# Numerical Solutions to the Schrö dinger Equation

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## Initialization

```
In[1]:= << Notation`;
        << PlotLegends`;

In[3]:= Developer`SetSystemOptions["EvaluateNumericalFunctionArgument" → False];
        Symbolize[a₊]
        Symbolize[a₋]
        Symbolize[α₁]
        Symbolize[α₂]
        Symbolize[β₂]
        Symbolize[k₀]
        Symbolize[σ₀]
        Symbolize[x₀]

In[12]:= a₊[f_] := Simplify[-D[f, q] + q f]
         a₋[f_] := Simplify[D[f, q] + q f]
         ψ0 = (1 / √π)^(1/2) Exp[-q^2 / 2];
         ψ[n_, q_] := Nest[a₊, ψ0, n] / Product[√(2 (i + 1)), {i, 0, n - 1}]
```

**Note to the student**

All the exercises in this notebook call for written responses not just code. You should clearly explain what you are doing, why you are doing it and why you believe (or don't believe) your results. You should discuss what your results mean and if appropriate what further lines of investigation might be fruitful.

***What to do if the code does not work***

This notebook is designed to run with *Mathematica* 6.0 to 7.01 . The code will probably work in higher versions of *Mathematica*, but large portions of the code will not work in version 5.2. If the code does not work in versions 6.0 or 7.01 the problem is almost certainly one of two things: 1) you forgot to run a line of code earlier in the notebook or 2) you used a variable or a name that is used for another propose in the notebook, and you now have a naming conflict.

**Note to the instructor**

I have tried to arrange the material in this notebook so that it can be used in a flexible manner. If you are short on time you can stop at the end of the section on eigenvalue problems. If you do this, the material can be covered in two weeks or less. But you will need to come up with a project for the students since both suggested projects involve the time-dependent behavior of wave packets. One possibility is to combine problems three and four into a project. The sections on wave packet splitting and charge oscillation are independent and depending on time and interest you may cover one or both.

**Prerequisites**

***Software***

Students should have a basic familiarity with *Mathematica*. They do not need to be *Mathematica* experts but they do need to know how to run code, make simple plots and understand the basics of *Mathematica* syntax.

***Mathematics***

The minimum mathematics prerequisite is a full year of calculus and an understanding of what a differential equation is and what an initial value problem is. Students should also have been exposed to the concept of an eigenvalue problem. Ideally students will have had or be currently enrolled in a course in differential equations.

***Physics***

The minimum physics prerequisite is a full year of calculus-based physics with a co-requisite of modern physics or an introductory quantum mechanics course. In particular, students need to have seen the Schrö dinger equation before. If they have not the instructor will have to introduce the Schrö dinger equation.

**Module Objectives**

After completion of this module students should:

- Understand how to solve an initial value problem numerically.
- Understand the difference between an initial value problem and a boundary value problem.
- Understand how to solve an boundary value problem numerically.
- Understand how to solve an eigenvalue problem numerically.
- Understand how to implement the method of lines.
- Understand how to check the accuracy of their solutions.
- Have developed a better intuition about wave functions and time dependent quantum phenomena.
- Have been exposed to topics in wave packet dynamics that are of current research interest.

**Competencies covered in this notebook**

***Modeling***

1.3 Create a conceptual model
1.4 Examine various mathematical representations of functions
1.5 Analyze issues in accuracy and precision
1.7 Demonstrate computational programming utilizing a higher level language

**Programming and Algorithms**

3.1 Describe the solution methodology for first-order linear differential and difference equations

**Numerical Methods**

4.4 Analyze techniques for computing eigenvalues-eigenvectors
4.6 Describe numerical methods for Ordinary Differential Equations
4.7 Describe numerical methods for Partial Differential Equations

# Introduction

Studying quantum mechanics in one-dimension allows you to learn the basics of quantum mechanics and to develop your quantum intuition without some of the mathematical complexities present in three-dimensions. In the old days (before 1974) one- dimensional quantum mechanics problems were just textbook problems, without real world applications. However in 1974 Dingle, Wiegmann and Henry at Bell Labs made a particle in a box [1]. Now experiments on one-dimensional quantum systems are common place. One-dimensional quantum systems lie at the heart of semiconductor devices such as quantum-well lasers [2]. In this module the methods needed for the numerical solution of the Schrö dinger equation are developed, and then used to model realistic semiconductor devices. We will also be interested in modeling the dynamics of wave packets in quantum wells since this is an area of great interest experimentally.

## The Schrö dinger Equation

We will very briefly review the Schrö dinger equation. If you are completely unfamiliar with the Schrö dinger equation you should consult a textbook on modern physics such as Thornton and Rex [3] or an introductory book on quantum mechanics such as Phillips [4]. Quantum mechanics tells us that particles have wave-like behavior and the Schrö dinger equation is the wave equation which describes this behavior.

### The time-dependent case

The one-dimensional Schrö dinger equation for a particle in a time-independent potential is

$$\frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+V(x)\Psi(x,t)=i\hbar\frac{\partial\Psi(x,t)}{\partial t}, \tag{0.1}$$

where $m$ is the mass of the particle, $V(x)$ is the potential that the particle moves in, and $\Psi(x, t)$ is the particle's wave function. The physical interpretation of the wave function is that $\Psi^*(x, t)\Psi(x, t)\,dx$ is the probability of finding the particle between $x$ and $x + dx$. The notation $\Psi^*$ denotes taking the complex conjugate which means that everywhere an $i$ appears in $\Psi$ you replace it by $-i$. For example if $\Psi(x, t) = e^{i(kx-\omega t)}$ then $\Psi^*(x, t) = e^{-i(kx-\omega t)}$ . In general the wave function $\Psi$ will be complex, not real.

For bound state problems we generally require that the wave function be normalized, which is to say that $\int\Psi^*(x, t)\Psi(x, t)\,dx = 1$ where the integral runs over all possible values of $x$. This condition simply means that if we look everywhere, we find the particle once and only once.

In quantum mechanics a particle does not have a definite position (at least not until we measure the particles position) but only has a probability of being found at a position. If we have a million hydrogen atoms all in the ground state and we measure the position of the electron in all million atoms, we will get a different answer for each atom. It does not make sense to talk about a definite position in a quantum system but only an average position. Since $\Psi^*(x, t)\Psi(x, t)$ is the probability distribution, the average position of a particle is $<x>=\int\Psi^*(x, t)\,x\,\Psi(x, t)\,dx$. In quantum mechanics angular brackets are used to denote an average. In general, the average or expectation value of an observable $O$ is $<O>=\int\Psi^* O\Psi\,dx$ and order matters! You can not interchange the operator $O$ and $\Psi^*$ or $\Psi$ except in special cases.

## The time-independent case

If the potential is time independent we can separate the time-dependent Schrö dingerequation into a spacial part and a temporal part. We look for a solution of the form $\Psi(x, t) = \psi(x)\,T(t)$. Substituting this into equation (0.1) gives

$$-\frac{\hbar^2}{2m}(1/\psi(x))\frac{d^2\psi(x)}{dx^2}+V(x) = \frac{i\hbar}{T(t)}\frac{dT(t)}{dt}. \tag{0.2}$$

Since the left-hand side depends only on $x$ and the right-hand side depends only on $t$, each side must be equal to a constant which we will call $E$. This gives

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\,\psi(x) \tag{0.3}$$

and

$$\frac{dT(t)}{dt}=(-i/\hbar)\,E\,T(t)\ . \tag{0.4}$$

Equation (0.4) is solved by $T(t) = A\,e^{-iEt/\hbar}$ and equation three is the time-independent Schrö dingerequation. In general, equation (0.3) cannot be satisfied for arbitrary values of $E$ but only for certain particular values of $E$. These values are known as the eigenvalues of the operator $\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)$ and are the allowed energies. The associated wave functions are known as the eigenfunctions.

### Particle in a box

This is best illustrated with an example. The simplest case is a particle in a one-dimensional box or infinite well of length $L$. The potential is

$V(x) = \begin{cases} \infty & x<0 \\ 0 & 0<x<L \\ \infty & x>L \end{cases}$ and is shown below in figure 1.

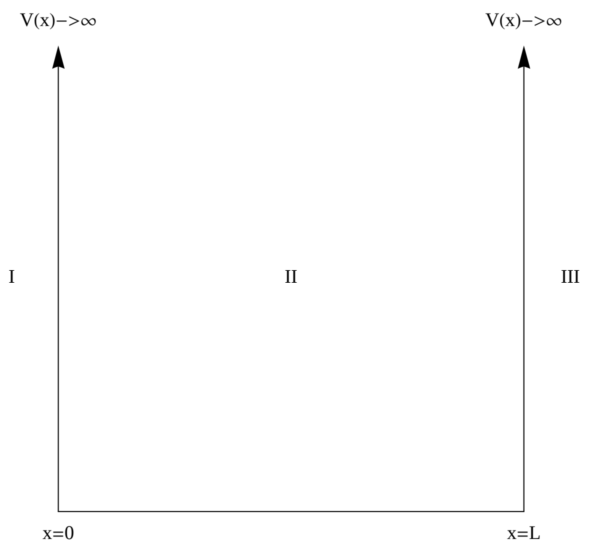


Figure1: An infinite potential well. The wave function must vanish in regions I and III and thus must vanish at the well boundaries..

In region II the time-independent Schrödinger equation is
$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\,\psi(x)$ which we can write as $\frac{d^2\psi(x)}{dx^2} + k^2\,\psi(x) = 0$ where $k^2 = 2\,m\,E/\hbar^2$. Note that $k$ has units of inverse length and is a wave-number. This is just the equation for a harmonic oscillator and thus has solutions $\psi(x) = A\,\cos(k\,x) + B\sin(k\,x)$. We need $\psi(0) = 0 \Rightarrow A = 0$. At the right boundary $\psi(L) = 0 \Rightarrow \sin(k\,L) = 0$. Thus, $k = n\,\pi/L$ where $n$ is a positive integer. Therefore $E = k^2\,\hbar^2/(2\,m) = n^2\,\hbar^2\,\pi^2/(2\,m\,L^2)$. Notice that it is the boundary conditions that give rise to the quantization of the energy levels. The remaining constant $B$ is fixed by the normalization condition $\int_0^L \psi^*\,\psi\,dx = 1 \Rightarrow B^2 \int_0^L \sin^2(n\,\pi\,x/L)\,dx = 1 \Rightarrow B = \sqrt{2/L}$ .

In practice we will be interested not in infinite wells, but in finite wells such as the well shown in Figure 2. The potential for a finite well is
$$V(x) = \begin{cases} 0 & x < 0 \\ -V_0 & 0 < x < L \\ 0 & x > L \end{cases}$$ where $V_0 > 0$.

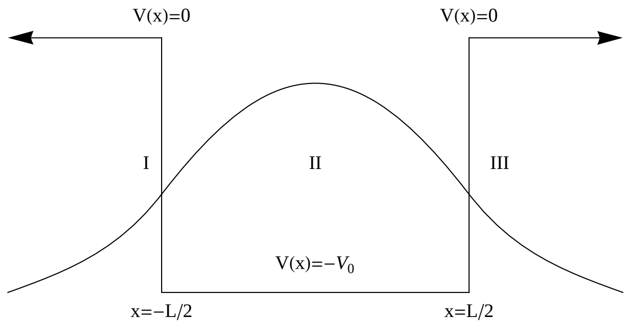


Figure 2: A finite well of depth $V_0$ and the ground state wave function. For a finite well there is a non-zero probability that the particle will be found outside the well. Since the ground state has an energy that is less then zero the particle would be classically forbidden in regions I and III. The wave function always falls off exponentially in classically forbidden regions.

**How do you make a quantum well?**

The quantum well studied by Dingle, Wiegmann and Henry was made by sandwiching a thin (on the order of 10-50 nanometers) layer of Gallium-Arsenic (GaAs) between two thick layers of Aluminum-Gallium-Arsenic (AlGaAs). This results in a quasi-one-dimensional well. Such wells are called quasi-one-dimensional because the charge carriers which could be electrons and or holes are free to move to the plane of the GaAs layer but are confined at the boundaries provided by the AlGaAs slabs. The physics of how the height of the well depends on the composition of the semiconductor is somewhat involved and would take us to far afield. Interested readers should consult Bastard [5] or Weisburch and Vinter[2].

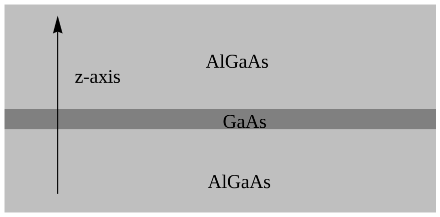


Figure 3: Schematic drawing of a single quantum well. Electrons and holes are free to move in the *x* and *y* directions but are confined in the *z* direction.

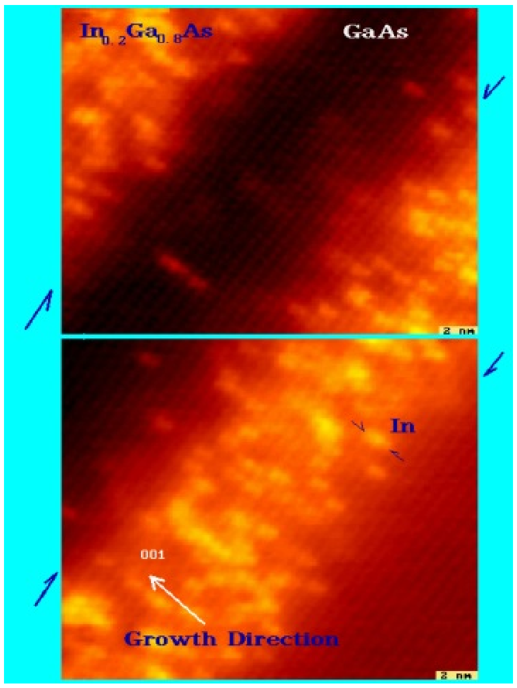
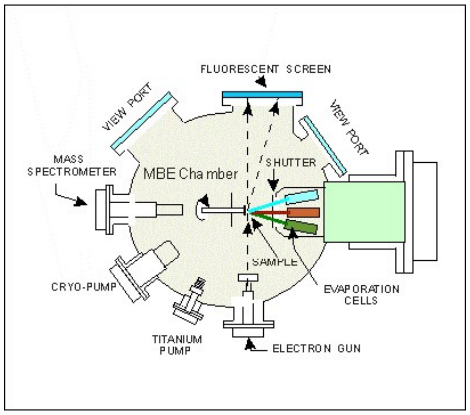


Figure 4: An image taken with a scanning tunneling microscope (STM) of a slice of a $In_{0.2}Ga_{0.8}As/GaAs$ multiple quantum well structure. Image is from Nikos Jä ger'sweb page.

One way to make a quantum well in the lab is to use molecular beam epitaxy or MBE. You can think of an MBE machine as a very high-tech and expensive paint sprayer. An MBE machine allows you to sputter materials onto a substrate in a vacuum. As a result you have good control over both the composition and thickness of the layers. A more detailed but accessible account of molecular beam epitaxy can be found in Ibach and Lüth [6]. If you lay down multiple thin layers of GaAs separated by thin layers of AlGaAs you can make multiple quantum wells. By varying the composition you can vary the depth of the wells. One can also make barriers. Although AlGaAs/GaAs is a popular choice, one can use other semiconductors. The well structure shown in figure 4 uses InGaAs/GaAs.



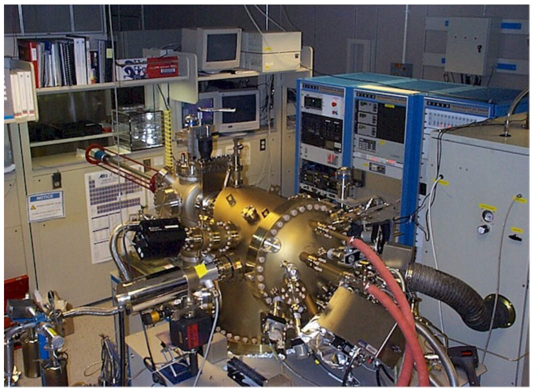


Figure 5: The left figure is a schematic of an MBE machine.Figure from http://users.rcn.com/qsa/waveeng.html.  On the right is a picture of Professor Andrew Steckel's MBE machine at the University of Cincinnati. Photograph is from http://www.nanolab.uc.edu/.

