Variational Principle: Harmonic Oscillator

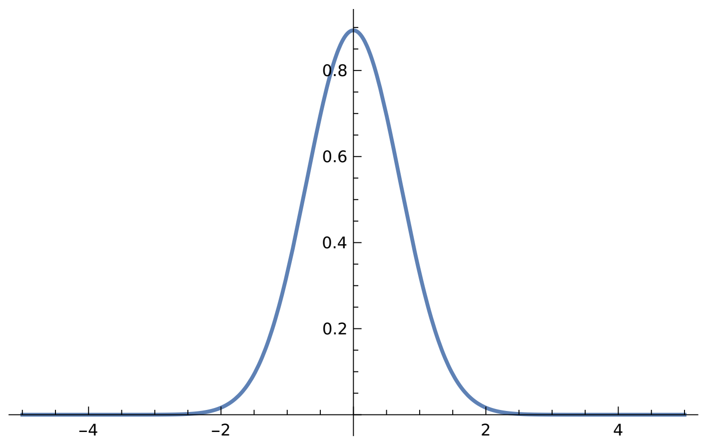
Ground State

1. Trial Wave Functions

In[1]:= `ψ[x_, α_] := Exp[-α x^2]`

In[31]:= `Plot[ψ[x, 1], {x, -5, 5}, PlotRange → All]`

Out[31]=



Norm

In[7]:= `Integrate[ψ[x, α] × ψ[x, α], {x, -Infinity, Infinity}, Assumptions → α > 0]`

Out[7]= $\frac{\sqrt{\frac{\pi}{2}}}{\sqrt{\alpha}}$

Normalized Trial Wave Functions

In[8]:= `ψ[x_, α_] := Exp[-α x^2] / Sqrt[`$\frac{\sqrt{\frac{\pi}{2}}}{\sqrt{\alpha}}$`]`

2. <H>(α)

In[12]:=
```
D[ψ[x, α], {x, 2}]
```

Out[12]=

$$\left(\frac{2}{\pi}\right)^{1/4} \alpha^{1/4} \left(-2\, e^{-x^2 \alpha} \alpha + 4\, e^{-x^2 \alpha} x^2 \alpha^2\right)$$

In[13]:=
```
H[x_, ϕ_] := -ℏ^2/(2 m) D[ϕ, {x, 2}] + 1/2 m ω^2 x^2 ϕ
```

In[14]:=
```
H[x, ψ[x, α]]
```

Out[14]=

$$\frac{e^{-x^2 \alpha}\, m\, x^2 \alpha^{1/4} \omega^2}{2^{3/4} \pi^{1/4}} - \frac{\alpha^{1/4}\left(-2\, e^{-x^2 \alpha} \alpha + 4\, e^{-x^2 \alpha} x^2 \alpha^2\right) \hbar^2}{2^{3/4}\, m\, \pi^{1/4}}$$

<H>(α)

In[16]:=
```
Integrate[ψ[x, α] × H[x, ψ[x, α]], {x, -Infinity, Infinity}, Assumptions → α > 0]
```

Out[16]=

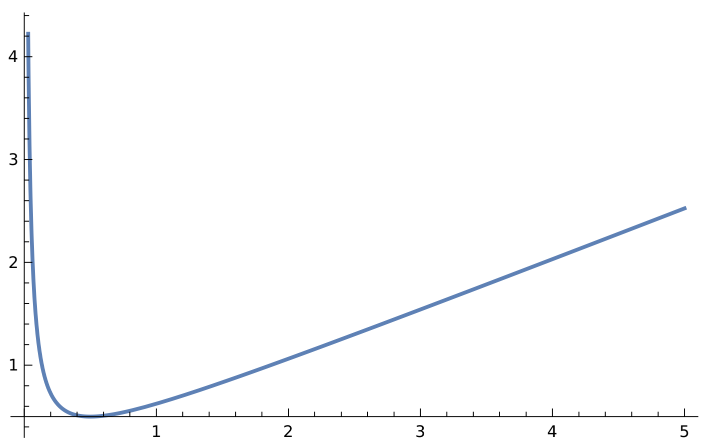
$$\frac{m\,\omega^2}{8\,\alpha} + \frac{\alpha\,\hbar^2}{2\,m}$$

