Solution to the Schrodinger Equation for a Linear 1-D Potential

$$V(x) = \alpha|x|$$

Since the potential is symmetric, then the solutions can be taken to be either symmetric or antisymmetric. Therefore, we can solve the equation for only $x > 0$, and the boundary condition at $x = 0$ will be either $\psi(0) = 0$ (for antisymmetric solutions) or $\psi'(0) = 0$ (for symmetric solutions).

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \alpha x\psi = E\psi$$

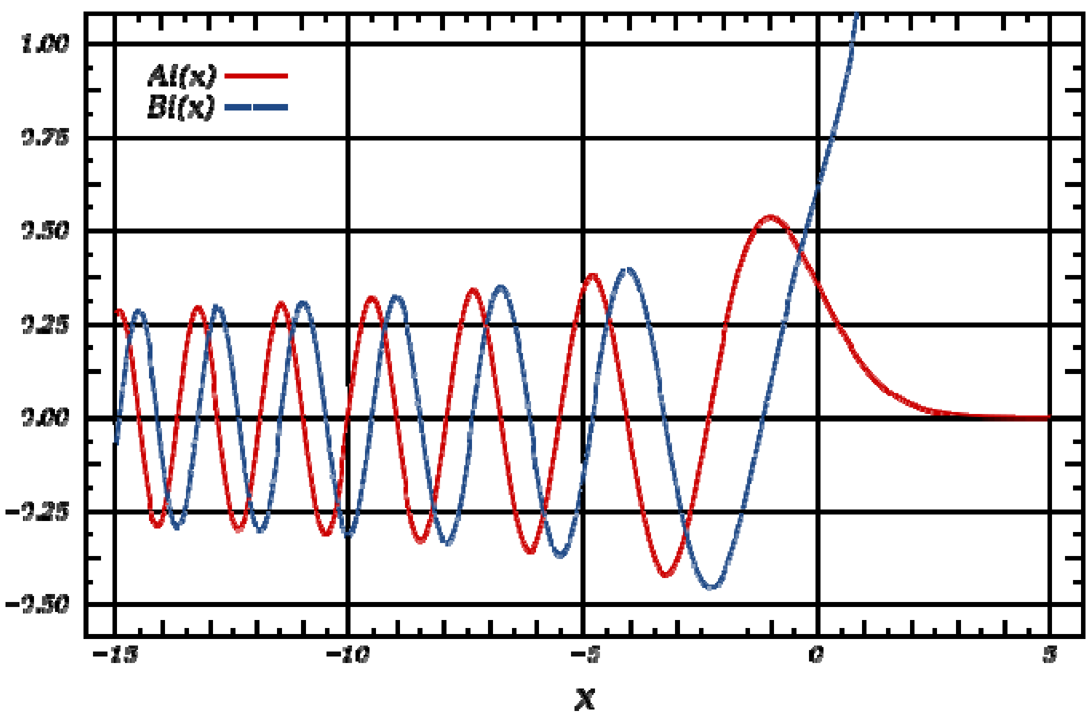
This can be rearranged as follows:

$$\frac{1}{\left(\frac{2m}{\hbar^2}\alpha\right)^{\frac{2}{3}}}\frac{d^2\psi}{dx^2} - \left(\frac{2m}{\hbar^2}\alpha\right)^{\frac{1}{3}}\left(x - \frac{E}{\alpha}\right)\psi = 0$$

Then it is clear that we want to make a change of variables $u \equiv \left(\frac{2m}{\hbar^2}\alpha\right)^{\frac{1}{3}}\left(x - \frac{E}{\alpha}\right)$, giving a neater looking equation

$$\frac{d^2\psi}{du^2} - u\psi = 0$$

which is known as the Airy equation. The solutions are the Airy functions $Ai(x)$ and $Bi(x)$ (1st kind and 2nd kind, respectively). For details, see http://en.wikipedia.org/wiki/Airy_function, from which the plot below was copied.



