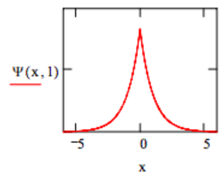
10.30: The Variation Method in Momentum Space

The following normalized trial wavefunction is proposed for a variational calculation on the harmonic oscillator.

$$\psi(x,a) := \sqrt{\frac{1}{a}}exp(\frac{-|x|}{a})$$

$$\int_{-\infty}^{\infty}\psi(x,a)^2dx \quad assume,\ a>0 \rightarrow 1$$

However, the graph below shows a cusp at x = 0, indicating that the wavefunction is not well-behaved and therefore cannot be used for quantum mechanical calculations.

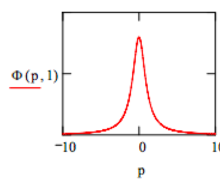


Therefore, the wavefunction is Fourier transformed into the momentum representation.

$$\Phi(p,a) := \int_{-\infty}^{\infty}\frac{exp(-ipx)}{\sqrt{2\pi}}\sqrt{\frac{1}{a}}exp(\frac{-|x|}{a})dx \mid_{simplify}^{assume,\ a>0} \rightarrow (-a^{\frac{1}{2}})\frac{2^{\frac{1}{2}}}{(ipa-1)\pi^{\frac{1}{2}}(ipa+1)}$$

Normalization is checked and the function is graphed.

$$\int_{-\infty}^{\infty}\Phi(p,a)^2dp \quad assume,\ a>0 \rightarrow 1$$



The momentum wavefunction appears to be well-behaved, so a variational calculation will be carried out in momentum space.

Assuming a m = k =1 and h = 2π, we have for the harmonic oscillator in momentum space.

- Momentum space integral: $\int_{-\infty}^{\infty} \blacksquare dp$
- Momentum operator: $p\blacksquare$
- Kinetic energy operator: $\frac{p^2}{2}$
- Position operator: $i\frac{d}{dp}\blacksquare$
- Potential energy operator: $\frac{-1}{2}\frac{d^2}{dp^2}\blacksquare$

Evaluate the energy integral in the momentum representation:

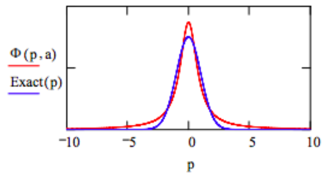
$$E(a) := \int_{-\infty}^{\infty}\Phi(p,a)\frac{p^2}{2}\Phi(p,a)dp... + \int_{-\infty}^{\infty}\Phi(p,a)\frac{-1}{2}\frac{d^2}{dp^2}\Phi(p,a)dp \mid_{assume,\ a>0}^{simplify} \rightarrow \frac{1}{4}\frac{2+a^4}{a^2}$$

Minimize energy with respect to the variational parameter:

a := 1 a := Minimize (E, a) a = 1.189 E(a) = 0.707

Display optimum wavefunction along with exact wavefunction:

$$Exact(p) := \frac{1}{\pi^{\frac{1}{4}}}e^{\frac{-1}{2}p^2}$$



Naturally the agreement with the exact solution is not favorable because of the poor quality of the original coordinate space wavefunction.

$$\frac{E(a)-0.5}{0.5}=41.421$$