## Numerical Solutions of Initial Value Problems

Before we can understand how to find the eigenvalues of an operator numerically, we must first understand how to solve an initial value problem numerically.

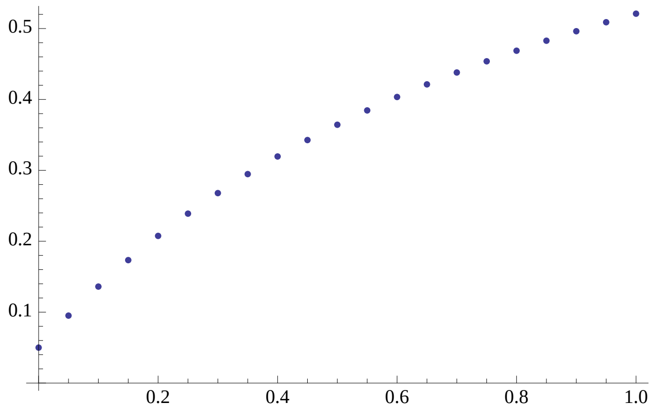
### The Euler method

Suppose we have a differential equation of the form $\mathrm{dy}(x)/\mathrm{dx} = f(x)$. If we replace $\mathrm{dy}/\mathrm{dx}$ by $(y[x_{i+1}] - y[x_i])/(x_{i+1} - x_i)$ then we can write $y[x_{i+1}] = (x_{i+1} - x_i)\, f(x_i) + y[x_i]$. This is the simplest method for numerical solution of a differential equation and is known as Euler's method.

```
Clear[Euler]
    Euler::usage = "Euler[f,y,y0,{t,tmin,tmax},n]  solves the differential equation
        dy/dt =f subject to the initial condition y[0]=y0 over the interval
     [tmin,tmax] using n steps and plots solution.The default value of n is 20.";

            Euler[f_, y_, y0_, {t_, tmin_, tmax_}, n_: 20] := Module[{h, ydata, tdata, data},
        h = N[(tmax - tmin) / n];
        y[1] = y0;
        ydata = Join[{y[1]}, Table[y[i + 1] = y[i] + h f /. t → i, {i, 1, n}]];
        tdata = Table[t, {t, tmin, tmax, h}];
        data = Transpose[{tdata, ydata}];
        ListPlot[data]]
```

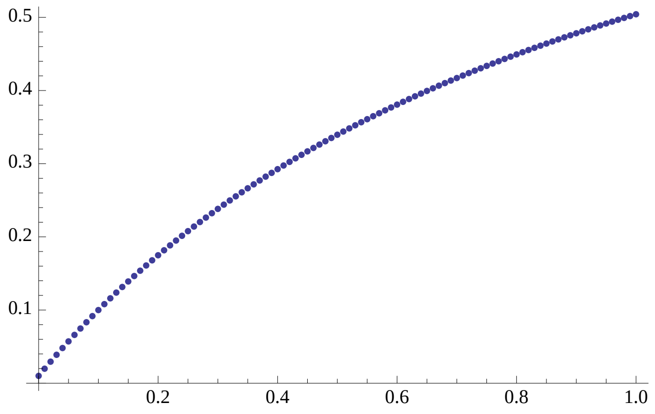
Here the Euler method is called on the equation $\mathrm{dy}(t)/\mathrm{dt} = (1 - y(t))^2$ with $y(0) = 0$. Twenty steps are taken over the interval zero to one.

```
plot1 = Euler[(1 - y[t])^2, y, 0, {t, 0, 1.}]
```



Here we take one hundred steps.

```
plot2 = Euler[(1 - y[t])^2, y, 0, {t, 0, 1.}, 100]
```



Our test equation is easy to solve exactly, so we can check the accuracy of our method.

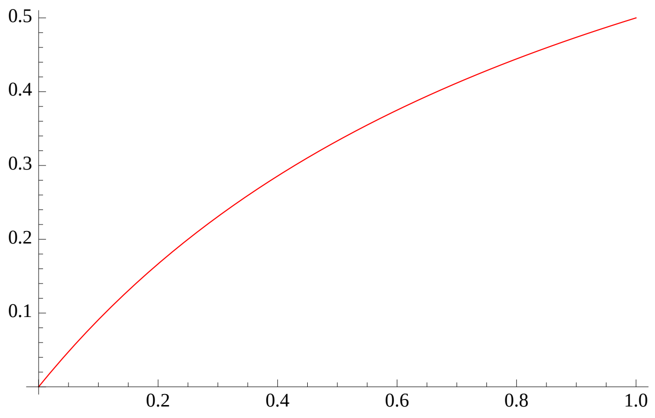
```
eqn = D[y[t], t] == (1 - y[t])^2
```

$y'[t] == (1 - y[t])^2$

```
Clear[y]
result =     First[DSolve[{eqn, y[0] == 0}, y[t], t]]
```

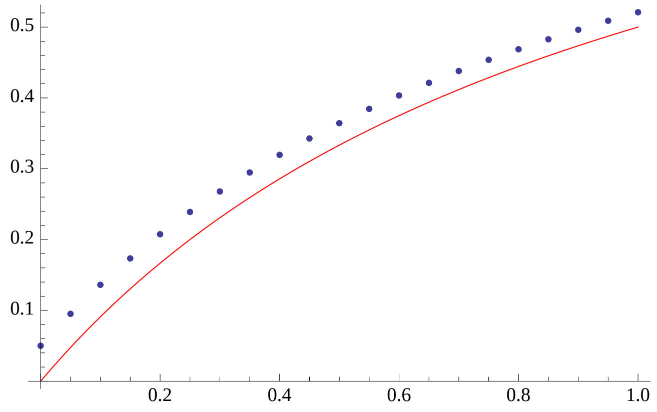
$\left\{y[t] \to \frac{t}{1+t}\right\}$

```
plot3 = Plot[y[t] /. result, {t, 0, 1}, PlotStyle -> RGBColor[1, 0, 0]]
```

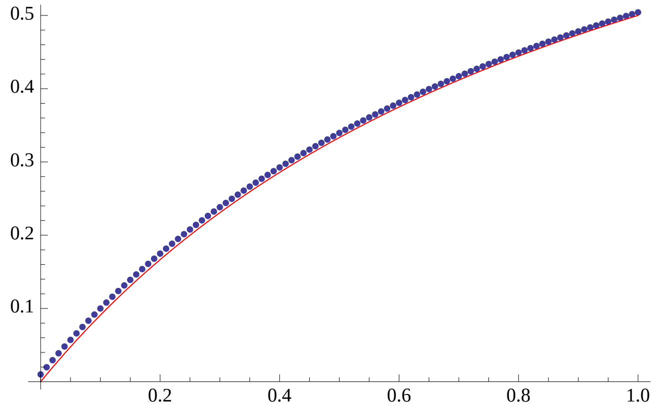


Comparing the exact solution (in red) with the numerical approximation shows that the method is not very accurate unless we take many steps.

```
Show[plot1, plot3]
```

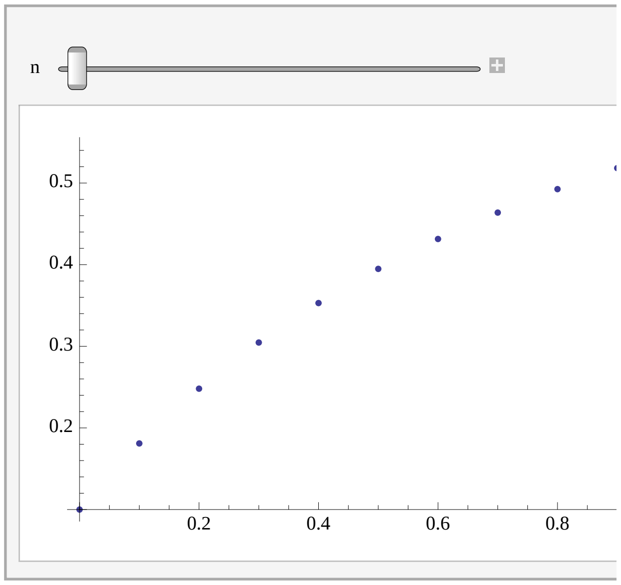


```
Show[plot2, plot3]
```



We can use Manipulate to explore how the accuracy for the solution depends on the number of points that we use.

```
Manipulate[Euler[(1 - y[t])^2, y, 0, {t, 0, 1.}, n], {n, 10, 100, 10}, SaveDefinitions → True]
```



***Exercise One***

Use the Euler method to solve the simple harmonic oscillator $\frac{d^2x(t)}{dt^2} + \omega^2 x(t) = 0$. Make a parametric plot of $x$ versus $v$ for several different step sizes. Comment on your result.

You should have noticed that convergence is slow (we need many steps) in the Euler method. We can do better by using a method that is higher order in $h$.

## Runge-Kutta methods

Once again consider $dy/dt = f(y, t)$ Now Taylor expand $y(t)$ about $\tau = t + h$. I will illustrate this by expanding to second order, but higher order expansions are common.

```
Clear[h];
equation1 = Simplify[Normal[Series[y[t + h], {h, 0, 2}]]]
```

$$y[t] + h\, y'[t] + \frac{1}{2} h^2 y''[t]$$

Since $y' = f$ and $y'' = df(y,t)/dt = \partial f/\partial t + (\partial y/\partial t)(\partial f/\partial y)$ we have

$$y(t+h) = y(t) + h\, f(y, t) + \left(h^2/2\right)(\partial f/\partial t + (\partial y/\partial t)(\partial f/\partial y)) \tag{0.5}$$

We can also formally write

$$y(t+h) = y(t) + \alpha_1 k_1 + \alpha_2 k_2 \text{ with } k_1 = h\, f(y, t) \text{ and } k_2 = h\, f(y + \beta_2 k_1, t + \beta_1 h) \tag{0.6}$$

where the $\alpha$'s and $\beta$'s are parameters to be determined by comparing equations (0.5) and (0.6) term by term. Doing this gives $\alpha_1 + \alpha_2 = 1$ and $\alpha_2 \beta_1 = \alpha_2 \beta_2 = 1/2$. Any choice for the $\alpha$'s and $\beta$'s that satisfies these equations will work. These methods are known as Runge-Kutta methods [7]. We can see exactly how works by expanding eq(0.6).

```
equation2 = y[t] + h α1 f[t, y[t]] + α2 h Series[f[t + h β1, y[t] + β2 h f[t, y[t]]], {h, 0, 2}]
```

$$y[t] + (\alpha_1 f[t, y[t]] + \alpha_2 f[t, y[t]])\, h + \alpha_2 \left(\beta_2 f[t, y[t]]\, f^{(0,1)}[t, y[t]] + \beta_1 f^{(1,0)}[t, y[t]]\right) h^2 + \frac{1}{2}\alpha_2 \left(\beta_2^2 f[t, y[t]]^2 f^{(0,2)}[t, y[t]] + 2\beta_2 f[t, y[t]]\, \beta_1 f^{(1,1)}[t, y[t]] + \beta_1^2 f^{(2,0)}[t, y[t]]\right) h^3 + O[h]^4$$

and using LogicalExpand to equate eq(1) and eq(2) term by term.

```
result = LogicalExpand[equation1 == equation2]
```

$$-\alpha_1 f[t, y[t]] - \alpha_2 f[t, y[t]] + y'[t] == 0 \;\&\&$$
$$\frac{y''[t]}{2} - \alpha_2 \left(\beta_2 f[t, y[t]]\, f^{(0,1)}[t, y[t]] + \beta_1 f^{(1,0)}[t, y[t]]\right) == 0 \;\&\&$$
$$-\frac{1}{2}\alpha_2 \left(\beta_2^2 f[t, y[t]]^2 f^{(0,2)}[t, y[t]] + 2\beta_2 f[t, y[t]]\, \beta_1 f^{(1,1)}[t, y[t]] + \beta_1^2 f^{(2,0)}[t, y[t]]\right) == 0$$

Keeping in mind that $y' = f(t, y)$ we see from the order $h^0$(first) equation that $\alpha_1 + \alpha_2 = 1$. To solve the order $h$ (second) equation remember that $y'' = df(y,t)/dt = \partial f/\partial t + (\partial y/\partial t)(\partial f/\partial y)$. We can use a replacement rule to make this substitution.

```
result /. D[y[t], {t, 2}] → D[f[t, y], t] + D[y[t], t] D[f[t, y], y]
```

$$-\alpha_1 f[t, y[t]] - \alpha_2 f[t, y[t]] + y'[t] == 0 \;\&\&$$
$$\frac{1}{2}\left(y'[t]\, f^{(0,1)}[t, y] + f^{(1,0)}[t, y]\right) - \alpha_2 \left(\beta_2 f[t, y[t]]\, f^{(0,1)}[t, y[t]] + \beta_1 f^{(1,0)}[t, y[t]]\right) == 0 \;\&\&$$
$$-\frac{1}{2}\alpha_2 \left(\beta_2^2 f[t, y[t]]^2 f^{(0,2)}[t, y[t]] + 2\beta_2 f[t, y[t]]\, \beta_1 f^{(1,1)}[t, y[t]] + \beta_1^2 f^{(2,0)}[t, y[t]]\right) == 0$$

Looking at the order $h$ equation we see that $1/2 - \alpha_2 \beta_1 = 0$ and $1/2 - \alpha_2 \beta_2 = 0$ as claimed.

In practice one commonly uses a fourth-order Runge-Kutta method with $y(t+h) = y(t) + (1/6)(k_1 + 2k_2 + 2k_3 + k_4)$where

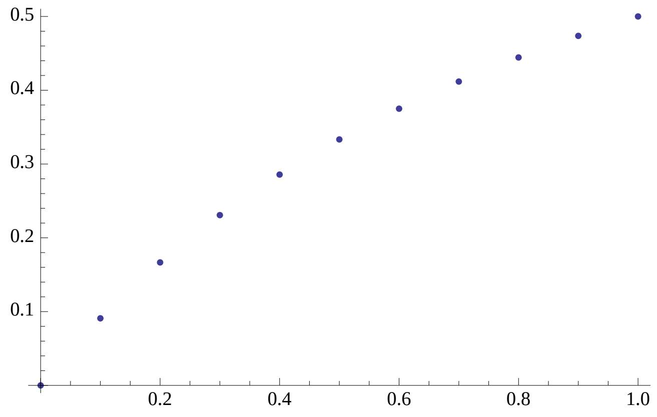
$k_1 = h\, f(y, t)$
$k_2 = h\, f(y + k_1/2, t + h/2)$
$k_3 = h\, f(y + k_2/2, t + h/2)$
$k_4 = h\, f(y + k_3, t + h)$

A simple fourth-order Runge-Kutta solver is implemented by the code below which is taken from Maeder[8].