To satisfy the boundary condition at $x \to \infty$ it is clear that we must choose the Airy function of the first kind, $Ai(x)$. To satisfy the boundary condition at $x = 0$ we have to know the zeroes of the Airy function or its derivative. Suppose that u_i^0 is the set of all zeroes of the Airy function, $Ai(u_i^0) = 0$, and v_i^0 is the set of all zeros of the derivative of the Airy function, $Ai'(v_i^0) = 0$, in both cases for $i = 1,2,3 \cdots \infty$. The values for the zeros can be found in handbooks or solved for numerically.

Even solutions (including the ground state): the requirement $\psi'(0) = 0$ leads to $Ai'(u(0)) = 0$, for which the solutions are $u(0) = \left(\frac{2m}{\hbar^2}\alpha\right)^{\frac{1}{3}}\left(-\frac{E}{\alpha}\right) = v_i^0$, from which we can solve for the energy eigenvalues (with $n = 1,3,5 \cdots \infty$):

$$E_n = -\alpha v_{(n+1)/2}^0 \left(\frac{2m}{\hbar^2}\alpha\right)^{-\frac{1}{3}} = -v_{(n+1)/2}^0 \left(\frac{\hbar^2\alpha^2}{2m}\right)^{\frac{1}{3}}$$

Odd solutions: the requirement $\psi(0) = 0$, leads to $Ai\big(u(0)\big) = 0$, for which the solutions are $u(0) = \left(\frac{2m}{\hbar^2}\alpha\right)^{\frac{1}{3}}\left(-\frac{E}{\alpha}\right) = u_i^0$, from which we solve for the energy eigenvalues (with $n = 2,4 \cdots \infty$):

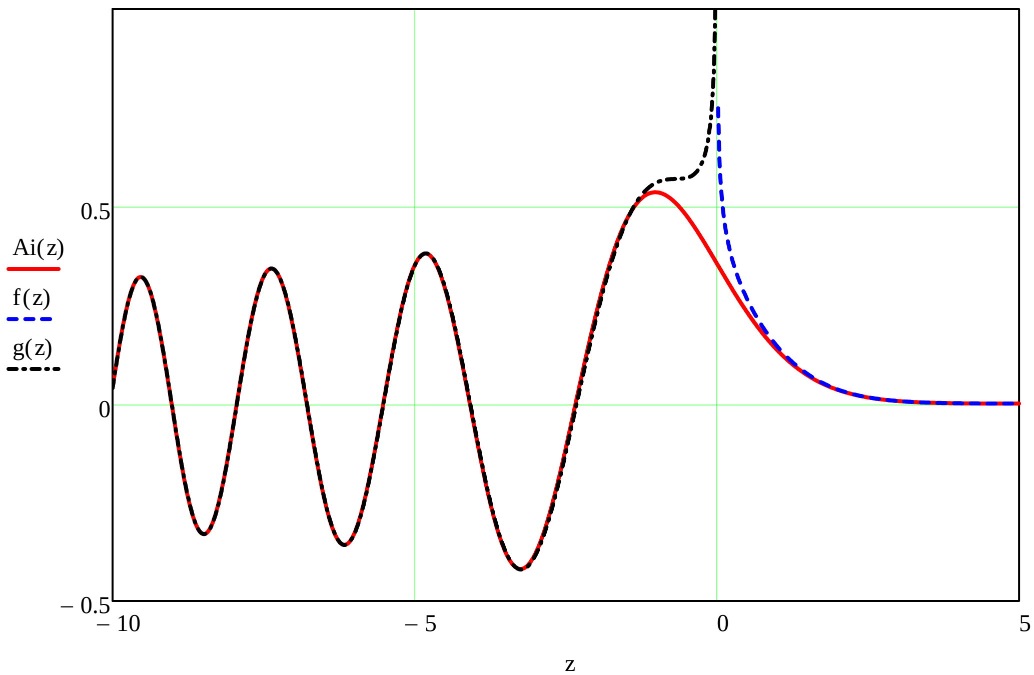
$$E_n = -\alpha u_{n/2}^0 \left(\frac{2m}{\hbar^2}\alpha\right)^{-\frac{1}{3}} = -u_{n/2}^0 \left(\frac{\hbar^2\alpha^2}{2m}\right)^{\frac{1}{3}}$$