In[17]:=
```
H1[α_] := m ω^2/(8 α) + α ℏ^2/(2 m)
```

3. Minimization

In[19]:=
```
Plot[H1[α] /. {m → 1, ℏ → 1, ω → 1}, {α, 0, 5}]
```

Out[19]=



In[21]:=
```
Solve[x^2 == -1, x]
```

Out[21]=

{{x → -i}, {x → i}}

In[23]:= `Solve[D[H1[α], α] == 0, α]`

Out[23]=

$$\left\{\left\{\alpha \to -\frac{m\,\omega}{2\,\hbar}\right\}, \left\{\alpha \to \frac{m\,\omega}{2\,\hbar}\right\}\right\}$$

Ground State Energy

In[25]:= $H1\left[\frac{m\,\omega}{2\,\hbar}\right]$

Out[25]=

$$\frac{\omega\,\hbar}{2}$$

Ground State

In[26]:= $\psi\left[x, \frac{m\,\omega}{2\,\hbar}\right]$

Out[26]=

$$\frac{e^{-\frac{m\,x^2\,\omega}{2\,\hbar}}\left(\frac{m\,\omega}{\hbar}\right)^{1/4}}{\pi^{1/4}}$$

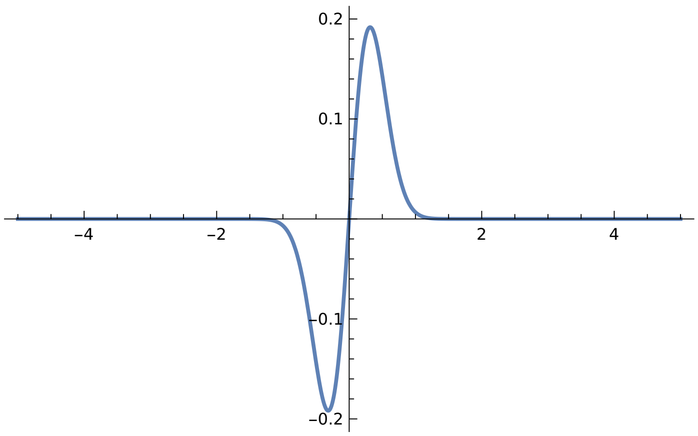
First Excited State (?)

1.

In[27]:= `γ[x_, α_] := x Exp[-α x^2]`

In[30]:= `Plot[γ[x, 5], {x, -5, 5}, PlotRange → All]`

Out[30]=



Normalized trial wave Functions

In[32]:=
```
Integrate[γ[x, α] × γ[x, α], {x, -Infinity, Infinity}, Assumptions → α > 0]
```

Out[32]=

$$\frac{\sqrt{\frac{\pi}{2}}}{4\,\alpha^{3/2}}$$

In[33]:=
```
γ[x_, α_] := x Exp[-α x^2] / Sqrt[Sqrt[π/2] / (4 α^(3/2))]
```

$$\gamma[x\_, \alpha\_] := x\,\mathrm{Exp}[-\alpha\, x^2] \Big/ \mathrm{Sqrt}\left[\frac{\sqrt{\frac{\pi}{2}}}{4\,\alpha^{3/2}}\right]$$

2.

In[34]:=
```
Integrate[γ[x, α] × H[x, γ[x, α]], {x, -Infinity, Infinity}, Assumptions → α > 0]
```

Out[34]=

$$\frac{3\,m\,\omega^2}{8\,\alpha} + \frac{3\,\alpha\,\hbar^2}{2\,m}$$

In[37]:=

$$\mathrm{H2}[\alpha\_] := \frac{3\,m\,\omega^2}{8\,\alpha} + \frac{3\,\alpha\,\hbar^2}{2\,m}$$

3.