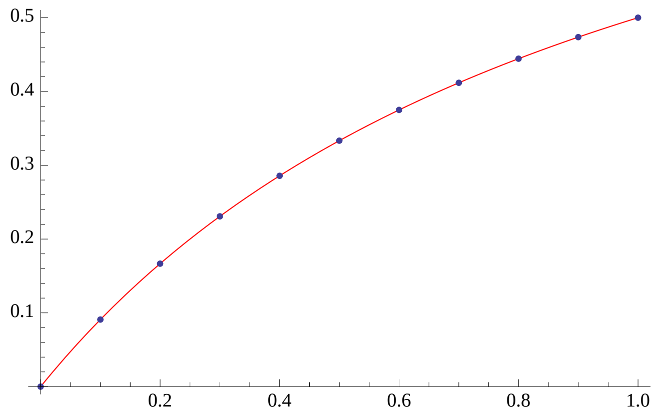
```
RKStep::usage =
 "RKStep[{f,y,y0,h]  uses a fourth order Runge-Kutta method to take a  single
   Runge-Kutta step of size h"; RKStep[f_, y_, y0_, h_] := Module[{},
  k1 = N[h f /. {y → y0}];
  k2 = N[h f /. {y → y0 + k1 / 2}];
  k3 = N[h f /. {y → y0 + k2 / 2}];
  k4 = N[h f /. {y → y0 + k3}];
  y0 + (1 / 6) (k1 + 2 k2 + 2 k3 + k4)]

Clear[RungeKutta]

RungeKutta::usage = "RungeKutta[{f,y,y0,{x,xmin,xmax},n]  uses a fourth order Runge-Kutta
    method to solve the differential equation
        dy/dx =f subject to the initial condition y[0]=y0 over the interval
    [xmin,xmax] using n steps and plots solution.The default value of n is 20.";


RungeKutta[f_, y_, y0_, {t_, tmin_, tmax_}, n_: 20] := Module[{h, ydata, tdata, data},
        h = (tmax - tmin) / n;
  tdata = Table[t, {t, tmin, tmax, h}];
  k1 = N[h f /. {y → y0}];
  k2 = N[h f /. {y → y0 + k1 / 2}];
  k3 = N[h f /. {y → y0 + k2 / 2}];
  k4 = N[h f /. {y → y0 + k3}];
  ListPlot[Transpose[{tdata, NestList[RKStep[f, y, #, h] &, y0, n]}]]]
```

Note the dramatic improvement in accuracy.

```
plot4 = RungeKutta[(1 - y)^2, y, 0, {t, 0, 1}, 10]
```



```
Show[plot3, plot4]
```

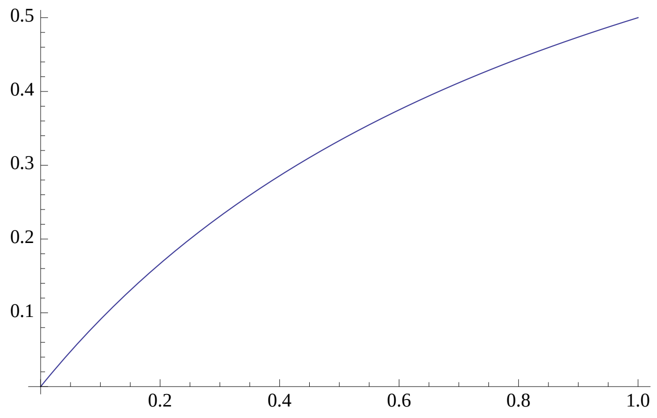


We will in general use NDSolve to solve initial value problems.

```
Clear[y]
result = NDSolve[{D[y[t], t] == (1 - y[t])^2, y[0] == 0}, y[t], {t, 0, 1}]
```

```
{{y[t] → InterpolatingFunction[{{0., 1.}}, <>][t]}}
```

```
Plot[y[t] /. result, {t, 0, 1}]
```



## Shooting Methods

Often we are interested in a boundary value problem rather than an initial value problem. For example suppose we want to solve $\frac{d^2 y}{d t^2} + 2\pi y = 0$ subject to the conditions that $y(0) = 0$ and $y(1) = 1/2$. How can we do that? We could pick an initial value for $y'(0)$, solve the initial value problem and compute $y(1)$. The value for $y(1)$ will of course be wrong. Pick a new value for $y'(0)$ and continue this process (using your favorite equation solver or minimization code) and continue until $y(1) = 1/2$. For example we pick (arbitrarily) $y'(0) = 1$and solve the initial value problem.

```
Clear[result]
result[t_] =
  First[y[t] /. NDSolve[{D[y[t], {t, 2}] + 2 π y[t] == 0, y[0] == 0, y'[0] == 1}, y[t], {t, 0, 1}]]
```

```
InterpolatingFunction[{{0., 1.}}, <>][t]
```

```
result[1]
```

```
0.236632
```

This gives a value for $y(1)$ of 0.23 which is too small. Try $y'(0) = 5$

```
Clear[result]
result[t_] =
 First[y[t] /. NDSolve[{D[y[t], {t, 2}] + 2 π y[t] == 0, y[0] == 0, y'[0] == 5}, y[t], {t, 0, 1}]]
result[
 1]
```

```
InterpolatingFunction[{{0., 1.}}, <>][t]

1.18316
```

This is too large. But, with the result bounded we can quickly iterate to a solution. Try it!

```
Clear[result]
result[t_] = First[
  y[t] /. NDSolve[{D[y[t], {t, 2}] + 2 π y[t] == 0, y[0] == 0, y'[0] == 2.113}, y[t], {t, 0, 5}]]
result[
 1]
```

```
InterpolatingFunction[{{0., 5.}}, <>][t]

0.500004
```

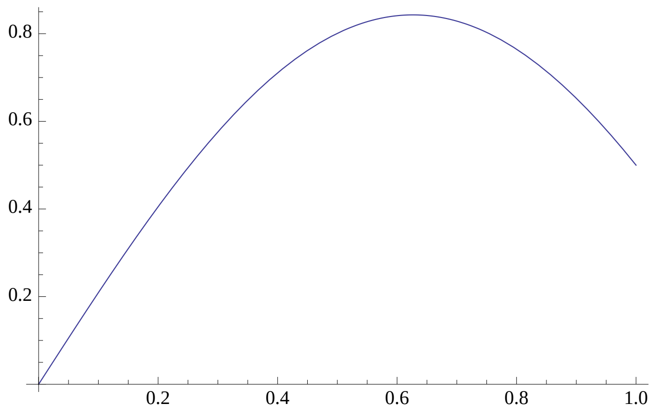
We can of course use an equation solver to do this for us.

```
Developer`SetSystemOptions["EvaluateNumericalFunctionArgument" → False];
shooting[equationList_List, y_[x_], {x_, xmin_, xmax_}, intialGuess_, yAtRightEnd_] :=
 Module[{result, solution},
  Clear[solution, result];
  solution[v_?NumericQ] :=
   NDSolve[Join[equationList, {y'[0] == v}], y[x], {x, xmin, xmax}][[1, 1, 2]];
  result = FindRoot[(solution[v] /. x → xmax) == yAtRightEnd,
     {v, intialGuess, 2 intialGuess}][[1, 2]];
  NDSolve[Join[equationList, {y'[0] == result}], y[x], {x, xmin, xmax}][[1, 1, 2]]
 ]
```

```
Clear[result]
result[t_] = shooting[{D[y[t], {t, 2}] + 2 π y[t] == 0, y[0] == 0}, y[t], {t, 0, 1}, 1, 1 / 2]
```

```
InterpolatingFunction[{{0., 1.}}, <>][t]
```

```
Plot[result[t], {t, 0, 1}]
```



***Exercise Two***

Use the code given below to visualize the shooting method. The variable "trials" is initialized to an empty list. Be sure you run this line of code.

```
trials = {};
```

We want to solve the boundary value problem $\frac{d^2 f(t)}{dt^2} + \sqrt{2}\ f(t) = 0,\ f(0) = 0,\ f(2\pi) = 1$ .

You can use the code below to explore how changing the value of $f'(0)$ changes the value of $f(2\pi)$. The target point will be shown in red. You should run the code several times with different values of $f'(0)$.

```
Clear[solution, v0]
v0 = Input["enter a value for V0"];

solution[t_] =
  NDSolve[{D[f[t], {t, 2}] + √2 f[t] == 0, f[0] == 0, f'[0] == v0}, f[t], {t, 0, 4 π}][[1, 1, 2]];
trials = AppendTo[trials, {{2 π, solution[2 π]}}];
plot1 = Plot[solution[t], {t, 0, 2 π}];
plot2 = ListPlot[trials, PlotStyle -> PointSize[0.025], PlotMarkers → Automatic];
Show[plot1, plot2, Graphics[{PointSize[0.025], RGBColor[1, 0, 0], Point[{2 π, 1}]}],
 PlotRange → All, PlotLabel → StringJoin["f[2π]=", ToString[solution[2 π]]]]
```

## Eigenvalue Problems

In quantum mechanics we frequently want to solve an eigenvalue problem. These are very much like shooting problems but harder. Suppose we want to find the bounds for a particle in a potential $V(x)$. To do this we must solve $-(\hbar^2/2m)\nabla^2\psi + V = E\psi$. If the wave function is to be normalizable it must go to zero at $\pm\infty$. We expect that this will happen only for certain values of E, the eigenvalues or allowed energies. The trick is integrate in from both the right and the left and vary E until you get a smooth join in the middle. More details on this method can be found in Pang [9]. We will assume that the wave function vanishes at sufficiently large distances.

### The Harmonic Oscillator

To see how this method works we will start by applying it to a simple harmonic oscillator. The time independent Schrö dingerequation for the harmonic oscillator is

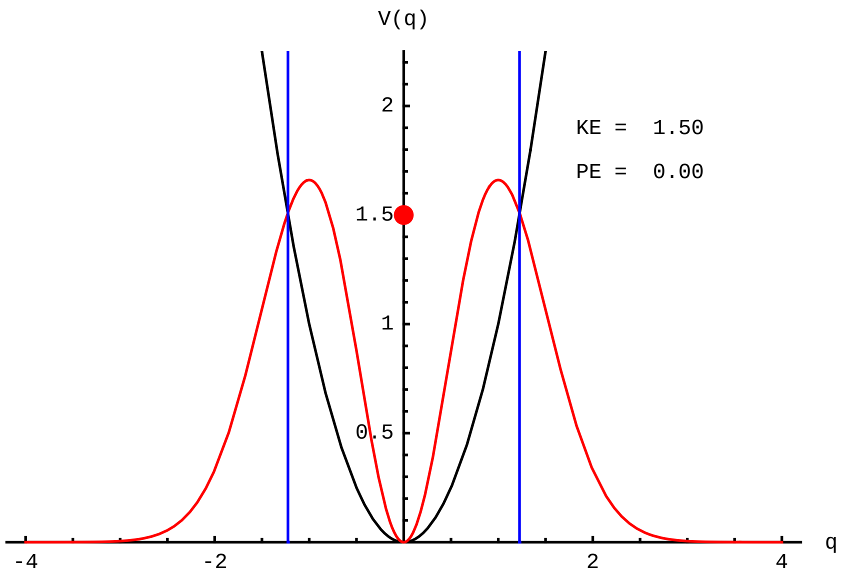
$$-(\hbar^2/2m)\frac{d^2\psi}{dx^2} + (1/2)kx^2\psi = E\psi. \tag{0.7}$$

The first step is to change to a dimensionless variable. This is always a good idea for numerical work. Let $q = \sqrt{m\omega/\hbar}\,x$ where $\omega^2 = k/m$. Then equation (0.7) becomes

$$\frac{-d^2\psi}{dq^2} + q^2 = 2\epsilon\psi \tag{0.8}$$

where we have written the energy as $E = \epsilon\hbar\omega$. Notice that $\epsilon$ is a dimensionless number since $\hbar\omega$ has units of energy. In these units the momentum operator $p \to -i\hbar\partial/\partial x = -i\sqrt{\hbar m\omega}\,\partial/\partial q$ and $p^2 \to -\hbar m\omega\partial^2/\partial q^2$.

I said earlier that we wanted to integrate in from both the right and the left and join the wave functions in the middle. But how do we pick the right and left starting points and where do we try to join the wave functions? We pick the right and left starting points at distances large enough so that the wave function can be taken to be zero there. To find such points we must first find the turning points. Recall that classically a turning point is where the particle's energy is equal to the potential energy of the potential well. At that point the particle's energy is all potential and it turns around and moves in the opposite direction.



The animation above shows a particle in the potential $V(q) = q^2$. The red dot represents the classical motion of the particle. The classical kinetic and potential energies are given in arbitrary units. The energy corresponds to the $n = 1$ quantum state. The blue lines show the classical turning points. The quantum mechanical probability distribution is shown in red for the $n = 1$ state. Note the exponential decay of the wave function outside of the turning points.

In our dimensionless units our potential is just $V(q) = q^2$.

For a simple harmonic oscillator the energy is given by $E = (n + 1/2)\hbar\omega$ where n is a non- negative integer. The energy of the ground state is $E_{\text{ground}} = \hbar\omega/2$ and the energy of the first excited state is $E_1 = 3/2\,\hbar\omega$ so the turning points for the first excited state are given by

```
In[16]:= turningPoints = Solve[n + 1 / 2 == q^2, q] /. n → 1
```

Out[16]= $\left\{\left\{q \to -\sqrt{\frac{3}{2}}\right\}, \left\{q \to \sqrt{\frac{3}{2}}\right\}\right\}$

I want the right most turning point, so I want the second solution.

```
In[17]:= RightTurningPoint = First[Last[turningPoints]]
```

Out[17]= $q \to \sqrt{\frac{3}{2}}$

We need to define the potential

```
V[q_] = q^2
```

$q^2$

and integrate in from both sides. The function leftψ[ϵ,q] is the result of integrating in from the left. We start the integration at $q = -4$ which is well past the left turning point. Since we are well past the turning point we can take the wave function to be zero at $q = -4$. Remember that the wave function decays exponentially past the turning points. Since the Schrö dingerequation is second order in the spatial variables, we need to specify the value of the first derivative as well. Since $\psi$ should increase as we integrate inward we will take the derivative to be small and positive at $q = -4$. We integrate in from $q = -4$ to the right turning point.

```
In[18]:= leftψ[ϵ_, q_] :=
           First[NDSolve[{-D[ψ[q], {q, 2}] + V[q] ψ[q] == 2 ϵ ψ[q], ψ'[-4] == 0.0001, ψ[-4] == 0},
              ψ[q], {q, -4, √(3 / 2)}]][[1, 2]];
```

The integration from the right is handled in exactly the same way except of course that we start our integrating to the right of the right turning point and integrate in.

```
In[19]:= rightψ[ϵ_, q_] :=
           First[NDSolve[{-D[ψ[q], {q, 2}] + V[q] ψ[q] == 2 ϵ ψ[q], ψ'[4] == 0.0001, ψ[4] == 0},
              ψ[q], {q, 4, √(3 / 2)}]][[1, 2]];
```

In order to re-scale the wave functions we need to compute two scale factors which I have called scaleLeft and scaleRight. These are just the left and right wave functions evaluated at the right turning point where we want to match the wave functions.

```
In[20]:= scaleLeft[ϵ_] := leftψ[ϵ, q] /. RightTurningPoint
         scaleRight[ϵ_] := rightψ[ϵ, q] /. RightTurningPoint
```

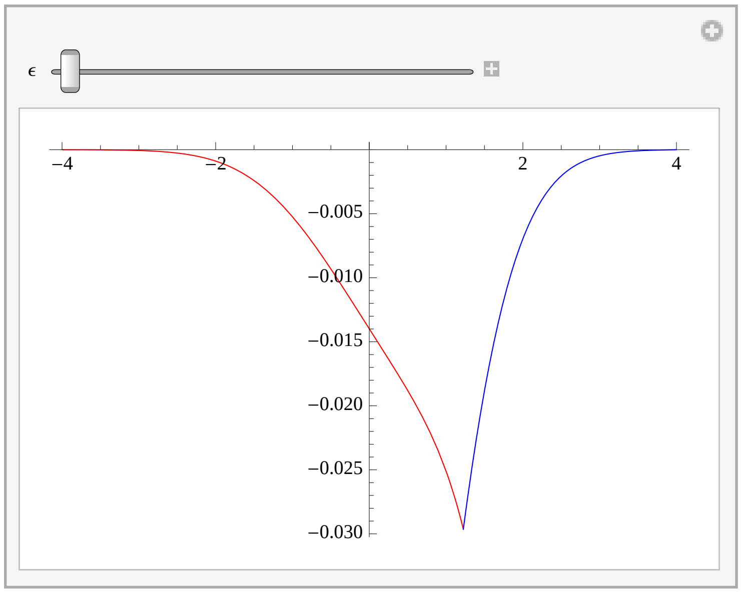
We now re-scale the wave function so that the left and right wave functions are equal at the right turning point.

```
In[22]:= scaledLeft[ϵ_, q_] := leftψ[ϵ, q] scaleRight[ϵ] / scaleLeft[ϵ]
```