Solutions of the Schrodinger equation for a symmetric, linearly sloping well V(x)=a*|x|

First some stuff on the Airy function of the first kind:

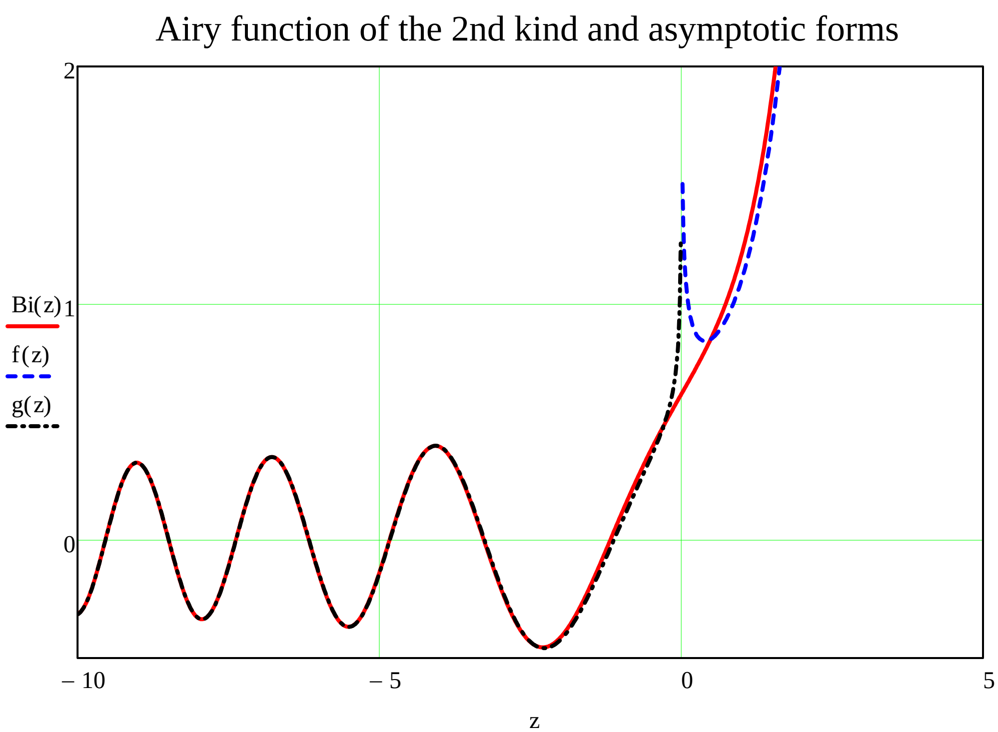
$$f(z) := \frac{1}{2\cdot\sqrt{\pi}\cdot z^{\frac{1}{4}}}\cdot e^{\frac{-2}{3}\cdot z^{\frac{3}{2}}} \qquad g(z) := \frac{1}{\sqrt{\pi}\cdot(-z)^{\frac{1}{4}}}\cdot\sin\left[\frac{2}{3}\cdot(-z)^{\frac{3}{2}} + \frac{\pi}{4}\right]$$

Airy function of the 1st kind and asymptotic forms



For completeness, here is the Airy function of the second kind (not used for a potential well):

$$f(z) := \frac{1}{\sqrt{\pi}\cdot z^{\frac{1}{4}}}\cdot e^{\frac{2}{3}\cdot z^{\frac{3}{2}}} \qquad g(z) := \frac{1}{\sqrt{\pi}\cdot(-z)^{\frac{1}{4}}}\cdot\cos\left[\frac{2}{3}\cdot(-z)^{\frac{3}{2}} + \frac{\pi}{4}\right]$$



