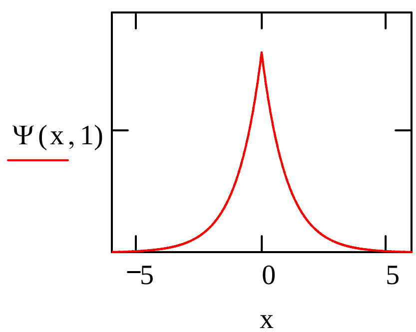
Variational Calculation on the Simple Harmonic Oscillator in Momentum Space

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

$$\Psi(x,a) := \sqrt{\frac{1}{a}}\cdot\exp\left(\frac{-|x|}{a}\right) \qquad \int_{-\infty}^{\infty}\Psi(x,a)^2\,dx \text{ assume}, a > 0 \;\rightarrow 1$$

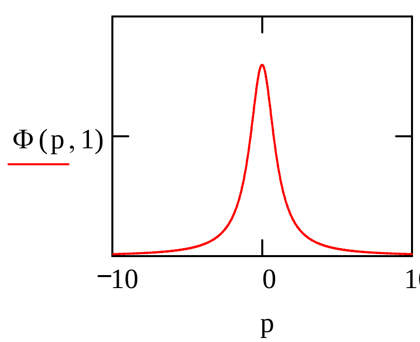
However, the graph below shows a cusp at x = 0, indicating that the wave function is not well-behaved and therefore cannot be used for quantum mechanical calculations.



Therefore, the wave function is Fourier transformed into the momentum representation.

$$\Phi(p,a) := \int_{-\infty}^{\infty}\frac{\exp(-i\cdot p\cdot x)}{\sqrt{2\cdot\pi}}\cdot\sqrt{\frac{1}{a}}\cdot\exp\left(\frac{-|x|}{a}\right)dx \;\Big|\begin{array}{l}\text{assume}, a > 0\\ \text{simplify}\end{array} \rightarrow \left(-a^{\frac{1}{2}}\right)\cdot\frac{2^{\frac{1}{2}}}{(i\cdot p\cdot a-1)\cdot\pi^{\frac{1}{2}}\cdot(i\cdot p\cdot a+1)}$$

Normalization is checked and the function is graphed. $\int_{-\infty}^{\infty}\Phi(p,a)^2\,dp \text{ assume}, a > 0 \;\rightarrow 1$



The momentum wave function 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: $p \cdot \blacksquare$ Kinetic energy operator: $\frac{p^2}{2}$

Position operator: $i \cdot \frac{d}{dp} \blacksquare$ Potential energy operator: $\frac{-1}{2} \cdot \frac{d^2}{dp^2} \blacksquare$

Evaluate the energy integral in the momentum representation:

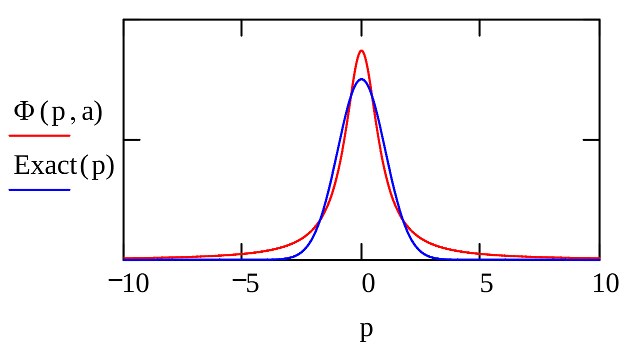
$$E(a) := \int_{-\infty}^{\infty} \Phi(p,a) \cdot \frac{p^2}{2} \cdot \Phi(p,a)\, dp \ldots + \int_{-\infty}^{\infty} \Phi(p,a) \cdot \frac{-1}{2} \cdot \frac{d^2}{dp^2} \Phi(p,a)\, dp \quad \left| \begin{array}{l} \text{simplify} \\ \text{assume}, a > 0 \end{array} \right. \rightarrow \frac{1}{4} \cdot \frac{2 + a^4}{a^2}$$

Minimize energy with respect to the variational parameter:

$a := 1$ $a := \text{Minimize}(E, a)$ $a = 1.189$ $E(a) = 0.707$

Display optimum wave function along with exact wave function: $\text{Exact}(p) := \frac{1}{\pi^{\frac{1}{4}}} \cdot e^{\frac{-1}{2} \cdot p^2}$

$p := -10, -9.99 .. 10$



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

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