In[38]:=
```
Solve[D[H2[α], α] == 0, α]
```

Out[38]=

$$\left\{\left\{\alpha \to -\frac{m\,\omega}{2\,\hbar}\right\}, \left\{\alpha \to \frac{m\,\omega}{2\,\hbar}\right\}\right\}$$

First Excited State Energy

In[39]:=

$$\mathrm{H2}\left[\frac{m\,\omega}{2\,\hbar}\right]$$

Out[39]=

$$\frac{3\,\omega\,\hbar}{2}$$

First Excited State

In[40]:= $\gamma\left[x, \frac{m\,\omega}{2\,\hbar}\right]$

Out[40]=

$$\frac{\sqrt{2}\, e^{-\frac{m\,x^2\,\omega}{2\,\hbar}}\, x}{\pi^{1/4}\sqrt{\frac{1}{\left(\frac{m\,\omega}{\hbar}\right)^{3/2}}}}$$

“Arbitrary” State

1.

In[41]:= `κ[x_, α_] := 1 / (x ^ 2 + α)`

In[42]:= `Integrate[κ[x, α] × κ[x, α], {x, -Infinity, Infinity}, Assumptions → α > 0]`

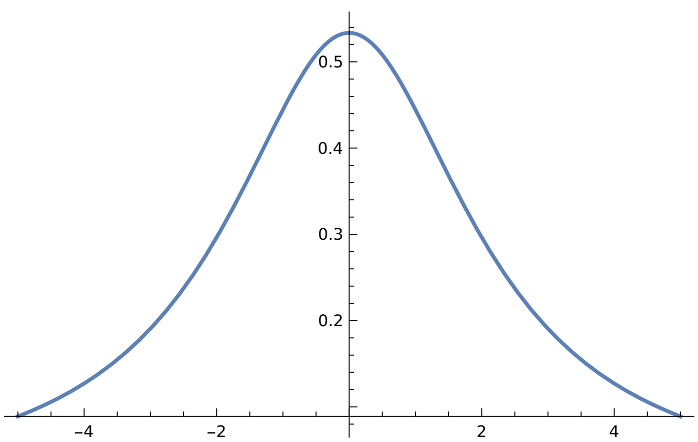
Out[42]=

$$\frac{\pi}{2\,\alpha^{3/2}}$$

In[43]:= `κ[x_, α_] := 1 / (x ^ 2 + α)` $\Big/$ `Sqrt`$\left[\frac{\pi}{2\,\alpha^{3/2}}\right]$

In[47]:= `Plot[κ[x, 5], {x, -5, 5}]`

Out[47]=



2.

In[48]:=
```
Integrate[κ[x, α] × H[x, κ[x, α]], {x, -Infinity, Infinity}, Assumptions → α > 0]
```

Out[48]=

$$\frac{1}{2} m \alpha \omega^2 + \frac{\hbar^2}{4 m \alpha}$$

In[49]:=
```
H3[α_] := 1/2 m α ω^2 + ħ^2/(4 m α)
```

$$H3[\alpha\_] := \frac{1}{2} m \alpha \omega^2 + \frac{\hbar^2}{4 m \alpha}$$

3.

In[50]:=
```
Solve[D[H3[α], α] == 0, α]
```

Out[50]=

$$\left\{\left\{\alpha \to -\frac{\hbar}{\sqrt{2} m \omega}\right\}, \left\{\alpha \to \frac{\hbar}{\sqrt{2} m \omega}\right\}\right\}$$

Ground State Energy

In[51]:=

$$H3\left[\frac{\hbar}{\sqrt{2} m \omega}\right]$$

Out[51]=

$$\frac{\omega \hbar}{\sqrt{2}}$$

In[56]:=

$$\left(\frac{\omega \hbar}{\sqrt{2}} - \frac{\omega \hbar}{2}\right) / (\omega \hbar) \text{ // FullSimplify // N}$$