Some approximations for getting the roots of the Ai(z) function and its derivative
(see Abramowitz & Stegun, Handbook of Mathematical Functions):

$$f(z) := z^{\frac{2}{3}}\cdot\left[1 + \frac{5}{48}\cdot z^{-2} - \frac{5}{36}\cdot z^{-4} + \frac{77125}{82944}\cdot z^{-6} + \left(-\frac{108056875}{6967296}\cdot z^{-8} + \frac{162375596875}{334430208}\cdot z^{-10}\right)\right]$$

$$x_0(n) := \mathrm{if}\left[n = 1, -2.338107, -f\left[3\cdot\pi\cdot\frac{(4\cdot n - 1)}{8}\right]\right]$$ Approximation from A&S for the roots of Ai.

$$g(z) := z^{\frac{2}{3}}\cdot\left(1 - \frac{7}{48}\cdot z^{-2} + \frac{35}{288}\cdot z^{-4} - \frac{181223}{207360}\cdot z^{-6} + \frac{18683371}{1244160}\cdot z^{-8} - \frac{91145884361}{191102976}\cdot z^{-10}\right)$$

$$xp_0(n) := \mathrm{if}\left[n = 1, -1.018793, -g\left[3\cdot\pi\cdot\frac{(4\cdot n - 3)}{8}\right]\right]$$ Approximation from A&S for the roots of the derivative of Ai.

Solution to the Schrodinger equation for a symmetric linear potential well:

$hbarc := 197$ Planck's constant times the speed of light in units of keV times picometers

$mc2 := 511$ Electron rest energy in keV

$$\alpha := \left(\frac{\sqrt{mc2}}{hbarc}\right) = 0.115 \qquad V(x) := \alpha\cdot|x|$$

The eigenvalues are found by requiring the derivative of psi to be zero at the origin (for the even solutions, including the ground state) or requiring pzi to be zero at the origin (for the odd states). This amounts to finding the zeroes of the Airy function or its derivative, using the approximate formulas found above.

$$E(n) := \mathrm{if}\left[\mathrm{mod}(n,2) = 0, -\left(\frac{hbarc^2\cdot\alpha^2}{2\cdot mc2}\right)^{\frac{1}{3}}\cdot x_0\left(\frac{n}{2}\right), -\left(\frac{hbarc^2\cdot\alpha^2}{2\cdot mc2}\right)^{\frac{1}{3}}\cdot xp_0\left(\frac{n+1}{2}\right)\right]$$

$m := 1 .. 15$ $E(m) =$

0.809
1.856
2.578
3.245
3.826
4.382
4.892
5.387
5.851
6.305
6.737
7.161
7.568
7.969
8.356

List of the first 15 energy eigenvalues

Variational result for the ground state (Problem 7.1): $b := \left(\frac{mc2\cdot\alpha}{\sqrt{2\pi}\cdot hbarc^2}\right)^{\frac{2}{3}} = 7.136\times10^{-3}$

$$E_{gs} := \frac{3}{2}\cdot\left(\frac{\alpha^2\cdot hbarc^2}{2\pi\cdot mc2}\right)^{\frac{1}{3}} \qquad E_{gs} = 0.813 \qquad \psi_{trial}(x) := \left(\frac{2\cdot b}{\pi}\right)^{\frac{1}{4}}\cdot e^{-b\cdot x^2}$$

Plot the solution

$a := 0$ $\quad b := 40$ $\quad n := 1$ Plot range and eigenvalue choice

$$\beta := \left(\frac{2\cdot mc2\cdot\alpha}{hbarc^2}\right)^{\frac{1}{3}} = 0.145$$

$$\psi(x) := Ai\left[\beta\cdot\left(x - \frac{E(n)}{\alpha}\right)\right]$$

The exact solution for the wave function (Airy function)