This ensures that the wave functions join, but it does not ensure that they smoothly join.  You can explore this using the code below.

```
In[23]:= Clear[ϵ]
         Developer`SetSystemOptions["EvaluateNumericalFunctionArgument" → False];
         WaveFunctionSolver[ϵ_] := Module[
           {V, RightTurningPoint, leftψ, rightψ, scaleRight, scaleLeft, scaledLeft, plot1, plot2},
           V[q_] = q^2;
           RightTurningPoint = q -> √(3 / 2);
         leftψ[ϵ] =
            First[NDSolve[{-D[ψ[q], {q, 2}] + V[q] ψ[q] == 2 ϵ ψ[q], ψ'[-4] == 0.0001, ψ[-4] == 0},
               ψ[q], {q, -4, √(3 / 2)}]][[1, 2]];
         rightψ[ϵ] = First[NDSolve[{-D[ψ[q], {q, 2}] + V[q] ψ[q] == 2 ϵ ψ[q], ψ'[4] == 0.0001, ψ[4] == 0},
               ψ[q], {q, 4, √(3 / 2)}]][[1, 2]];
         scaleLeft[ϵ] = leftψ[ϵ] /. RightTurningPoint;
           scaleRight[ϵ] = rightψ[ϵ] /. RightTurningPoint;
           scaledLeft[ϵ] = leftψ[ϵ] scaleRight[ϵ] / scaleLeft[ϵ];
           plot1 = Plot[scaledLeft[ϵ], {q, -4, RightTurningPoint[[2]]}, PlotStyle → Red];
           plot2 = Plot[rightψ[ϵ], {q, RightTurningPoint[[2]], 4}, PlotStyle → Blue];
           Show[plot1, plot2, PlotRange → {{-4, 4}, All}]]
```

```
Manipulate[WaveFunctionSolver[ϵ], {ϵ, 0, 2}, SaveDefinitions → True]
```



For a smooth join we must match the derivatives as well. I have called these DRight and DLeft.

```
In[26]:= DRight[ϵ_, q_] := D[rightψ[ϵ, q], q]
```

```
In[27]:= DLeft[ϵ_, q_] := D[scaledLeft[ϵ, q], q]
```

We can now find the allowed energy (or eigenvalue) by finding the value of ϵ for which the derivatives match.

```
In[28]:= Energy = ϵ /. FindRoot[
           (DLeft[ϵ, q] /. RightTurningPoint) == (DRight[ϵ, q] /. RightTurningPoint), {ϵ, 1.5, 1.7}]

Out[28]= 1.50001
```

This compares well with the exact answer of 3/2. With the energy in hand we can calculate the wave function.

```
In[29]:= Clear[result]
         result[q_] = First[ψ[q] /. NDSolve[
              {-D[ψ[q], {q, 2}] + V[q] ψ[q] == 2 Energy ψ[q], ψ'[-4] == 0.0001, ψ[-4] == 0}, ψ[q], {q, -4, 4}]]

Out[30]= InterpolatingFunction[( -4.   4. ), <>][q]
```

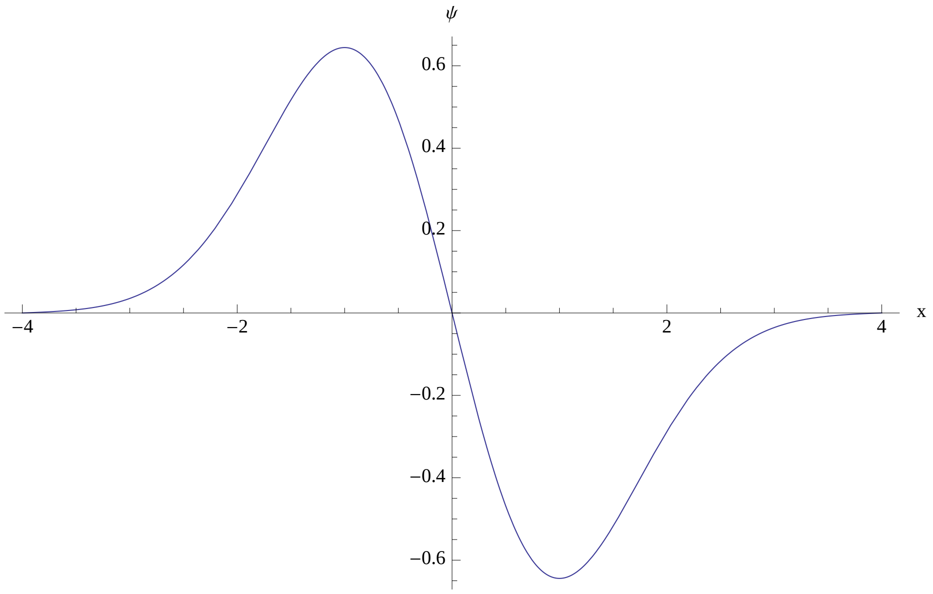
```
In[31]:= normalization = 1 / Sqrt[NIntegrate[result[q]^2, {q, -4, 4}]]

Out[31]= 102.429
```

The normalized wave function is plotted below. We have found (as we should) the $n = 1$ state.

```
In[32]:= wavefunction[q_] = normalization result[q];
```

In[33]:=
```
plot1 = Plot[wavefunction[q], {q, -4, 4},
  PlotLabel -> "Numerical Solution \n \n", AxesLabel → {"x", "ψ"}, ImageSize → 72 × 6]
```

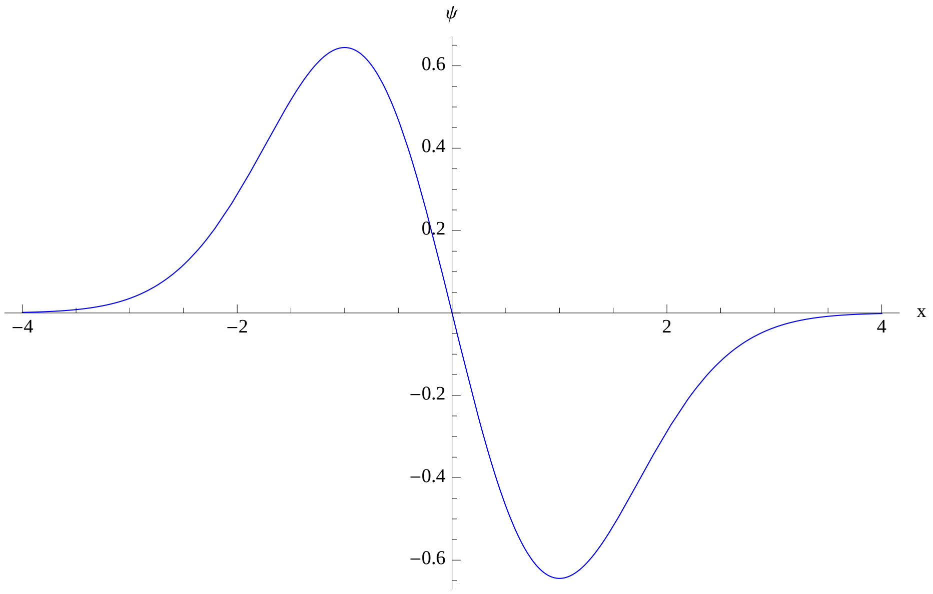
Numerical Solution

Out[33]=


We can compare this with the exact solution. Notice the minus sign! Our solution differs from $\psi[1, q]$ by a minus sign. Since both expectation values and the probability density depend n the product of $\psi^*$and $\psi$ this minus sign has no physical consequence. Here I have plotted the two wave functions one above the other. If you try to plot them on the same plot you will find that they overlay one another.

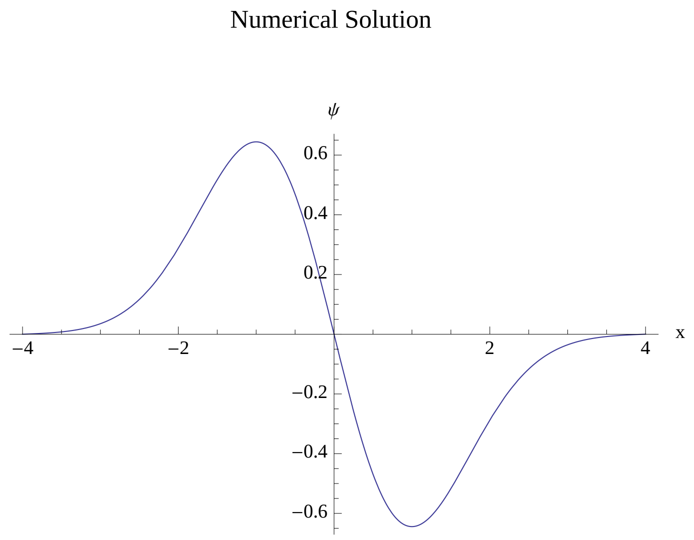
In[34]:=
```
plot2 = Plot[Evaluate[-ψ[1, q]], {q, -4, 4},
  PlotStyle → RGBColor[0, 0, 1], PlotLabel -> "Exact Solution \n \n",
  AxesLabel → {"x", "ψ"}, ImageSize → 72 × 6, DisplayFunction → Identity]
```

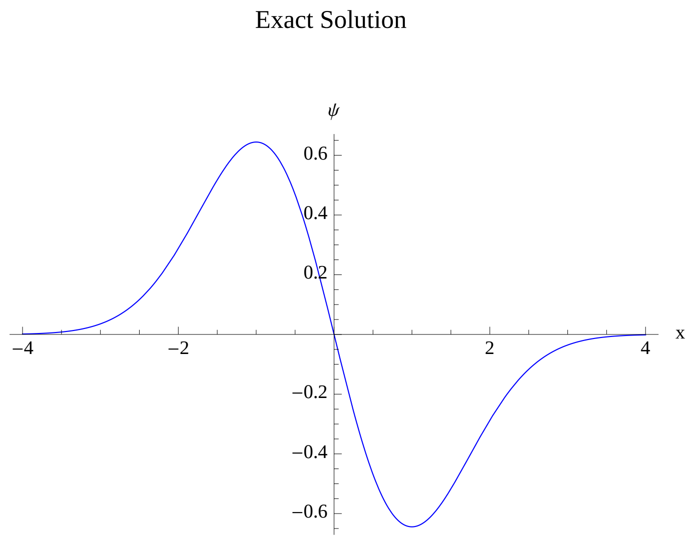
Exact Solution

Out[34]=


```
In[35]:= Show[GraphicsArray[{{plot1}, {plot2}}], ImageSize → 72 × 6]
```

Out[35]=





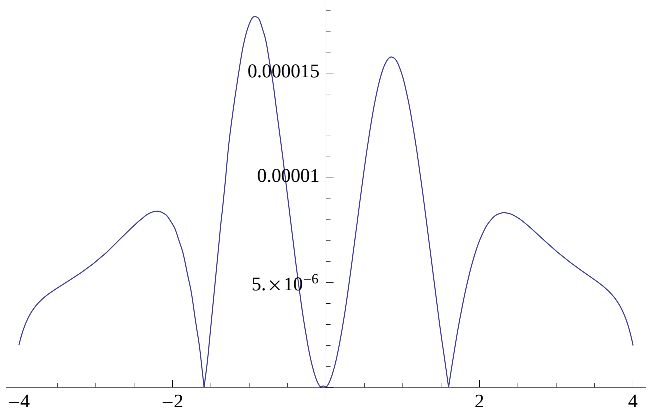
A better measure of the quality of our numerical solution is to compute a metric that measures the distance between the numerical solution and the exact solution. I have chosen to compare the difference between the probability distribution for the numerical result and the exact result. I then take the square root of the square of the difference so that I always get a positive result. It may seem like we should then divide by the exact probability density to get a fractional difference, but this will cause problems when the probability density has a zero.

In[36]:= $\texttt{ProbablityMetric[q\_]} = \sqrt{\left(\texttt{wavefunction[q]}^2 - \psi\texttt{[1, q]}^2\right)^2}$ ;

We can now plot the metric and you can see that we do pretty well.

```
In[37]:= Plot[ProbablityMetric[q], {q, -4, 4}, PlotRange → All]
```

Out[37]=



We can do the same thing for the energy except that here we can divide by the exact energy to get a fractional difference since the energy is a positive number.

In[38]:= EnergyMetric = $\sqrt{(\text{Energy} - 3/2)^2} \Big/ (3/2)$

Out[38]= $9.55467\times10^{-6}$

Once we have the wave function we can compute expectation values for an operator we are interested in. Here we see one advantage of working in dimensionless coordinates. We can compute $<q>$ and $<q^2>$ and then transform back to $<x>$ and $<x^2>$ without needing numerical values for $k$ and $m$. The value of $<q>$ should be zero and it is. You may get a warning message about poor convergence. This is standard when trying to numerically evaluate an integral whose true value is zero. Try numerically integrating $\sin(x)$ from 0 to $2\pi$.

```
In[39]:= qAverage = NIntegrate[ wavefunction[q] q wavefunction[q], {q, -4, 4}]
```

Out[39]= $-2.48994\times10^{-6}$

In[40]:= qSquareAverage = NIntegrate[ wavefunction[q] $q^2$ wavefunction[q], {q, -4, 4}]

Out[40]= 1.4998

We can now convert back from $q$ to $x$. Since $x = \sqrt{\hbar/(m\,\omega)}\;q$ we have $<x^2> = \hbar/(m\,\omega)\;<q^2>$.

```
In[41]:= xSquareAverage = ℏ / (m ω) qSquareAverage
```

Out[41]= $\dfrac{1.4998\,\hbar}{m\,\omega}$

To compute the expectation value of the momentum, we need to differentiate the wave function since $p \to -i\hbar\,\partial/\partial x = -i\sqrt{\hbar\,m\,\omega}\;\partial/\partial q$. I have called the derivative of the wave function d$\psi[q]$.

```
In[42]:=
dψ[q_] = Evaluate[ D[ wavefunction[q], q]]
```

Out[42]= 102.429 InterpolatingFunction[( −4. 4. ), <>][q]

The average momentum is zero as it should be.

```
In[43]:= pAverage = NIntegrate[Evaluate[ wavefunction[q] dψ[q]], {q, -4, 4}]
```

NIntegrate::ncvb :
NIntegrate failed to converge to prescribed accuracy after 9 recursive bisections in $q$ near {$q$} = {−1.078}. NIntegrate obtained $7.06971\times10^{-9}$ and $8.8384\times10^{-11}$ for the integral and error estimates. ≫

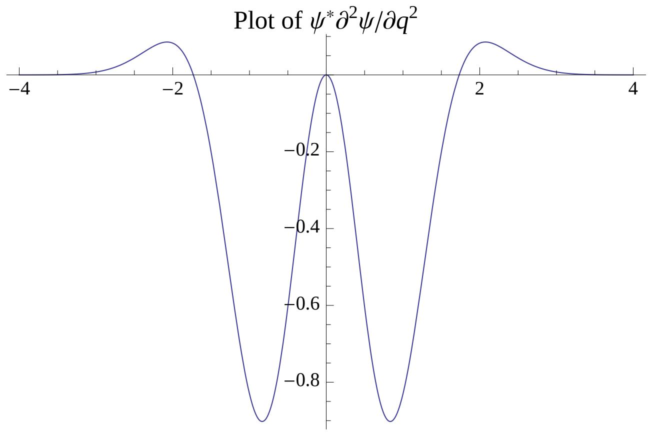
Out[43]= $7.06971\times10^{-9}$

To compute $< p^2 >$ we use the fact that $p^2 \to -\hbar\, m\, \omega\, \partial^2 / \partial q^2$. I have called the second derivative of $\psi$ with respect to $q$, d2$\psi$[$q$].

```
In[44]:= d2ψ[q_] = Evaluate[ D[ wavefunction[q], {q, 2}]]

Out[44]= 102.429 InterpolatingFunction[( -4.   4. ), <>][q]

In[45]:= pSquareAverage = (-ℏ m ω ) NIntegrate[ wavefunction[q] d2ψ[q], {q, -4, 4}]

Out[45]= 1.50023 m ω ℏ
```

In some versions you will get a warning about poor convergence and this time it is unexpected since the integral is non-vanishing. Plotting the integral shows that it is well behaved.

```
In[46]:= Plot[wavefunction[q] d2ψ[q], {q, -4, 4}, PlotLabel → "Plot of ψ*∂²ψ/∂q²"]

Out[46]=
```



Turning up the number of recursive bisections used for **NIntegrate** gets rid of the warning message (if you got one) but does not change the answer. See the note in the help browser for an explanation of how NIntegrate works.

```
In[47]:= NIntegrate[ wavefunction[q] d2ψ[q], {q, -4, 4}, MaxRecursion → 12]

Out[47]= -1.50023
```

It is now easy to compute $\Delta x = \sqrt{< x^2 > - < x >^2}$ and $\Delta p = \sqrt{< p^2 > - < p >^2}$. Since both $< x >$ and $< p >$ vanish we have

```
In[48]:= Δp = √pSquareAverage
```

Out[48]= $1.22484 \sqrt{m\, \omega\, \hbar}$

and

```
In[49]:= Δx = √xSquareAverage
```

Out[49]= $1.22466 \sqrt{\frac{\hbar}{m\, \omega}}$

Checking the uncertainty principle bound $\Delta x\, \Delta p \geq \hbar/2$

```
In[50]:= PowerExpand[Δx Δp]

Out[50]= 1.50002 ℏ
```

shows that we have good agreement with the exact result for a harmonic oscillator which is $\Delta x\, \Delta p = (n + 1/2)\, \hbar$. Since we have found the $n = 1$ state we expect $\Delta x\, \Delta p = (3/2)\hbar$.