Out[56]=

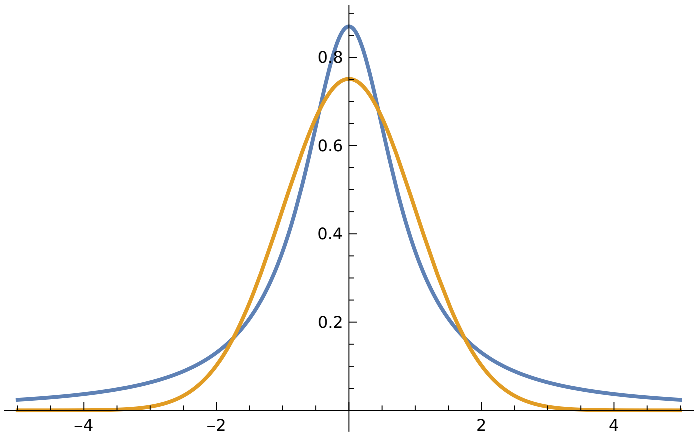
0.207107

Ground State

In[58]:=

$$\texttt{Plot}\left[\texttt{Evaluate@}\left(\left\{\kappa\left[x, \frac{\hbar}{\sqrt{2}\, m\, \omega}\right], \psi\left[x, \frac{m\, \omega}{2\, \hbar}\right]\right\} \texttt{/. } \{m \to 1, \hbar \to 1, \omega \to 1\}\right), \{x, -5, 5\}\right]$$

Out[58]=



Observables

<X^2>

In[60]:=

$$\texttt{Integrate}\left[\psi\left[x, \frac{m\, \omega}{2\, \hbar}\right] x^{\wedge}2\ \psi\left[x, \frac{m\, \omega}{2\, \hbar}\right], \left\{x, -\texttt{Infinity}, \texttt{Infinity}\right\}, \texttt{Assumptions} \to \frac{m\, \omega}{\hbar} > 0\right]$$

Out[60]=

$$\frac{\hbar}{2\, m\, \omega}$$

In[62]:=

$$\texttt{Integrate}\left[\kappa\left[x, \frac{\hbar}{\sqrt{2}\, m\, \omega}\right] x^{\wedge}2\ \kappa\left[x, \frac{\hbar}{\sqrt{2}\, m\, \omega}\right], \left\{x, -\texttt{Infinity}, \texttt{Infinity}\right\}, \texttt{Assumptions} \to \frac{\sqrt{\hbar}}{\sqrt{m}\, \sqrt{\omega}} > 0\right]$$

Out[62]=

$$\frac{\hbar}{\sqrt{2}\, m\, \omega}$$

In[64]:= $\left(\frac{\hbar}{\sqrt{2}\ m\ \omega} - \frac{\hbar}{2\ m\ \omega}\right) \Big/ \left(\frac{\hbar}{2\ m\ \omega}\right)$ // FullSimplify // N

Out[64]=

0.414214

< X^4 >

In[65]:= Integrate$\left[\psi\left[x, \frac{m\ \omega}{2\ \hbar}\right] x\,^\wedge 4\ \psi\left[x, \frac{m\ \omega}{2\ \hbar}\right], \{x, -\text{Infinity}, \text{Infinity}\}, \text{Assumptions} \to \frac{m\ \omega}{\hbar} > 0\right]$

Out[65]=

$$\frac{3\ \hbar^2}{4\ m^2\ \omega^2}$$

In[66]:= Integrate$\left[\kappa\left[x, \frac{\hbar}{\sqrt{2}\ m\ \omega}\right] x\,^\wedge 4\ \kappa\left[x, \frac{\hbar}{\sqrt{2}\ m\ \omega}\right],\right.$

$\left.\{x, -\text{Infinity}, \text{Infinity}\}, \text{Assumptions} \to \frac{\sqrt{\hbar}}{\sqrt{m}\ \sqrt{\omega}} > 0\right]$

••• Integrate: Integral of $\frac{4\ 2^{1/4}\ x^4\ \sqrt{m\ \omega\ \hbar^3}}{\pi\left(2\ m\ x^2\ \omega + \sqrt{2}\ \hbar\right)^2}$ does not converge on $\{-\infty, \infty\}$.

Out[66]=

$$\text{Integrate}\left[\frac{2^{1/4}\ x^4\left(\frac{\hbar}{m\ \omega}\right)^{3/2}}{\pi\left(x^2 + \frac{\hbar}{\sqrt{2}\ m\ \omega}\right)^2}, \{x, -\infty, \infty\}, \text{Assumptions} \to \frac{\sqrt{\hbar}}{\sqrt{m}\ \sqrt{\omega}} > 0\right]$$