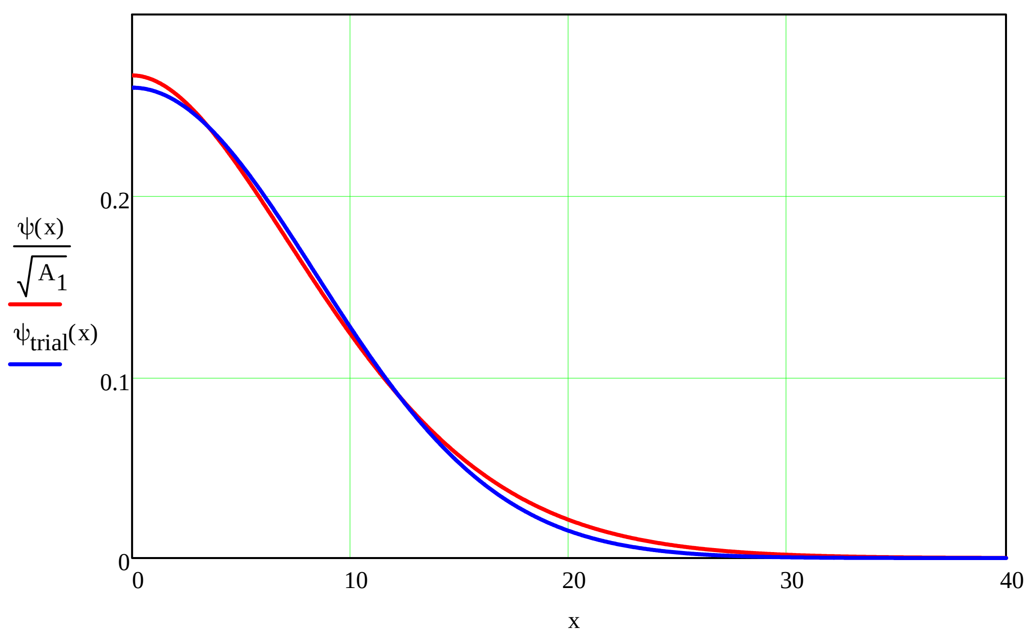
$$A_1 := 2\left[\int_0^{\infty} (|\psi(x)|)^2\, dx\right] = 4.044$$

Integral for the normalization factor

$\alpha = 0.115$

$n = 1$ $\quad E(n) = 0.809$ $\quad y_{max} := 0.3$

Two solutions to the linear potential



Solution to the 1D Schrodinger equation for a potential that goes as the 4th power of x, by numerical integration and by the variational method.

Units are keV, pm, and fs for Energy, Length, and Time respectively. These units keep all of the numbers near unity for the case of an electron in a nanometer scale well. Purely for convenience, I multiply hbar times c, the electron mass by c^2, and the frequency by 1/c. The factors of c all cancel out in the end.

$\mathrm{hbarc} := 197$ Planck's constant times the speed of light in units of keV times picometers

$\mathrm{mc2} := 511$ Electron rest energy in keV

$$\alpha := \left(\frac{\mathrm{mc2}}{\mathrm{hbarc}^2}\right)^2 = 1.734 \times 10^{-4}$$

Example choice of the strength of the potential

P.E. function:

$$V(x) := \alpha \cdot x^4$$

My solutions for the energies, in keV, of the first two states:

