# Variational Method

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## Introduction

The application of Variational Method takes the form of roughly four steps.

### Step 1

First one must choose an appropriate normalized trial wave function that takes into account all the physical properties of the ground state. The trial wave function should scale based on a parameter $a$, which will account for various unknown properties, as $|\psi_0\rangle = |\psi_0(a)\rangle$. The closer the trial wave function to the true wave function, the better the estimate of the ground state energy.

### Step 2

Once we have a normalized trial wave function, we can calculate the energy, which has the following expression:

$$E_0(a) = \frac{\langle\psi_0(a)|\hat{H}|\psi_0(a)\rangle}{\langle\psi_0(a)|\psi_0(a)\rangle} \tag{1}$$

### Step 3

Next we minimize $E_0(a)$ and solve for $a$

$$\frac{\partial E_0(a)}{\partial a} = 0 \tag{2}$$

### Step 4

Lastly once we have found $a_0$, we plug it back into $E_0$ and thus have found our upper bound for the ground state energy.

### Things to Note

One thing to note is that the ground state energy estimate we find doing the variational method is greater or equal to the true ground state energy.

$$E_{est} \geq E_{true} \tag{3}$$

## Problem

Use the variational method to estimate the energy of the ground state of a one-dimensional harmonic oscillator by making use of the following two trial functions:

$$(a) \quad \psi_0(x,a) = Ae^{-a|x|} \qquad (b) \quad \psi_0(x,a) = \frac{A}{(x^2+a)} \qquad (c*) \quad \psi_0(x,a) = \frac{A}{(1+ax^2)^2}$$

where $a$ is a positive real number and where A is the normalization constant.[1]

### (a) $\psi_0(x,a) = Ae^{-a|x|}$

First we must find the normalization constant A

$$\begin{aligned}
\langle\psi_0|\psi_0\rangle &= A^2\int_{-\infty}^{0} e^{2ax}dx + A^2\int_0^\infty e^{-2ax}dx \\
&= 2A^2\int_0^\infty e^{-2ax}dx \\
&= \frac{A^2}{a} \\
\Rightarrow A &= \sqrt{a}
\end{aligned} \tag{4}$$

Now lets find the expectation value for the Hamiltonian given our normalized trial wave function

$$\langle\psi_0|\hat{H}|\psi_0\rangle = \int_{-\infty}^{\infty} e^{-a|x|}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2A^2x^2\right)e^{-a|x|}dx \tag{5}$$

Lets look at the potential term first

$$\begin{aligned}
\langle\psi_0|V(x)|\psi_0\rangle &= \frac{1}{2}m\omega^2A^2\int_{-\infty}^{\infty} x^2e^{-2a|x|}dx \\
&= m\omega^2A^2\int_0^\infty x^2e^{-2ax}dx \\
&= \frac{m\omega^2}{4a^2}
\end{aligned} \tag{6}$$

Now lets solve the kinetic term

$$\begin{aligned}
-\frac{\hbar^2}{2m}\langle\psi_0|\frac{d^2}{dx^2}|\psi_0\rangle &= -\frac{\hbar^2}{2m}A^2\int_{-\infty}^{\infty} e^{-a|x|}\frac{d^2e^{-a|x|}}{dx^2}dx \\
&= -\frac{\hbar^2a^2}{m}A^2\int_0^\infty e^{-2ax}dx \\
&= -\frac{\hbar^2a^2}{2m}
\end{aligned} \tag{7}$$

Due to our carelessness this lead to a negative kinetic energy. Thus the correct way to calculate the kinetic energy term is by doing as such:

$$\begin{aligned}
-\frac{\hbar^2}{2m}\langle\psi_0|\frac{d^2}{dx^2}|\psi_0\rangle &= \frac{\hbar^2}{2m}A^2\int_{-\infty}^{\infty}\left|\frac{de^{-a|x|}}{dx}\right|^2 dx \\
&= \frac{\hbar^2a^2}{2m}
\end{aligned} \tag{8}$$

Adding the kinetic and potential term we get

$$E_0 = \frac{\hbar^2 a^2}{2m} + \frac{m\omega^2}{4a^2} \tag{9}$$

Then we minimize $E_0(a) = \dfrac{\langle\psi_0(a)|\hat{H}|\psi_0(a)\rangle}{\langle\psi_0(a)|\psi_0(a)\rangle}$:

$$\begin{aligned} \frac{\partial E_0}{\partial a} &= 0 \\ \frac{\hbar^2 a_0}{m} - \frac{m\omega^2}{2a_0^3} &= 0 \\ \Rightarrow a_0 &= \sqrt{\frac{mw}{\sqrt{2}\hbar}} \end{aligned} \tag{10}$$

Plugging $a_0$ back into (9):

$$\begin{aligned} E_0 &= \frac{\hbar^2 m\omega}{2m\sqrt{2}\hbar} + \frac{m\omega^2\sqrt{2}\hbar}{4mw} \\ &= \frac{\hbar\omega}{\sqrt{2}} \\ &= 0.707\hbar\omega \end{aligned} \tag{11}$$