### A more complicated potential

It's all well and good to find the allowed energies and the wave functions when we already know the answer, but what about when we don't. Suppose we have a more complicated potential for which we can not find analytic solutions to the Schrö dingeequation. Shown below is a "Mexican Hat" type potential in dimensionless coordinates.

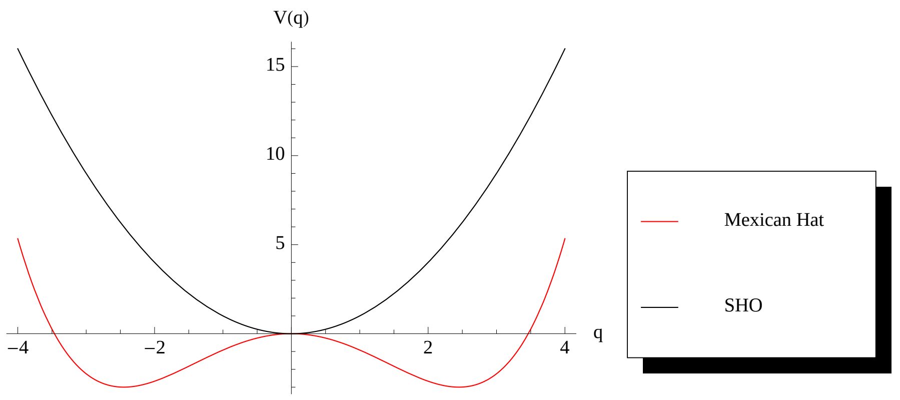
```
In[51]:= V[q_] = -q^2 + q^4 / 12
```

Out[51]= $\frac{q^4}{12} - q^2$

I have plotted the potential below along with the simple harmonic oscillator potential for comparison.

```
In[52]:= Plot[{V[q], q^2}, {q, -4, 4}, PlotStyle → {RGBColor[1, 0, 0], RGBColor[0, 0, 0]},
          AxesLabel → {"q", "V(q)"}, PlotLegend → {"Mexican Hat", "SHO"},
          LegendPosition → {1, -1 / 2}, ImageSize → 6 × 72]
```

Out[52]=



In dimensionless coordinates the Schrö dingeequation is $\frac{-d^2\psi}{d q^2} - q^2 + q^4/12 = 2\,\epsilon\,\psi$.

Once again we will need the turning points. The turning points are found by solving $V(q) = E_i$ where $E_i$ is some energy (in our units a dimensionless number). Our choice for $E_i$will determine which bound state we find. Suppose we pick $E_i = 2$. Then the turning points are given by

```
In[53]:= turningPoints = Solve[V[q] == 2., q]
```

Out[53]= $\{\{q \to -3.70756\}, \{q \to 0. - 1.32135\,i\}, \{q \to 0. + 1.32135\,i\}, \{q \to 3.70756\}\}$

We want the right turning point, which is the last solution.

```
In[54]:= RightTurningPoint = First[Last[turningPoints]]
```

Out[54]= $q \to 3.70756$

I now integrate in from the left starting at $q = -5$ which is outside the left turning point and stopping at the right turning point.

```
In[55]:= leftψ[ϵ_, q_] :=
           First[NDSolve[{-D[ψ[q], {q, 2}] + V[q] ψ[q] == 2 ϵ ψ[q], ψ'[-5] == 0.0001, ψ[-5] == 0},
              ψ[q], {q, -5, q /. RightTurningPoint}]][[1, 2]];
```

I do the same thing from the right, starting at $q = 5$ and integrating in to the right turning point.

```
In[56]:= rightψ[ϵ_, q_] :=
           First[NDSolve[{-D[ψ[q], {q, 2}] + V[q] ψ[q] == 2 ϵ ψ[q], ψ'[5] == 0.0001, ψ[5] == 0},
              ψ[q], {q, 5, q /. RightTurningPoint}]][[1, 2]];
```

I then adjust ϵ until I get a smooth match at the right turning point.

```
In[57]:= Energy = 2 ϵ /. FindRoot[
            (DLeft[ϵ, q] /. RightTurningPoint) == (DRight[ϵ, q] /. RightTurningPoint), {ϵ, 1, 1.1}]
```

Out[57]= 2.33468

I can now calculate the wave function and the normalization.

```
In[58]:= result[q_] = First[ψ[q] /. NDSolve[
             {-D[ψ[q], {q, 2}] + V[q] ψ[q] == Energy ψ[q], ψ'[-5] == 0.0001, ψ[-5] == 0}, ψ[q], {q, -5, 5}]]

Out[58]= InterpolatingFunction[( -5.   5. ), <>][q]
```

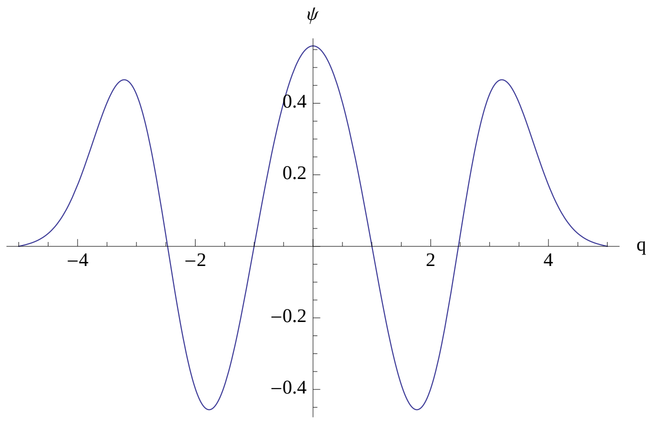
```
In[59]:= normalization = 1 / Sqrt[NIntegrate[result[q]^2, {q, -5, 5}]]

Out[59]= 374.659
```

The normalized wave function is

```
In[60]:= wavefunction[q_] = normalization result[q]

Out[60]= 374.659 InterpolatingFunction[( -5.   5. ), <>][q]
```

```
In[61]:= plot1 = Plot[wavefunction[q], {q, -5, 5}, AxesLabel → {"q", "ψ"}]
```

Out[61]=

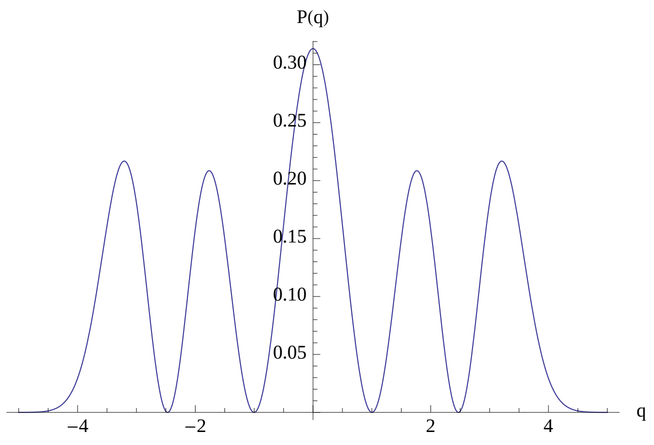


and the probability density is

```
In[62]:= plot2 = Plot[wavefunction[q]^2, {q, -5, 5}, AxesLabel → {"q", "P(q)"},
           PlotLabel → StringJoin["E = ", ToString[Energy ], "\n \n"]]
```

Out[62]=

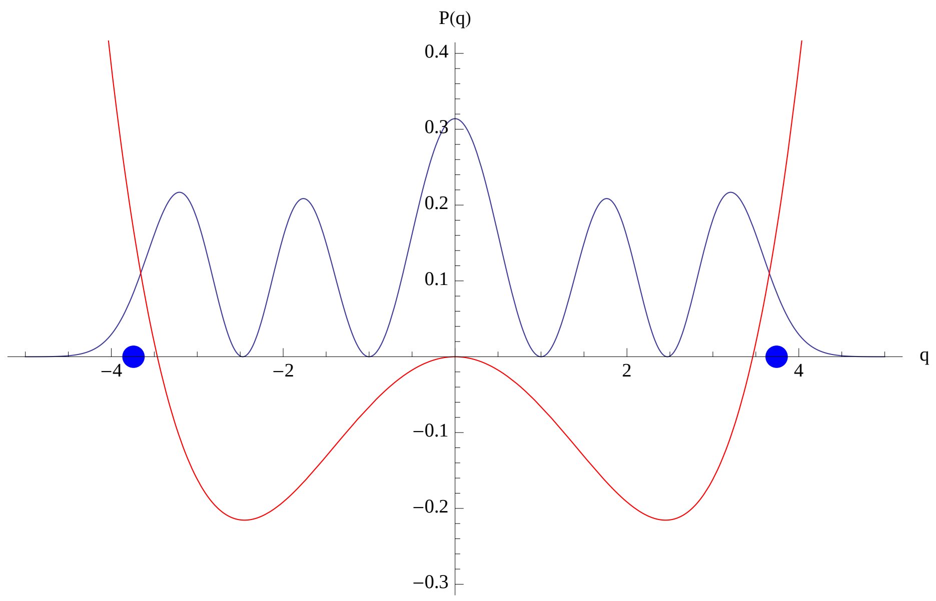
E = 2.33468



If we scale the potential we can plot the probability density and the potential on the same graph.

In[65]:=
```
plot4 =
  Plot[V[q] / V[4.5], {q, -5, 5}, PlotStyle → RGBColor[1, 0, 0], DisplayFunction → Identity];
points = Graphics[{RGBColor[0, 0, 1], PointSize[0.025],
    {Point[{q /. First[Solve[V[q]  == Energy, q]], 0}],
     Point[{q /. Last[Solve[V[q]  == Energy, q]], 0}]}}];
Show[plot2, plot4, points, PlotRange → {0.4, -0.3}, DisplayFunction → $DisplayFunction,
 ImageSize → 6 × 72]
```

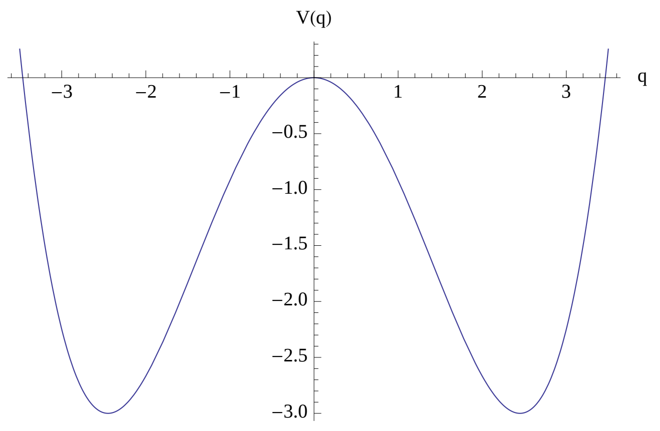
E = 2.33468

Out[67]=


The probability density is shown in light blue. The potential is shown in red and has been scaled for visual clarity. The left and right turning points are shown in blue. Note the exponential fall-off of the probability density outside the turning points.

The state that we have found is clearly not the ground state. To find the ground state we need to start lower in the well. A plot of the well

In[68]:=
```
Plot[V[q], {q, -3.5, 3.5}, AxesLabel → {"q", "V(q)"}]
```

Out[68]=


shows that the bottom of the well is  at -3.  If we start around $E = -2$ we find that the turning points are

In[69]:=
```
turningPoints = Solve[V[q] == -2., q]
```

Out[69]= $\{\{q \to -3.07638\}, \{q \to -1.59245\}, \{q \to 1.59245\}, \{q \to 3.07638\}\}$

Note that there are 4 real turning points.

```
In[70]:= RightTurningPoint = First[Last[turningPoints]]

Out[70]= q → 3.07638

In[71]:= Energy = 2 ϵ /. FindRoot[
            (DLeft[ϵ, q] /. RightTurningPoint) == (DRight[ϵ, q] /. RightTurningPoint), {ϵ, -2.5, -2.6}]

Out[71]= -1.71124

In[72]:= result[q_] = First[ψ[q] /. NDSolve[
             {-D[ψ[q], {q, 2}] + V[q] ψ[q] == Energy ψ[q], ψ'[-5] == 0.0001, ψ[-5] == 0}, ψ[q], {q, -5, 5}]]

Out[72]= InterpolatingFunction[( -5.   5. ), <>][q]
```

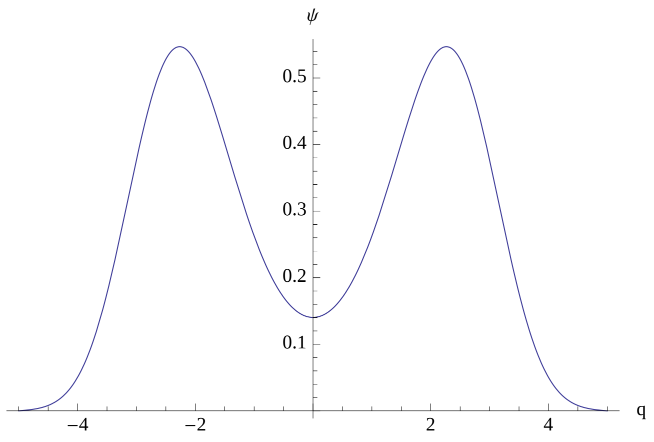
```
In[73]:= normalization = 1/Sqrt[NIntegrate[result[q]^2, {q, -5, 5}]]
```

$$\text{normalization} = 1\Big/\sqrt{\text{NIntegrate}\left[\text{result}[q]^2, \{q, -5, 5\}\right]}$$

```
Out[73]= 73.7615
```

The normalized wave function is

```
In[74]:= wavefunction[q_] = normalization result[q]

Out[74]= 73.7615 InterpolatingFunction[( -5.   5. ), <>][q]

In[75]:= plot1 = Plot[wavefunction[q], {q, -5, 5}, AxesLabel → {"q", "ψ"}]

Out[75]=
```

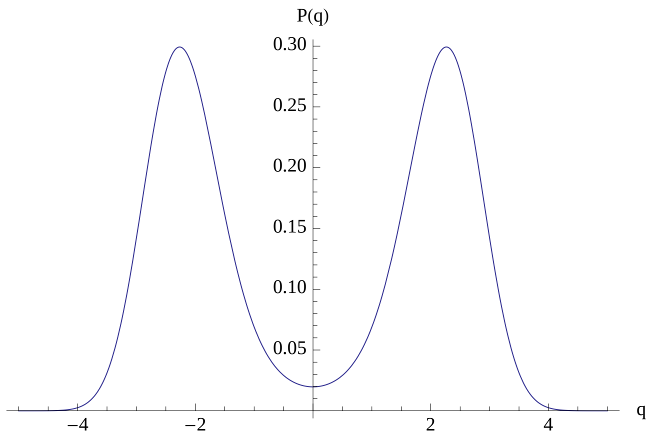


and the probability density is

In[76]:=
```
plot2 = Plot[wavefunction[q]^2, {q, -5, 5}, AxesLabel → {"q", "P(q)"},
  PlotLabel → StringJoin["E = ", ToString[Energy ], "\n \n"]]
```