$E_0 := 0.667928 \qquad E_1 := 2.39362$

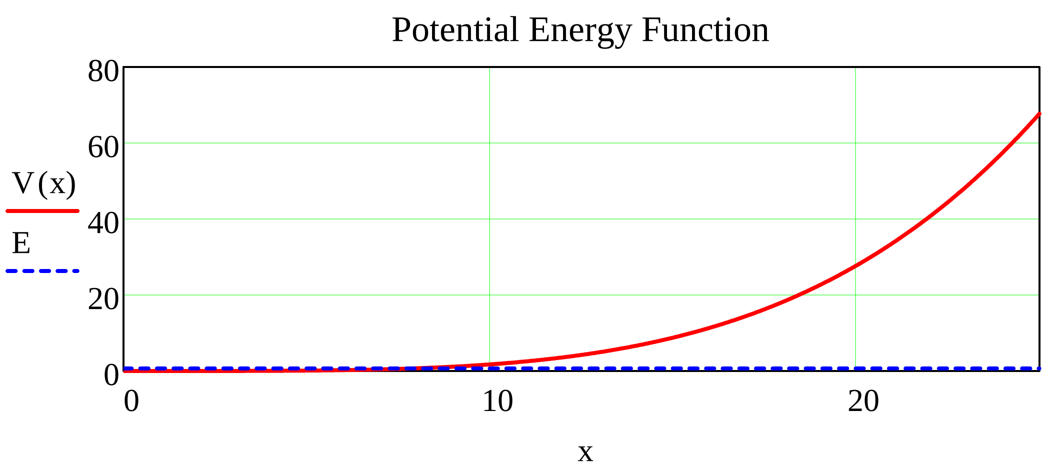
$a := 0 \qquad b := 25$

Range for the numerical integration. It is convenient to start from the center of the potential, because we know that there either the wave function must be zero (for odd solutions) or else its slope should be zero (for even solutions). The units here are picometers (pm).

Solution of the Schrodinger Equation by the shooting ("wag the dog") method

In the following, you have to adjust the energy by hand, look to see if the solution works, try a different value of energy if not, and so forth. Obviously this iteration could be automated by a program, but this is just for illustration.

$E := 0.667928$ The assumed energy of the solution to the time-independent Schrodinger equation. You have to home in on correct values by trial and error.



MathCad syntax for defining a set of differential equations to integrate (other options exist in MathCad for solving differential equations, but this is the most visually appealing syntax).

Given

$$\frac{d^2}{dx^2}\psi(x) + \frac{2mc2}{hbarc^2}(E - V(x)) \cdot \psi(x) = 0$$

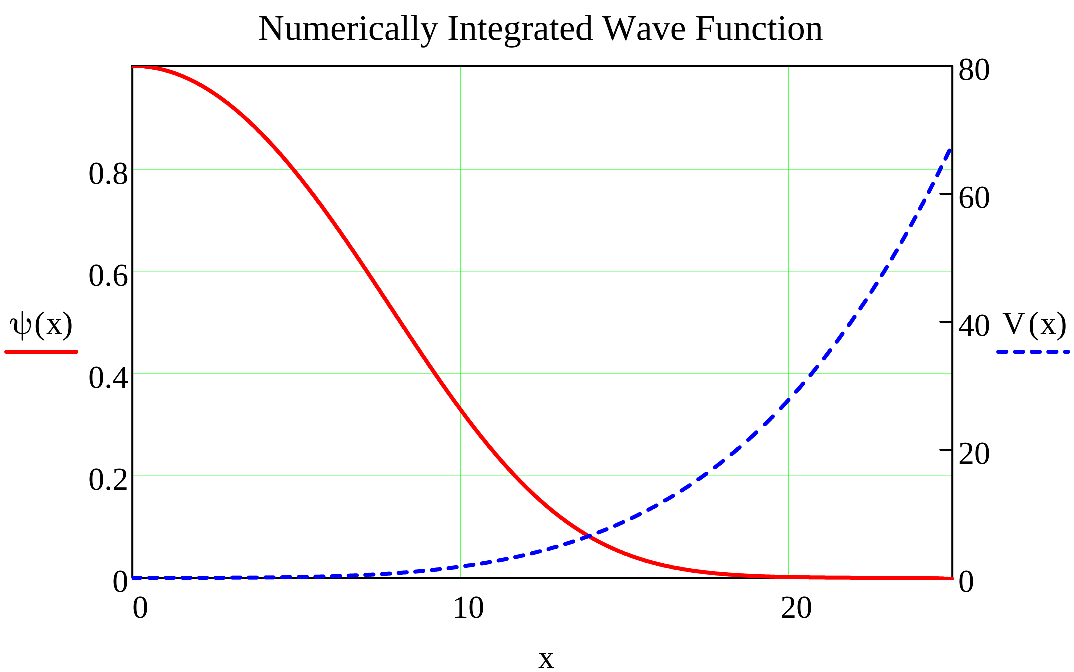
Time independent S.E. in 1D

$\psi(a) = 1$ $\psi'(a) = 0$

Conditions for starting the integration. The potential is even, so the ground state solution must be even and therefore have zero derivative at the origin. The first excited state is odd, so in that case the wave function is zero at the origin.