## (b) $\psi_0(x,a) = \dfrac{A}{(x^2+a)}$

For our wavefunction to be normalized

$$\begin{aligned} \langle\psi_0|\psi_0\rangle &= A^2 \int_{-\infty}^{\infty} \frac{1}{(a+x^2)^2} dx \\ &= A^2 \frac{\pi}{2a^{3/2}} \\ \Rightarrow A &= \left(\frac{4a^3}{\pi^2}\right)^{1/4} \end{aligned} \tag{12}$$

The expectation value of the Hamiltonian for this normalized wave function can be found by

$$\begin{aligned} \langle\psi_0(a)|\hat{H}|\psi_0(a)\rangle &= A^2 \int_{-\infty}^{\infty} \frac{1}{x^2+a} \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx} + \frac{1}{2}m\omega^2 x^2\right) \frac{1}{x^2+a} dx \\ &= -\frac{A^2\hbar^2}{2m} \int_{-\infty}^{\infty} \frac{6x^2-2a}{(x^2+a)^4} dx + \frac{1}{2}m\omega^2 A^2 \int_{-\infty}^{\infty} \frac{x^2}{(x^2+a)^2} dx \\ &= \frac{\hbar^2}{4ma} + \frac{1}{2}m\omega^2 a \end{aligned} \tag{13}$$

Minimizing $E_0(a) = \frac{\langle \psi_0(a)|\hat{H}|\psi_0(a)\rangle}{\langle \psi_0(a)|\psi_0(a)\rangle}$ we obtain

$$\begin{aligned} \frac{\partial E(a)}{\partial a} &= 0 \\ \Rightarrow -\frac{\hbar^2}{4ma_0^2} + \frac{1}{2}m\omega &= 0 \\ \Rightarrow a_0 &= \frac{\hbar}{\sqrt{2}m\omega} \end{aligned} \tag{14}$$

Plugging the expression for $a_0$ into (13) we obtain

$$\begin{aligned} E_0 &= \frac{\hbar\omega}{\sqrt{2}} \\ &= 0.707\hbar\omega \end{aligned} \tag{15}$$

The reason we found the same estimation for parts (a) and (b) is that the two trial wave function are connected through a Fourier Transform. Specifically:

$$\mathcal{F}\left[\frac{1}{t^2+a}\right](x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{1}{t^2+a}e^{ixt}dt = Ae^{-b|x|} \tag{16}$$

where $A = \sqrt{\frac{\pi}{2a}}$ and $b = \sqrt{a}$. Therefore it is reasonable that the two trial wavefunctions yielded the same result for the ground state energy.

## (c) $\psi_0(x, a) = \frac{A}{(1+ax^2)^2}$

We want to try one more wave function, in order to get a different estimate for the ground state energy for comparison. Since the true harmonic oscillator ground state wave function is a Gaussian function, a good educated guess would be to use a Lorentzian function (also known as Cauchy - Lorentz distribution or Breit - Wigner distribution). The Lorentzian describes a decaying system over time, since it is the Fourier transform of an exponentially decaying oscillation, and therefore describes many of the physical attributes of our harmonic oscillator.
As before, we begin by normalizing our wavefunction

$$\begin{aligned} \langle \psi_0|\psi_0\rangle &= A^2\int_{-\infty}^{\infty}\frac{1}{(1+ax^2)^4}dx \\ &= A^2\frac{5\pi}{16\sqrt{a}} \end{aligned} \tag{17}$$

and we obtain the normalization constant:

$$A = \left(\frac{16\sqrt{a}}{5\pi}\right)^{1/2} \tag{18}$$

The expectation value of the Hamiltonian for this normalized wave function can be found by

$$\langle \psi_0|\hat{H}|\psi_0\rangle = A^2\int_{-\infty}^{\infty}\frac{1}{(1+ax^2)^2}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx} + \frac{1}{2}m\omega^2x^2\right)\frac{1}{(1+ax)^2}dx \tag{19}$$

Starting from the potential term:

$$\begin{aligned}
\langle\psi_0|V(x)|\psi_0\rangle &= \frac{m\omega^2 A^2}{2}\int_{-\infty}^{\infty}\frac{x^2}{(1+ax)^4}dx \\
&= \frac{m\omega^2 A^2}{2}\left(\frac{\pi}{16a^{3/2}}\right) \\
&= \frac{m\omega^2}{10a}
\end{aligned} \tag{20}$$

Moving on to the kinetic term:

$$\begin{aligned}
-\frac{\hbar^2}{2m}\langle\psi_0|\frac{d^2}{dx^2}|\psi_0\rangle &= -\frac{\hbar^2}{2m}A^2\int_{-\infty}^{\infty}\frac{1}{(1+ax^2)^2}\frac{d^2}{dx^2}\left(\frac{1}{(1+ax^2)^2}\right)dx \\
&= -\frac{\hbar^2}{2m}A^2\left[\int_{-\infty}^{\infty}\frac{24a^2x^2}{(1+ax^2)^6} - \int_{-\infty}^{\infty}\frac{4a}{(1+ax^2)^5}\right] \\
&= -\frac{\hbar^2}{2m}A^2\left(\frac{21\pi\sqrt{a}}{32} - \frac{35\pi\sqrt{a}}{32}\right) \\
&= \frac{\hbar^2}{2m}\cdot\frac{16\sqrt{a}}{5\pi}\cdot\frac{14\pi\sqrt{a}}{32} \\
&= \frac{7\hbar^2 a}{10m}
\end{aligned} \tag{21}$$