E = −1.71124

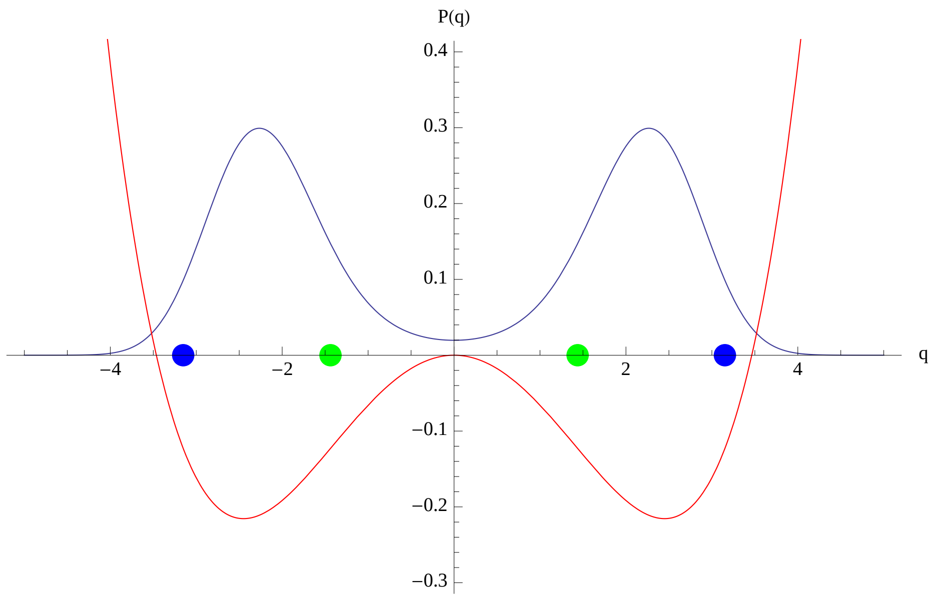
Out[76]=



In[77]:=
```
plot4 =
  Plot[V[q] / V[4.5], {q, -5, 5}, PlotStyle → RGBColor[1, 0, 0], DisplayFunction → Identity];
outerPoints = Graphics[{RGBColor[0, 0, 1], PointSize[0.025],
    {Point[{q /. First[Solve[V[q]  == Energy]], 0}],
     Point[{q /. Last[Solve[V[q]  == Energy]], 0}]}}];
innerPoints = Graphics[{RGBColor[0, 1, 0], PointSize[0.025], {Point[
      {q /. Solve[V[q]  == Energy][[2]], 0}], Point[{q /. Solve[V[q]  == Energy][[3]], 0}]}}];
Show[plot2, plot4, outerPoints, innerPoints, PlotRange → {0.4, -0.3},
 DisplayFunction → $DisplayFunction, ImageSize → 6 × 72]
```

E = −1.71124

Out[80]=



The probability density is shown in light blue. The potential is shown in red and has been scaled for visual clarity. The left and right outer turning points are shown in blue.The inner turning points are shown in green. Note the exponential fall-off of the probability density outside the turning points (both inner and outer).

***Exercise Three***

Investigate the bound states for a potential given by

```
V[x_] = x^4 + .7 x^3 - 2 x^2 - 1.13 x - 2
```

and be sure to comment on your results.

***Conceptual Question***

Devise your own well. Be sure to plot it. Without calculation sketch the wave functions for the first two bound states for your well. Now find the bound states and their wave functions numerically. Do these agree with your sketch? If not, which result (if either) is right? What strategy did you use for deciding which result (sketch or numerical calculation) was right? Blind faith in a numerical result is not a strategy!

**Time-Dependent States**

We can fairly easily look at time-dependent states as well. Call $\psi_1$the state with energy $E = -1.71$. This is the state that we just found . Call the state with $E = 2.33$ , $\psi_2$. Suppose we start with equal mixtures of each state. Then $\Psi(x,t) = \frac{1}{\sqrt{2}} e^{-i E_1 t/\hbar} \psi_1 + \frac{1}{\sqrt{2}} e^{-i E_2 t/\hbar} \psi_2$ . The code below generates both $\psi_1$ and $\psi_2$. There is nothing new in the code it is just collected from above.

```
V[q_] = -q^2 + q^4 / 12;
turningPoints = Solve[V[q] == -2., q];
RightTurningPoint = First[Last[turningPoints]];
leftψ[ϵ_, q_] :=
  First[NDSolve[{-D[ψ[q], {q, 2}] + V[q] ψ[q] == 2 ϵ ψ[q], ψ'[-6] == 0.0001, ψ[-6] == 0},
     ψ[q], {q, -6, q /. RightTurningPoint}]][[1, 2]];
rightψ[ϵ_, q_] := First[NDSolve[{-D[ψ[q], {q, 2}] + V[q] ψ[q] == 2 ϵ ψ[q],
       ψ'[6] == 0.0001, ψ[6] == 0}, ψ[q], {q, 6, q /. RightTurningPoint}]][[1, 2]];
Energy = 2 ϵ /. FindRoot[(DLeft[ϵ, q] /. RightTurningPoint) ==
      (DRight[ϵ, q] /. RightTurningPoint), {ϵ, -2.5, -2.6}];
result[q_] = First[ψ[q] /. NDSolve[{-D[ψ[q], {q, 2}] + V[q] ψ[q] == Energy ψ[q],
       ψ'[-6] == 0.0001, ψ[-6] == 0}, ψ[q], {q, -6, 6}]];
normalization = 1 / Sqrt[NIntegrate[result[q]^2, {q, -6, 6}]] ;
ψ1[q_] = normalization result[q];
E1 = Energy;

V[q_] = -q^2 + q^4 / 12;
turningPoints = Solve[V[q] == 2., q];
RightTurningPoint = First[Last[turningPoints]];
leftψ[ϵ_, q_] :=
  First[NDSolve[{-D[ψ[q], {q, 2}] + V[q] ψ[q] == 2 ϵ ψ[q], ψ'[-6] == 0.0001, ψ[-6] == 0},
     ψ[q], {q, -6, q /. RightTurningPoint}]][[1, 2]];
rightψ[ϵ_, q_] := First[NDSolve[{-D[ψ[q], {q, 2}] + V[q] ψ[q] == 2 ϵ ψ[q],
       ψ'[6] == 0.0001, ψ[6] == 0}, ψ[q], {q, 6, q /. RightTurningPoint}]][[1, 2]];
Energy = 2 ϵ /. FindRoot[(DLeft[ϵ, q] /. RightTurningPoint) ==
      (DRight[ϵ, q] /. RightTurningPoint), {ϵ, 1, 1.1}];
result[q_] = First[ψ[q] /. NDSolve[{-D[ψ[q], {q, 2}] + V[q] ψ[q] == Energy ψ[q],
       ψ'[-6] == 0.0001, ψ[-6] == 0}, ψ[q], {q, -6, 6}]];
normalization = 1 / Sqrt[NIntegrate[result[q]^2, {q, -6, 6}]] ;
ψ2[q_] = normalization result[q];
E2 = Energy;
```

We can now superimpose the states to get our time-dependent wave function.

```
Ψ[q_, t_] = (1 / Sqrt[2]) Exp[- ⅈ E1 t] ψ1[q] + (1 / Sqrt[2]) Exp[-ⅈ E2 t] ψ2[q]
```

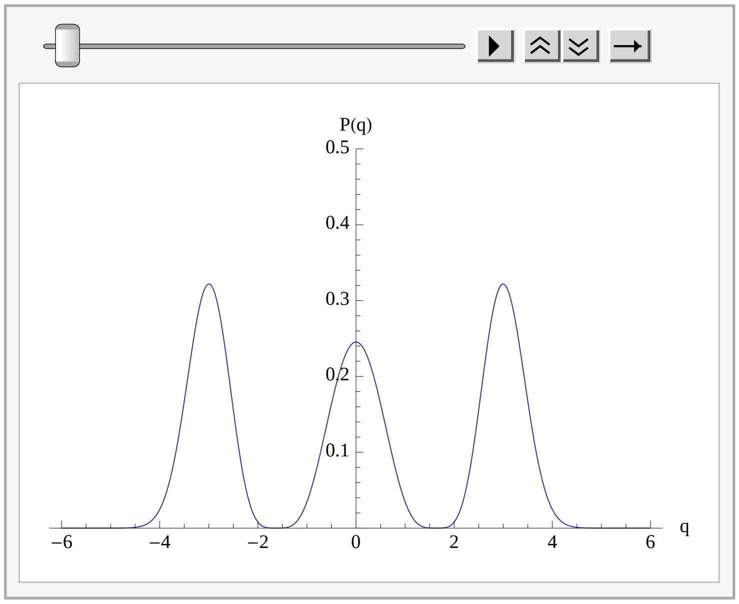
```
0.46279 ⅇ^(-2.3344 ⅈ t) InterpolatingFunction[{{-6., 6.}}, <>][q] +
  0.0651926 ⅇ^(1.71125 ⅈ t) InterpolatingFunction[{{-6., 6.}}, <>][q]
```

```
ΨStar[q_, t_] = Conjugate[(1/√2) Exp[- ⅈ E1 t] ψ1[q] + (1/√2) Exp[-ⅈ E2 t] ψ2[q]]
```

```
Conjugate[0.46279 ⅇ^(-2.3344 ⅈ t) InterpolatingFunction[{{-6., 6.}}, <>][q] +
  0.0651926 ⅇ^(1.71125 ⅈ t) InterpolatingFunction[{{-6., 6.}}, <>][q]]
```

The time dependent probability density is plotted below.

```
ListAnimate[
 Table[Plot[ΨStar[q, t] Ψ[q, t], {q, -6, 6}, PlotRange → {0, 0.5}, AxesLabel → {"q", "P(q)"}],
  {t, 0, 2 π / Abs[E1 + E2] - 6 π / (40 Abs[E1 + E2]), 2 π / (80 Abs[E1 + E2])}]]
```



**_Exercise Four_**

Make a time dependent state out of the first two states for a particle in a potential given by

```
V[x_] = x^4 + .7 x^3 - 2 x^2 - 1.13 x - 2
```

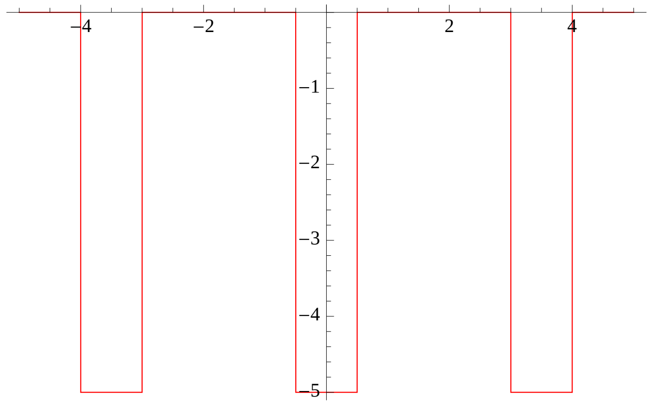
Calculate $< x >$ for this state and plot the time-dependent probability density. Comment on your results.

**Multiple Wells**

Multiple quantum wells can be handled in the same way. Plotted below is a potential made of three finite square wells.

```
V[q_] := Piecewise[{{0, q < -4}, {-5, -4 < q < -3}, {0, -3 < q < -1 / 2},
    {-5, -1 / 2 < q < 1 / 2}, {0, 1 / 2 < q < 3}, {-5, 3 < q < 4}, {0, q > 4}}]
```

```
plot1 = Plot[{V[q]}, {q, -5, 5},
  PlotPoints -> 100, PlotStyle → RGBColor[1, 0, 0], Exclusions → None]
```



This problem can be solved analytically, but if we want a numerical solution we can proceed exactly as we did previously.

```
RightTurningPoint = q -> 4
```

```
q → 4
```

```
leftψ[ϵ_, q_] :=
  First[NDSolve[{-D[ψ[q], {q, 2}] + V[q] ψ[q] == ϵ ψ[q], ψ'[-5] == 0.0001, ψ[-5] == 0},
     ψ[q], {q, -5, q /. RightTurningPoint}]][[1, 2]];

rightψ[ϵ_, q_] :=
  First[NDSolve[{-D[ψ[q], {q, 2}] + V[q] ψ[q] == ϵ ψ[q], ψ'[5] == 0.0001, ψ[5] == 0}, ψ[q],
     {q, 5, q /. RightTurningPoint}]][[1, 2]];

Energy = ϵ /. FindRoot[
   (DLeft[ϵ, q] /. RightTurningPoint) == (DRight[ϵ, q] /. RightTurningPoint), {ϵ, -5, -4.5}]
```

```
-2.43285
```

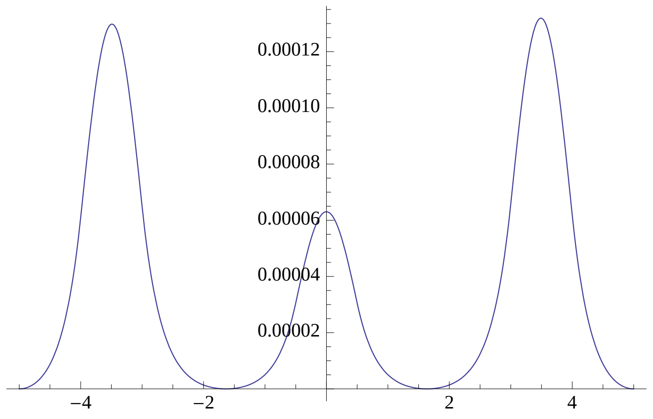
```
result[q_] = First[ψ[q] /. NDSolve[
    {-D[ψ[q], {q, 2}] + V[q] ψ[q] == Energy ψ[q], ψ'[-5] == 0.0001, ψ[-5] == 0}, ψ[q], {q, -5, 5}]]
```

```
InterpolatingFunction[{{-5., 5.}}, <>][q]
```

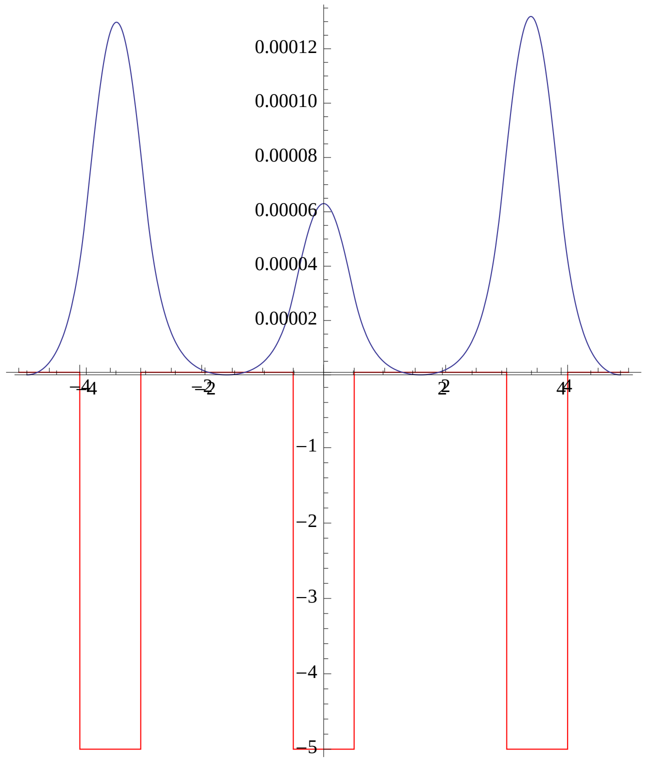
```
normalization = 1 / Sqrt[NIntegrate[result[q]^2, {q, -5, 5}]]
```

```
2864.66
```

```
plot2 = Plot[normalization result[q]^2, {q, -5, 5}, PlotRange -> All]
```



```
Show[GraphicsArray[{{plot1}, {plot2}}, GraphicsSpacing → -2.86]]
```