$\psi := \mathrm{Odesolve}(x, b)$

Solve the differential equation numerically. By default the Adams/BDF algorithm is used, but by right clicking on Odesolve you can choose other methods, such as 4th order Runge-Kutta with fixed or adaptive step size.



$E = 0.667928$

When the wave function approaches zero as x gets large, then we have a valid stationary state.

$$\mathrm{Norm} := 2\left(\int_0^b \psi(x)^2\, dx\right) = 12.349$$

Normalization factor for plotting below

Variational upper bounds:

Ground state:

Exact results below:

$$\frac{3}{4}\cdot\left(\frac{3\cdot\alpha\cdot hbarc^4}{4\cdot mc2^2}\right)^{\frac{1}{3}} = 0.681 \qquad E_0 = 0.668$$

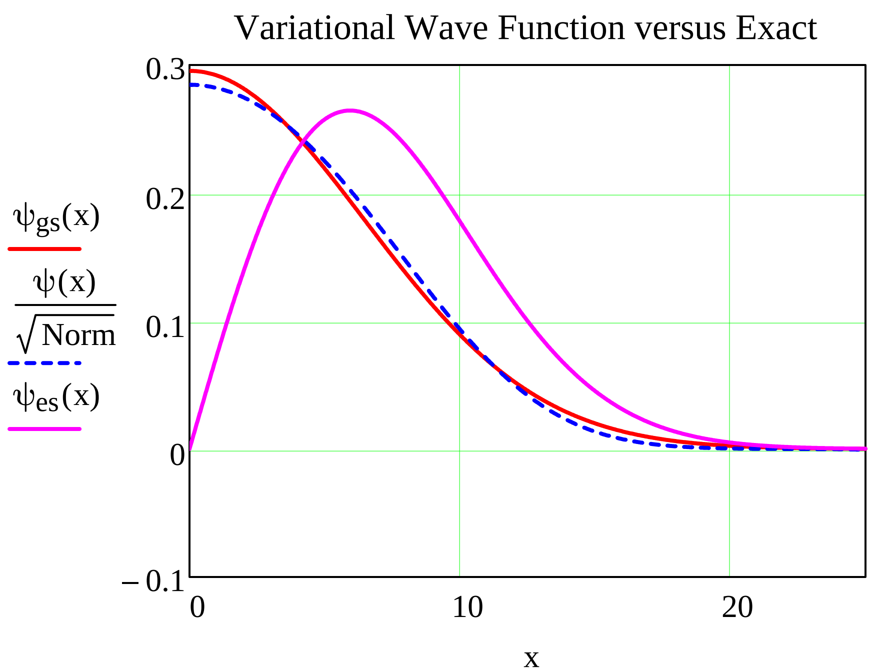
First excited state:

$$\frac{9}{4}\cdot\left(\frac{5\cdot\alpha\cdot hbarc^4}{4\cdot mc2^2}\right)^{\frac{1}{3}} = 2.424 \qquad E_1 = 2.394$$

The variational upper bounds were derived by taking the expectation value of a gaussian function for the ground states and x times a gaussian for the first excited state.

$$\beta_1 := \sqrt[3]{\frac{3}{4}\cdot\alpha\cdot\frac{mc2}{hbarc^2}} = 0.012 \qquad \beta_2 := \sqrt[3]{\frac{5\cdot\alpha\cdot mc2}{4\cdot hbarc^2}} = 0.0142$$

$$\psi_{gs}(x) := \left(\frac{2\cdot\beta_1}{\pi}\right)^{\frac{1}{4}}\cdot e^{-\beta_1\cdot x^2} \qquad \psi_{es}(x) := \sqrt{\frac{2}{\sqrt{\pi}}\left(2\cdot\beta_2\right)^{\frac{3}{2}}}\cdot x\cdot e^{-\beta_2\cdot x^2}$$



