Simple example of using the shooting method to determine the normalized wavefunction of a bound particle

Always start a worksheet with "restart". Hence you can !!! at any time to recalculate the worksheet.

> *restart*;

Write out the time dependent wave function with the potential energy expression:

> $Seq := -\frac{\hbar^2}{2 \cdot m} \cdot diff(\psi(x), x, x) + U(x) \cdot \psi(x) = E \cdot \psi(x);$

$U(x) := \frac{1}{4} \cdot \beta \cdot x^4;$

$$Seq := -\frac{1}{2} \frac{\hbar^2 \left(\frac{d^2}{dx^2} \psi(x)\right)}{m} + U(x)\, \psi(x) = E\, \psi(x)$$

$$U := x \rightarrow \frac{1}{4} \beta x^4 \qquad \textbf{(1)}$$

Define initial conditions assuming the symmetry of the problem (this is the first excited state).

> $ic := \psi(0) = 0, D(\psi)(0) = \psi slope;$

$$ic := \psi(0) = 0, D(\psi)(0) = \psi slope \qquad \textbf{(2)}$$

Make sure all constants are defined except for E

> $\hbar := 1 : m := 1 : \beta := 1 :$

$\psi slope := 1 :$

Use the shooting method to obtain a value for E. Test the accuracy of the trial E by plotting the wave function - does it approach 0 at the boundaries?

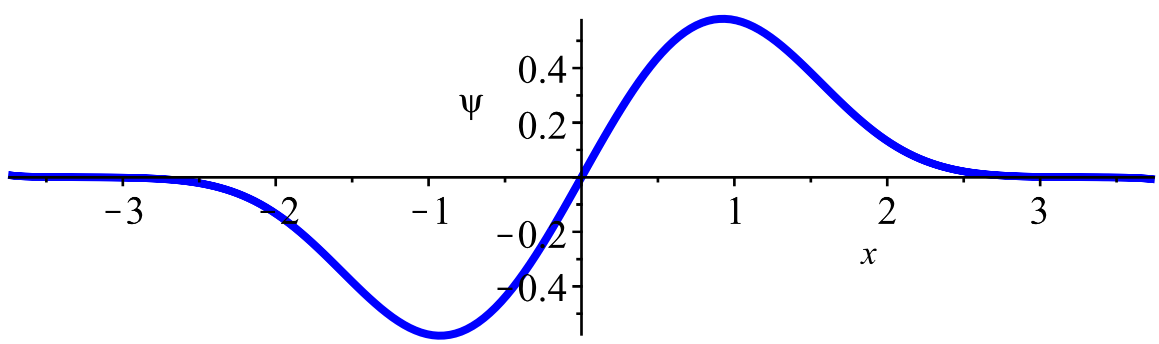
> $Etrial := 1.507902 :$

solution_procedures := *dsolve*([*eval*(*Seq*, *E* = *Etrial*), *ic*], [psi(*x*)],
numeric,
output = *listprocedure*);

> *L* := 3.75 : # *boundary. The larger L, the more significant digits required for E*

plots:-odeplot(*solution_procedures*, [*x*, ψ(*x*)], *x* = −*L*..*L*, *thickness* = 3, *color* = *blue*);

solution_procedures := [*x* = **proc**(*x*) ... **end proc**, ψ(*x*) = **proc**(*x*) ... **end proc**, $\frac{d}{dx}\psi(x)$ = **proc**(*x*) ... **end proc**]



Create a normalization integral and evaluate it. Do this by calling the procedure for calculating ψ(x) from the solution procedures. This integral is equal to the amplitude squared, A^2.
Solve for A.

> $Normalize\_integral := Int\left(\left(eval\left(\psi(x), solution\_procedures\right)(x)\right)^2, x=-L..L\right);$

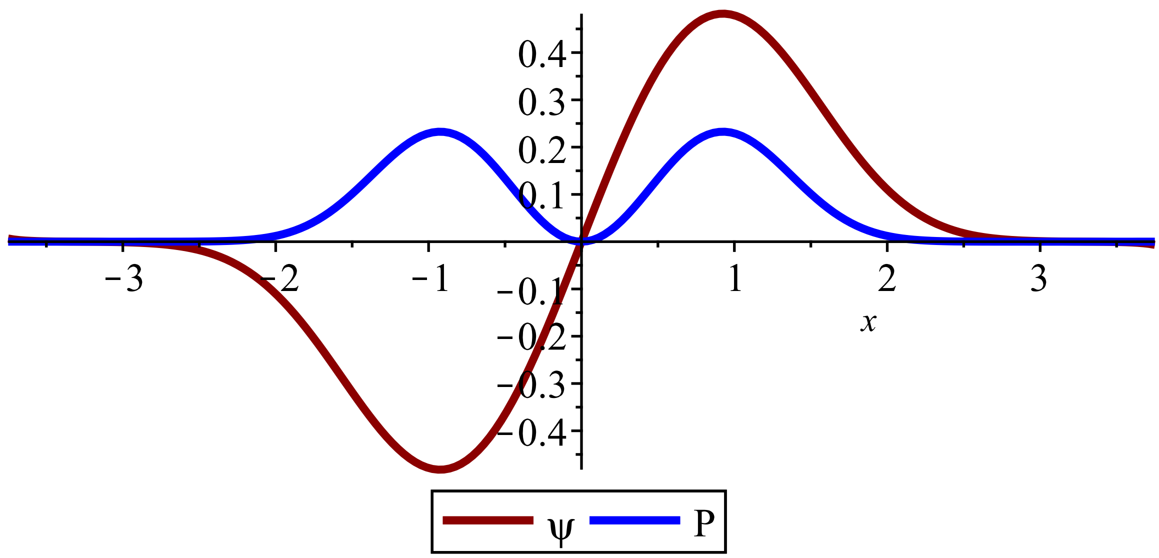
$A := evalf(Normalize\_integral)^{\frac{1}{2}};$

$$Normalize\_integral := \int_{-3.75}^{3.75} psi(x)(x)^2 \, dx$$

$$A := 0.830750142340569 \quad (3)$$

Show a plot ψ and ψ^2 once the system is normailzed:

> $plots\text{:-}odeplot\big(solution\_procedures,$
$[[x, A\cdot \mathrm{psi}(x)], [x, (A\cdot \mathrm{psi}(x))^2]], x=-L..L,$
$thickness=3, color=[\text{"DarkRed"}, blue], legend=[\text{"}\psi\text{"}, \text{"P"}]\big);$



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