## Wave Packets and Scattering

### Introduction to wave packets

So far we have looked at states that were either energy eigenstates or a superposition of a small number of energy eigenstates. However for some problems, such as scattering problems, we want solutions that are not energy eigenstates but are solutions to the full time-dependent Schrö dingerequation.

$$\frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+V(x)\,\Psi(x,t)=i\,\hbar\,\frac{\partial\Psi(x,t)}{\partial t}.$$

Suppose for the moment that we have a free particle so that $V(x, t) = 0$. The time dependent Schrö dinger equation is then

$$\frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}=i\,\hbar\,\frac{\partial\Psi(x,t)}{\partial t} \qquad (0.9)$$

and has solutions of the form $\Psi(x, t) = A\,e^{i(k\,x-\omega\,t)}$. Plugging this into equation (0.9) gives $\frac{\hbar}{2m}k^2 = \omega$, which is a dispersion relation relating the wave number $k$ to the angular frequency $\omega$. Remember that the wave number is related to the wavelength by $k = 2\,\pi/\lambda$ and that the momentum of a particle is $p = \hbar\,k$. The Schrö dingerequation is linear so a sum of solutions is also a solution. Thus a wave function of the form

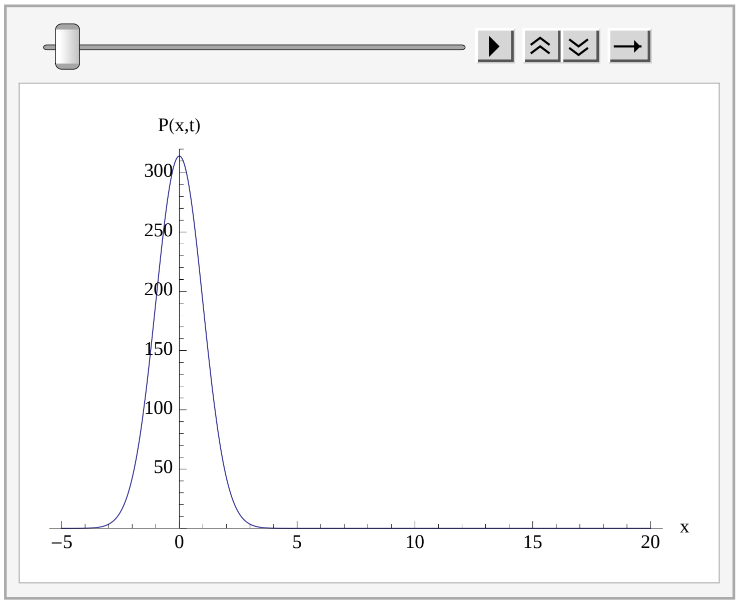
$$\Psi(x,t) = \sum_i A_i\,e^{i(k_i\,x-\omega_i\,t)} \qquad (0.10)$$

is also a solution. In equation (0.10) the sum runs over the allowed wave numbers $k_i$. If we have just one wave number, the particle has a definite momentum but is not spatially localized. This is easily seen by computing $P(x, t) = \Psi^*(x, t)\,\Psi(x, t)$ which is a constant if $\Psi(x, t) = A\,e^{i(k\,x-\omega\,t)}$ indicating that the particle has an equal probability of being found anywhere in space. This is consistent with the uncertainly principle, since $\Delta p = 0$ we must have $\Delta x = \infty$. The situation is different if we have a state with many wave numbers. Suppose we have a state with 101 different wave numbers. The code below generates such a state. The wave numbers are gaussian distributed around 5. The units are chosen so that $\hbar = 1$ and the particle has unit mass.

```
Clear[A]
ℏ = 1;
m = 1;
Table[A[k] = Exp[-(k - 5)^2], {k, 0, 10, .1}];
ψ[x_, t_] = Sum[A[k] Exp[ⅈ (k x - k^2 ℏ t / (2 m))], {k, 0, 10, .1}];
ψStar[x_, t_] = ψ[x, t] /. Complex[a_, b_] → Complex[a, -b];
P[x_, t_] = ψStar[x, t] ψ[x, t];
```

Plotting the probability density shows that our state is localized in space (although $\Delta x \neq 0$) and is right moving.

```
ListAnimate[Table[Plot[Chop[P[x, t]], {x, -5, 20},
   PlotRange → {0, 320}, AxesLabel → {"x", "P(x,t)"}], {t, 0, 3, .1}]]
```



Notice that this state looks like a particle. States like this are called wave packets.

**Exercise Five**

Plot similar states but with Gaussian distributions around $k = 10$ and $k = 20$. Interpret your results physically.

Change the variance of your Gaussian distribution and interpret your results in light of the uncertainty principle.

What happens when a wave packet scatters off a potential barrier or well? To answer this question we need to solve the time-dependent Schrö ding equation. That means we need to solve

$$\frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\,\Psi(x,t) = i\,\hbar\,\frac{\partial\Psi(x,t)}{\partial t}$$

with the initial condition $\Psi(x, 0) = \psi(x)$ and subject to the appropriate boundary conditions. In general we want the wave function to vanish at $\pm\infty$ at any finite time. Thus, we want $\Psi(-\infty, t) = \Psi(\infty, t) = 0$. This is hard to do on a computer so we will put our system in a "large" box and demand that the wave function vanish at the box boundaries. We will see shortly what "large" means in this context.

## Method of Lines

We will solve the time-dependent Schrö dingerequation using a technique called the method of lines. This is a general technique for solving partial differential equations that are initial value problems. You can not use it to solve Laplace's equation for example since that is not an initial value problem. *Mathematica's* differential equation solver **NDSolve** has the method of lines built into it, but we should understand how the method of lines works before we go ahead and use it.

To broaden our experience we will start with something other than the Schrö dingerequation. Suppose we have a partial differential equation of the form $\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}$. This is the heat equation with a thermal diffusivity of $\kappa$. We could of course also think of this as a diffusion equation. Physically $T$ is the temperature of our one-dimensional object, which we can take to be of length $L$, and it is a function of both $x$ and $t$. We want to solve this equation subject to the initial condition $T(x, 0) = f(x)$ where $f(x)$ is the initial temperature profile of the object and subject to the boundary conditions $T(0, t) = T_1$ and $T(L, t) = T_2$.

The idea is to reduce our partial differential equation to a system of ordinary differential equations by making the spatial derivatives discrete. We will use a central difference method so that $\frac{dT}{dx} \to \frac{T(x+h/2,t)-T(x-h/2,t)}{h}$ and $\frac{d^2T}{dx^2} \to \frac{T(x+h,t)-2\,T(x,t)+T(x-h,t)}{h^2}$.

This reduces our partial differential equation to a set of coupled ordinary differential equations. For example if we take $L = 1$and $h = 1/10$ we get the following equations

```
equations = Table[D[T[x, t], t] == (T[x + h, t] - 2 T[x, t] + T[x - h, t]) / h^2,
   {x, 1 / 10, 9 / 10, 1 / 10}] /. h → 1 / 10
```

$$\left\{T^{(0,1)}\left[\frac{1}{10}, t\right] == 100\left(T[0, t] - 2\,T\left[\frac{1}{10}, t\right] + T\left[\frac{1}{5}, t\right]\right),\right.$$
$$T^{(0,1)}\left[\frac{1}{5}, t\right] == 100\left(T\left[\frac{1}{10}, t\right] - 2\,T\left[\frac{1}{5}, t\right] + T\left[\frac{3}{10}, t\right]\right),$$
$$T^{(0,1)}\left[\frac{3}{10}, t\right] == 100\left(T\left[\frac{1}{5}, t\right] - 2\,T\left[\frac{3}{10}, t\right] + T\left[\frac{2}{5}, t\right]\right),$$
$$T^{(0,1)}\left[\frac{2}{5}, t\right] == 100\left(T\left[\frac{3}{10}, t\right] - 2\,T\left[\frac{2}{5}, t\right] + T\left[\frac{1}{2}, t\right]\right),$$
$$T^{(0,1)}\left[\frac{1}{2}, t\right] == 100\left(T\left[\frac{2}{5}, t\right] - 2\,T\left[\frac{1}{2}, t\right] + T\left[\frac{3}{5}, t\right]\right),$$
$$T^{(0,1)}\left[\frac{3}{5}, t\right] == 100\left(T\left[\frac{1}{2}, t\right] - 2\,T\left[\frac{3}{5}, t\right] + T\left[\frac{7}{10}, t\right]\right),$$
$$T^{(0,1)}\left[\frac{7}{10}, t\right] == 100\left(T\left[\frac{3}{5}, t\right] - 2\,T\left[\frac{7}{10}, t\right] + T\left[\frac{4}{5}, t\right]\right),$$
$$T^{(0,1)}\left[\frac{4}{5}, t\right] == 100\left(T\left[\frac{7}{10}, t\right] - 2\,T\left[\frac{4}{5}, t\right] + T\left[\frac{9}{10}, t\right]\right),$$
$$\left.T^{(0,1)}\left[\frac{9}{10}, t\right] == 100\left(T\left[\frac{4}{5}, t\right] - 2\,T\left[\frac{9}{10}, t\right] + T[1, t]\right)\right\}$$

Since $T(0, t) = T_1$and $T(1, t) = T_2$ we have a set of nine coupled ODE's all which are posed as initial value problems. This set of equations can now be sent of to an ODE solver for solution. Of course in practice we will need a finer spatial grid and will thus have many more equations.

An efficient way to implement a finite difference in *Mathematica* is by rotating a list. The *Mathematica* functions RotateRight and RotateLeft rotate a list one element to the right or left respectively. The central difference for the second derivative can be implemented by rotating the list to the right subtracting twice the original list and adding the list rotated to the left. Notice that this effectively sets $h = 1$. This is done by the code below. We will worry shortly about how setting $h$ to 1 effects the scaling of the physical dimensions.

```
Laplacian[data_List, h_: 1] := (RotateRight[data] - 2 data +
RotateLeft[data]) / h^2;
```

The best way to understand exactly what the code does is to test it on a small symbolic list.

```
test = {f[x0], f[x1], f[x2], f[x3], f[x4]}
```

```
{f[x0], f[x1], f[x2], f[x3], f[x4]}
```

```
Laplacian[test, h]
```

$$\left\{\frac{-2 f[x0] + f[x1] + f[x4]}{h^2}, \frac{f[x0] - 2 f[x1] + f[x2]}{h^2}, \frac{f[x1] - 2 f[x2] + f[x3]}{h^2}, \frac{f[x2] - 2 f[x3] + f[x4]}{h^2}, \frac{f[x0] + f[x3] - 2 f[x4]}{h^2}\right\}$$

Notice that it does exactly what we want except at the beginning in ends of the list where the values are wrapped around. If we had periodic boundary conditions, this would be perfect but often the boundaries are held at specified values. In that case, we want to drop the first and last elements and then add the fixed boundary values back to the list. The function **InteriorLaplacian** simply takes all but the first and last elements returned by the function **Laplacian**.

```
InteriorLaplacian[data_List] := Take[Laplacian[data],
    {2, -2}]
```

```
InteriorLaplacian[test]
```

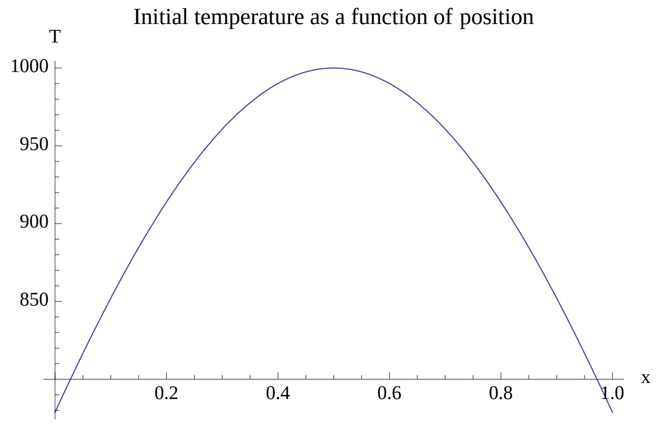
```
{f[x0] - 2 f[x1] + f[x2], f[x1] - 2 f[x2] + f[x3], f[x2] - 2 f[x3] + f[x4]}
```

The function InteriorLaplacian implements the second spatial derivative. We must also implement the time derivative. This is done by the function **NewT**. Notice that this is just the Euler method that we used earlier.

```
Clear[δ, κ];
NewT[data_List, δ_, κ_] := Take[data,
    {2, -2}] + δ κ InteriorLaplacian[data];
```

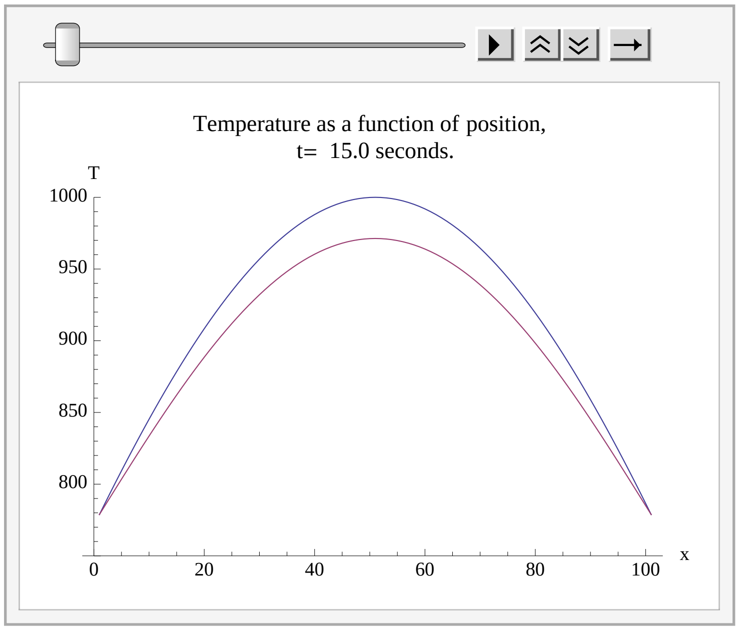
All that remains to be done now is to generate the initial data, the boundary conditions and to iterate. Suppose that we have a rod of unit length with an initial temperature  of 1000 K in the center of the rod and that the temperature is Gaussianly distributed across the rod. Thus, the initial temperature looks like

```
Plot[1000 Exp[- (x - 1 / 2)^2], {x, 0, 1}, AxesLabel → {"x", "T"},
 PlotLabel → "Initial temperature as a function of position"]
```



We will use this temperature distribution as our initial data. The step size with which we sample the initial data will control the spatial grid. In the code below $h$ controls the spatial grid and $\delta$ controls the size of the Euler step. The thermal diffusively  $\kappa$ has been set to 10. The code below produces a 25 frame animation of $T(x, t)$. Each frame of the animation represents 3000 time steps. We should think about what our units are here. We have arbitrarily set the length of the rod to one. If that is one meter then $h = 1$ cm. The time scale is controlled by $\delta$. If we take $\delta = 5 \cdot 10^{-3}\, s$ then the time between frames in the animation is 15 $s$. The thermal diffusivity $\kappa$ has units of length$^2$/time. The length scale of $\kappa$ is determined by $h$ so $\kappa = 10\,\text{cm}^2/s$. If we work in  meters and seconds then $\kappa = 10^{-3}\, m^2/s$. The initial temperature is shown in the light blue curve.

```
Clear[h, δ, κ]
h = 0.01;
δ = 0.005;
κ = 10;
iData = Table[1000 Exp[- (x - 1 / 2)^2], {x, 0, 1, h}];
T = iData;
leftEnd = 1000 Exp[- (1 / 2)^2] // N;
rightEnd = 1000 Exp[- (1 - 1 / 2)^2] // N;

ListAnimate[Table[Do[
    T = NewT[T, δ, κ];
    T = Prepend[T, leftEnd];
    T = Append[T, rightEnd],
       {j, 1, 3000}];


  ListPlot[{iData, T}, PlotJoined -> True, PlotRange -> {750, 1000}, AxesLabel → {"x", "T"},
   PlotLabel → StringJoin["Temperature as a function of position, \n t=" ,
     ToString[PaddedForm[δ 3000 i, {4, 1}]], " seconds."]],

  {i,
   1,
   25}]]
```