Adding the two terms we obtain:

$$E_0(a) = \frac{7\hbar^2 a}{10m} + \frac{m\omega^2}{10a} \tag{22}$$

Minimizing $E_0(a) = \dfrac{\langle\psi_0(a)|\hat{H}|\psi_0(a)\rangle}{\langle\psi_0(a)|\psi_0(a)\rangle}$ we obtain

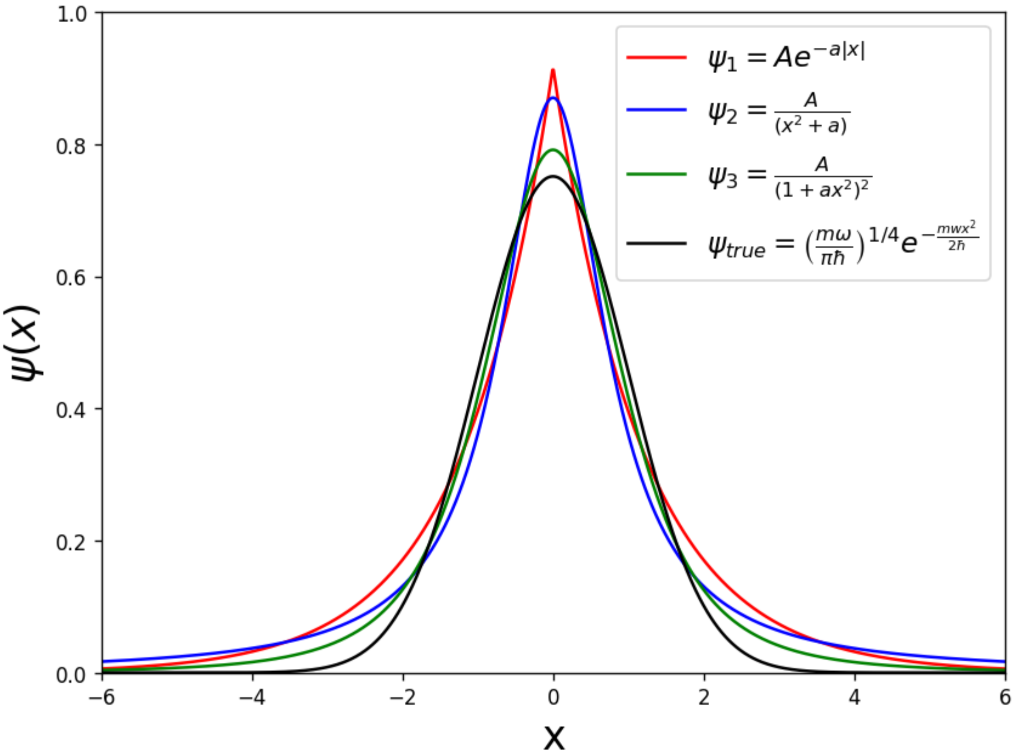
$$\begin{aligned}
&\frac{\partial E(a)}{\partial a} = 0 \\
\Rightarrow &\frac{7\hbar^2}{10m} - \frac{m\omega^2}{10a_0^2} = 0 \\
\Rightarrow &a_0 = \frac{m\omega}{\sqrt{7}\hbar}
\end{aligned} \tag{23}$$

Plugging the expression for $a_0$ into (22) we obtain

$$\begin{aligned}
E_0 &= \frac{7\hbar^2}{10m}\frac{m\omega}{\sqrt{7}\hbar} + \frac{m\omega^2}{10}\frac{\sqrt{7}\hbar}{m\omega} \\
&= \frac{\sqrt{7}hw}{5} \\
&= 0.529\hbar\omega
\end{aligned} \tag{24}$$

## Comparison

| Trial Wave Function | $E_0$ | Deviation from $E_0 = 0.5\hbar\omega$ |
|---|---|---|
| $\psi_1(x,a) = Ae^{-a\|x\|}$ | $0.707\hbar\omega$ | 41.4% |
| $\psi_2(x,a) = \dfrac{A}{(x^2+a)}$ | $0.707\hbar\omega$ | 41.4% |
| $\psi_3(x,a) = \dfrac{A}{(1+ax^2)^2}$ | $0.529\hbar\omega$ | 5.8% |




## Disclaimer

The variational method can also be used to find the approximate values for the energies of the first few excited states. However, these conditions can be included in the variational problem by means of Lagrange multipliers, that is, by means of a constrained variational principle. In this way, we can in principle evaluate any other excited state. However, the variational procedure becomes increasingly complicated as we deal with higher excited states. As a result, the method is mainly used to determine the ground state.

## References

[1] Zettili, Nouredine. 2009. *Quantum mechanics: concepts and applications.* Chichester, U.K.: Wiley.