1}]`

Out[22]=



minimum value is at b=sqrt(2)

In[21]:= $\frac{b}{4} + \frac{1}{2\,b}$ `/. b → √2.`

Out[21]= 0.707107

therefore the upper bound on the energy is .707 $\hbar\omega$, not too impressive. Probably could have done better with a wavefunction that fell off faster at large s

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

In[23]:= `Integrate[Exp[-2 b s^2], {s, -∞, ∞}]`

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

properly normalized wavefunction

In[24]:= `psi = (2 b / π)^(1/4) Exp[-b s^2]`

Out[24]= $b^{1/4}\, e^{-b s^2} \left(\frac{2}{\pi}\right)^{1/4}$

In[25]:= `Integrate[-1/2 psi D[psi, {s, 2}], {s, -∞, ∞}]`

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

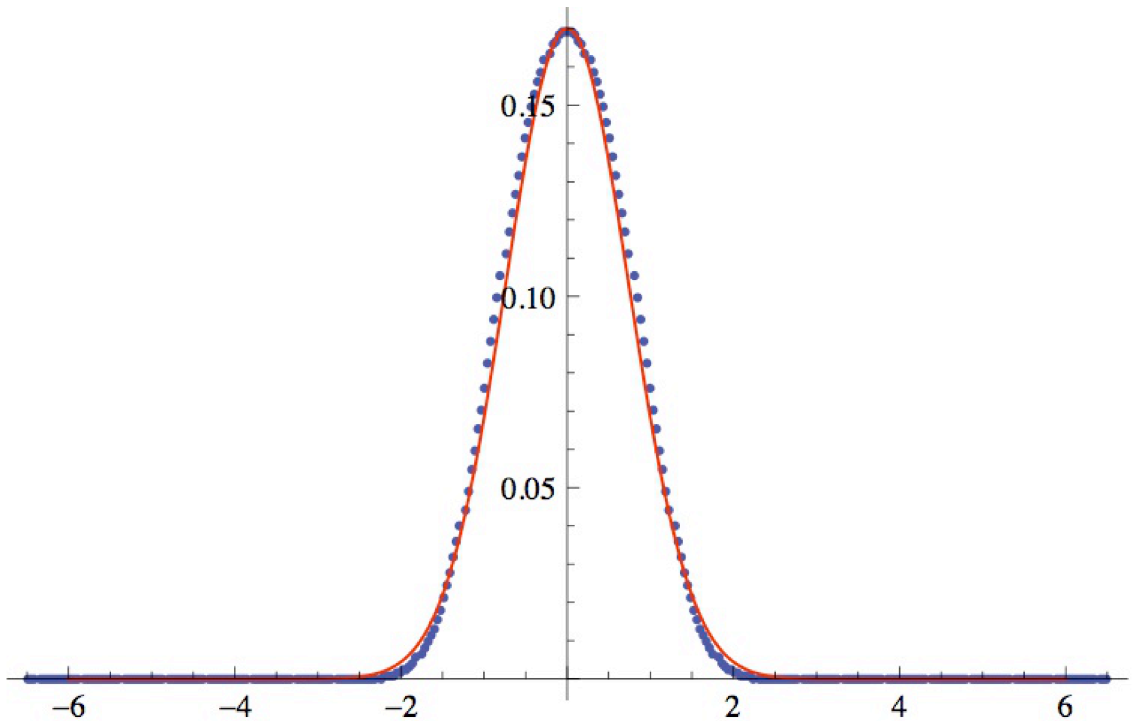
In[26]:= `Integrate[ q psi s^4 psi, {s, -∞, ∞}]`

Out[26]= $\frac{3\,q}{16\,b^2}$

In[27]:= `% + %% /. b → (.75 q)^(1/3)`

Out[27]= $0.68142\, q^{1/3}$

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

In[34]:= $\texttt{psi} = \frac{a\, s}{1 + b\, s^4}$

Out[34]= $\frac{a\, s}{1 + b\, s^4}$

In[35]:= `Integrate[psi^2, {s, -∞, ∞}]`

Out[35]= $\frac{a^2 \pi}{4 \sqrt{2}\, b^{3/4}}$

In[36]:= `Solve[% == 1, a]`

Out[36]= $\left\{\left\{a \to -\frac{2 \times 2^{1/4}\, b^{3/8}}{\sqrt{\pi}}\right\}, \left\{a \to \frac{2 \times 2^{1/4}\, b^{3/8}}{\sqrt{\pi}}\right\}\right\}$

In[37]:= $\texttt{psi} = \frac{2 \times 2^{1/4}\, b^{3/8}}{\sqrt{\pi}} \frac{s}{1 + b\, s^4}$

Out[37]= $\frac{2 \times 2^{1/4}\, b^{3/8}\, s}{\sqrt{\pi}\, \left(1 + b\, s^4\right)}$

In[38]:= $\text{Integrate}\left[\frac{-1}{2}\ \text{psi}\ \text{D[psi, \{s, 2\}], \{s, }-\infty, \infty\}\right]$

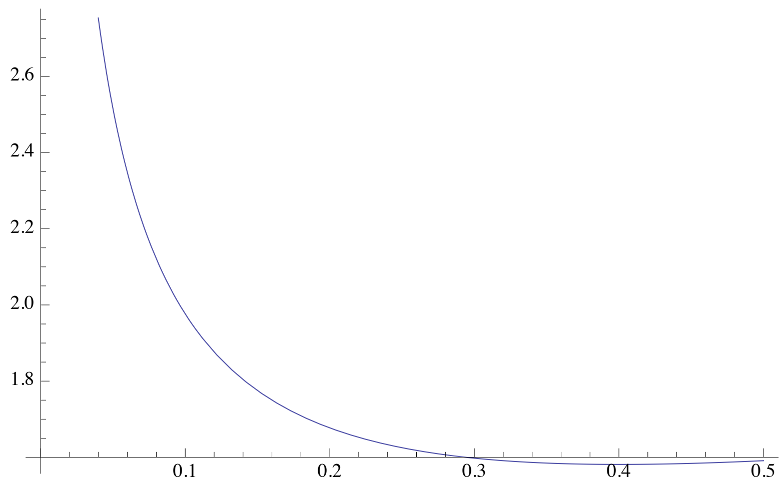
Out[38]= $\frac{5\sqrt{b}}{4}$

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

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

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

Out[42]=



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

Out[43]= 1.58114

correct value is 1.5 so this is pretty close!