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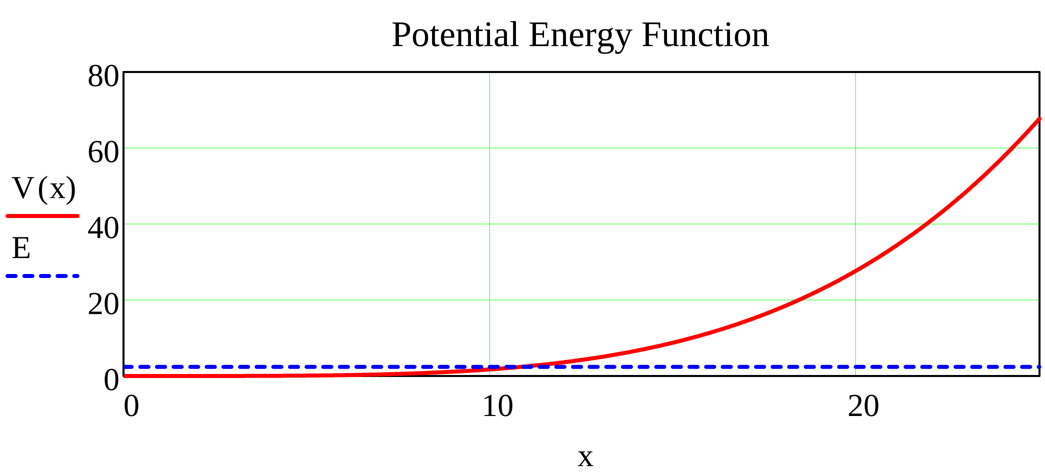

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Time independent S.E. in 1D

$$\psi(a) = 0 \qquad \psi'(a) = 1$$

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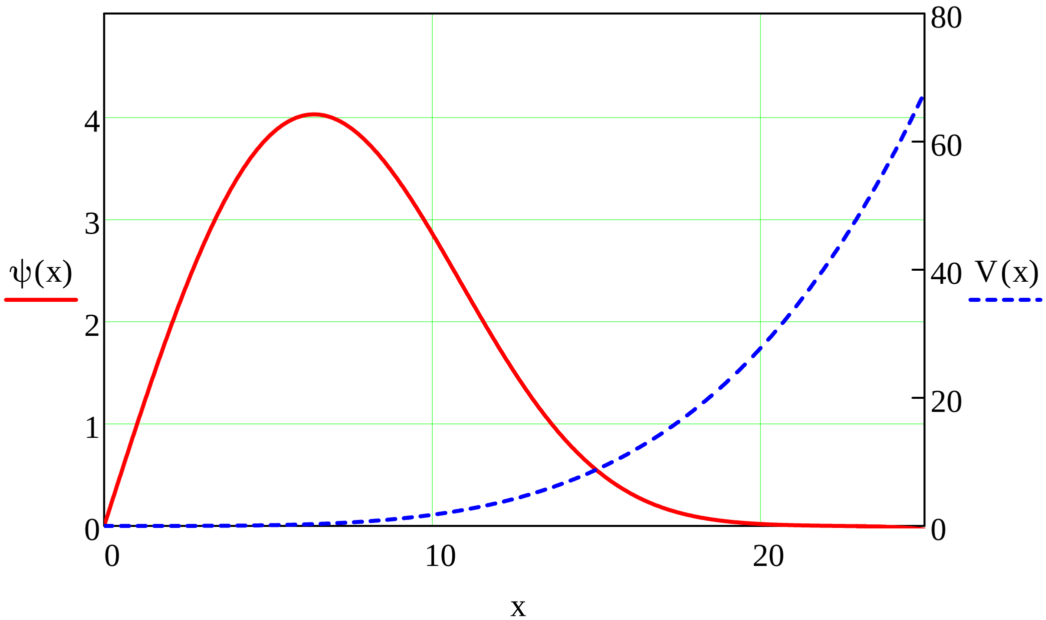
Numerically Integrated Wave Function



$$E = 2.39362$$

When the wave function approaches zero as x gets large, then we have a valid stationary state.

$$\mathrm{Norm} := 2\left(\int_0^b \psi(x)^2\, dx\right) = 228.39$$

Normalization factor for plotting below

Variational upper bounds:

Ground state:

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