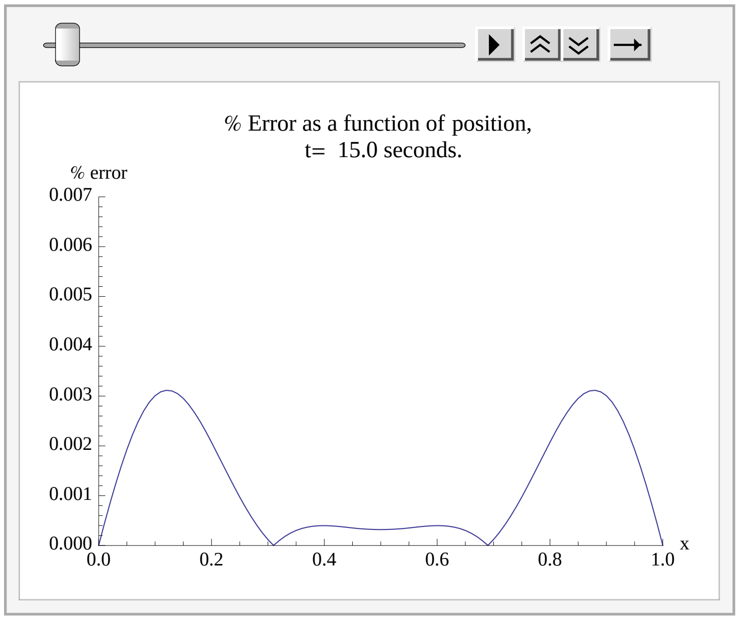


We should ask how accurate our solution is. *Mathematica's* built-in function NDSolve can solve initial value problems of this kind. NDSolve is much more sophisticated than our code. NDSolve uses the method of lines but incorporates (among other things) adaptive steps sizes based on error estimates. The default accuracy goal is one part in $10^6$. We can solve the same equation with NDSolve (note the dramatic speed up in computation time) and compare the two solutions.

```
κ = 10^-3;
Clear[T, result];
result[x_, t_] = NDSolve[{D[T[x, t], t] == κ D[T[x, t], {x, 2}], T[x, 0] == 1000 Exp[- (x - 1 / 2)^2],
     T[0, t] == 1000 Exp[- (1 / 2)^2], T[1, t] == 1000 Exp[- (1 / 2)^2]},
    T[x, t], {x, 0, 1}, {t, 0, 375}][[1, 1, 2]]

InterpolatingFunction[{{0., 1.}, {0., 375.}}, <>][x, t]
```

To compare the two solutions, I will subtract the solution returned by NDSolve from the one returned by my code, square the result, take the square root, divide by the equilibrium temperature and multiply by 100.

```
Clear[h, δ, κ]
h = 0.01;
δ = 0.005;
κ = 10;
iData = Table[1000 Exp[- (x - 1 / 2)^2], {x, 0, 1, h}];
T = iData;
leftEnd = 1000 Exp[- (1 / 2)^2] // N;
rightEnd = 1000 Exp[- (1 - 1 / 2)^2] // N;

ListAnimate[Table[Do[
    T = NewT[T, δ, κ];
    T = Prepend[T, leftEnd];
    T = Append[T, rightEnd],
       {j, 1, 3000}];
  ndsolveData = Table[result[x, δ 3000 i], {x, 0, 1, h}];
  percentError = 100 √((T - ndsolveData)^2) / leftEnd;
  xData = Table[x, {x, 0, 1, h}];
        ListPlot[Transpose[{xData, percentError}],
   PlotJoined -> True, AxesLabel → {"x", "% error"}, PlotRange → {{0, 1}, {0, .007}},
   PlotLabel → StringJoin["% Error as a function of position, \n t=" ,
     ToString[PaddedForm[δ 3000 i, {4, 1}]], " seconds."]],

  {i,
   1,
   25}]]
```



Looking at the animation shows that the two solutions are very close.

**Exercise Six**

Redo the above animation for different values of *δ*and *h*. Make sure that a least one of your choices breaks the code and produces significant numerical error.

Now that we understand how the method of lines works we will use *Mathematica*'s built in function **NDSolve** to solve the Schrö dingequation.

## The dynamics of wave packets

We are now in a position to explore a number of interesting topics in wave packet dynamics, several of which are of current research interest.

### Wave packet scattering off barriers

The standard textbook treatment of barriers considers a single plane wave incident on a barrier and computes the probability of reflection or transmission. This is time-independent. Here I want to consider the more complicated problem of a wave packet scattering off a barrier or barriers and calculate the time evolution of the packet. The first computer generated movies of wave packet scattering were done by Goldberg, Schey and Schwartz [10]. The example I want to consider is the scattering of a Gaussian wave packet of a set of two barriers. The time-dependent Schrö dinger equation is coded below.

```
Clear[V, ℏ, m, ψ]
eqn = ⅈ ℏ D[ψ[x, t], t] == -(ℏ^2 / 2 m) D[ψ[x, t], {x, 2}] + V[x] ψ[x, t]
```

$$i\,\hbar\,\psi^{(0,1)}[x,t] = V[x]\,\psi[x,t] - \frac{1}{2}\,m\,\hbar^2\,\psi^{(2,0)}[x,t]$$

The initial wave shape is taken to be a Gaussian wave packet centered at $x_0$with average momentum of $\hbar\, k_0$ and a width determined by $\sigma_0$. Note that the factor of $e^{i\,k_0\,x}$ makes this a right-moving wave packet. For simplicity we will work with a unit mass particle and in "natural units" where $\hbar = 1$. The initial wave shape provides the initial condition that we need to solve the Schrö dinger equation but we also need two boundary conditions. Physically we want the wave funcion to vanish at $\pm\infty$. To implement this condition numerically we will put our system in a box of length $L$ and require that the wave function vanish at the boundaries of the box.

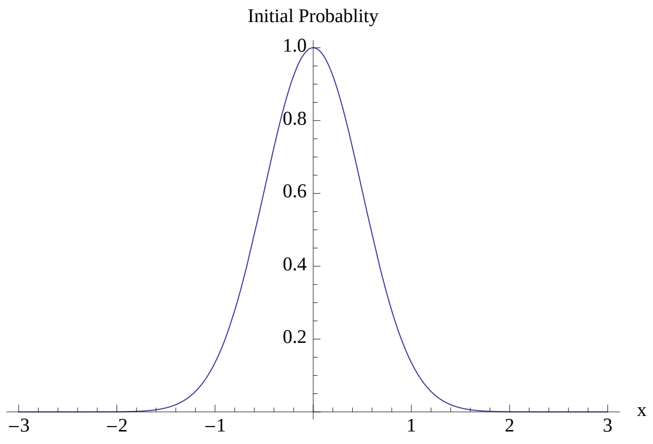
```
InitialWaveFunction = Exp[ⅈ k₀ x] Exp[-(x - x₀)^2 / (2 σ₀^2)]
```

$$e^{i\,k_0\,x-\frac{(x-x_0)^2}{2\,\sigma_0^2}}$$

```
Clear[ψ, k0]
m = 1;
ℏ = 1;
k₀ = 1;
x₀ = 0;
σ₀ = 1 / √2 ;
L = 30;
```

It is important to realize that what we start with is a wave function. To get the initial probability distribution we have to multiply the wave function by its complex conjugate. The initial probability distribution is plotted below.

```
InitialWaveShape = InitialWaveFunction (InitialWaveFunction /. ⅈ → -ⅈ);

Plot[InitialWaveShape, {x, -3, 3}, AxesLabel → {"x", "Initial Probablity"}]
```

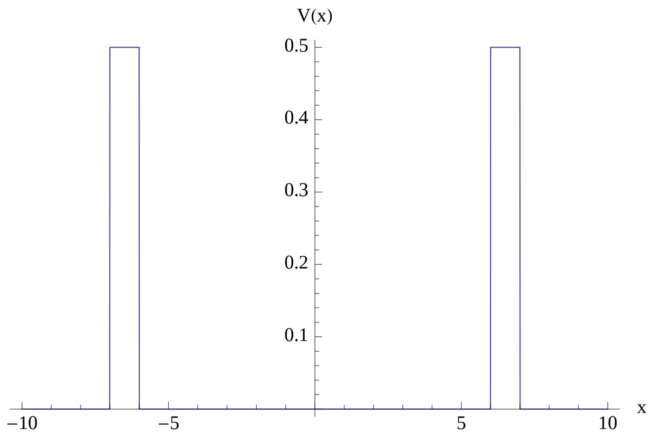


The next step is to define the barriers. I have chosen a barrier height of 1/2. To understand what this means physically, recall that the average momentum of the initial wave packet is $p = \hbar\, k_0$ so the average energy is $E = p^2 / 2\,m = 1/2$. The barriers are plotted below.

```
V[x_] = Piecewise[{{0, x < -7}, {1 / 2, -7 ≤ x ≤ -6}, {0, -6 ≤ x ≤ 6}, {1 / 2, 6 ≤ x ≤ 7}, {0, x > 7}}]
```

$$\begin{cases} 0 & x < -7 \\ \frac{1}{2} & -7 \le x \le -6 \\ 0 & -6 \le x \le 6 \\ \frac{1}{2} & 6 \le x \le 7 \end{cases}$$

```
well = Plot[V[x], {x, -10, 10}, Exclusions → None, AxesLabel → {"x", "V(x)"}]
```



We are now ready to solve the time-dependent Schrö dinger equation. We can just call NDSolve with the appropriate initial condition and boundary conditions. Remember that the double bracket notation is used to ask for a part of an expression, so [[1,1,2]] gives the second sub-part of the first sub-part of the first part. I have also used the function TimeUsed to see how long this computation took. TimeUsed[] gives the amount of CPU time used in the current kernel session. On my machine the calculation takes 24 seconds.

```
Clear[result]
a = TimeUsed[];
result[x_, t_] = NDSolve[{eqn, ψ[x, 0] == InitialWaveFunction, ψ[-L, t] == 0, ψ[L, t] == 0},
   ψ[x, t], {x, -L, L}, {t, 0, 15}][[1, 1, 2]]
TimeUsed[] -
 a

InterpolatingFunction[{{-30., 30.}, {0., 15.}}, <>][x, t]

24.1734
```

We can now multiply the result with its complex conjugate to get the probability density as a function of both space and time. I have used **Chop** to get rid of any small imaginary terms that might arise due to numerical noise.

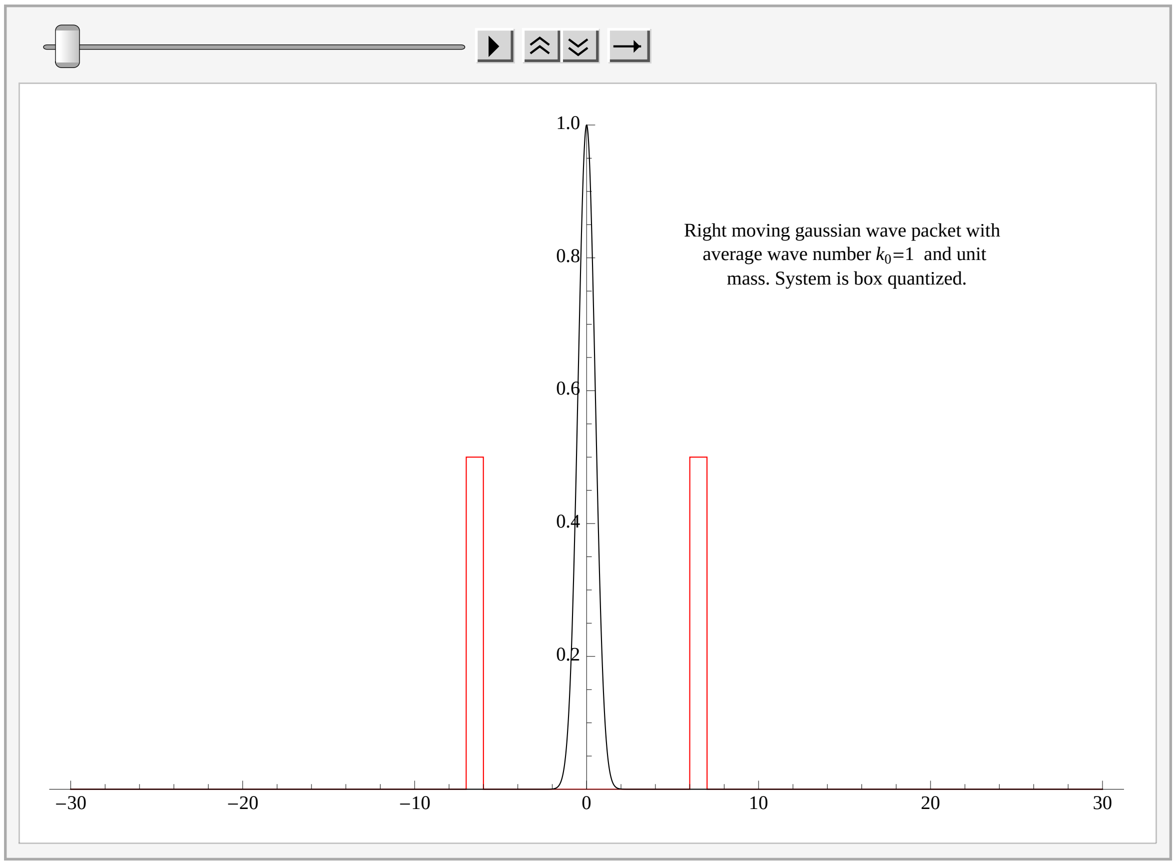
```
Clear[a, b]
wave[x_, t_] := Chop[Times[result[x, t], (result[x, t] /. Complex[a_, b_] → Complex[a, -b])]]
```

The best way to understand the physics of this result is to make an animation of the wave packet. I first generate a plot caption

```
caption = Graphics[
   Text[StyleForm["Right moving gaussian wave packet with \n average wave number k0=1  and
       unit \n mass. System is box quantized.", FontFamily -> "Times"], {15, .8}]];
```

and then animate the motion, showing both the wave packet and the barriers on the same plot.

```
ListAnimate[Table[Show[Plot[{V[x], wave[x, t]}, {x, -30, 30}, Exclusions → None,
    PlotStyle → {RGBColor[1, 0, 0], RGBColor[0, 0, 0], RGBColor[0, 0, 0]},
    PlotRange → {0, 1}, PlotPoints → 200], caption, ImageSize → 7 × 72], {t, 0, 15, .15}]]
```

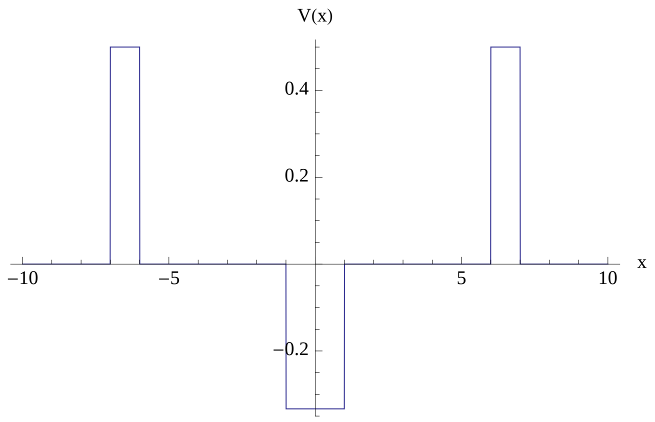


Right moving gaussian wave packet with average wave number $k_0$=1 and unit mass. System is box quantized.
1.0
0.8
0.6
0.4
0.2
−30
−20
−10
0
10
20
30

As you watch the animation you will see the wave packet move to the right (it's a right moving wave after all) and spread out. As it strikes the right barrier we see that there is some probability of reflection and some probability of transmission. When the packet reaches the right wall of the box the wave function is forced vanish by the boundary conditions. This is what causes the sinusoidal ripples!

### Exercise Seven

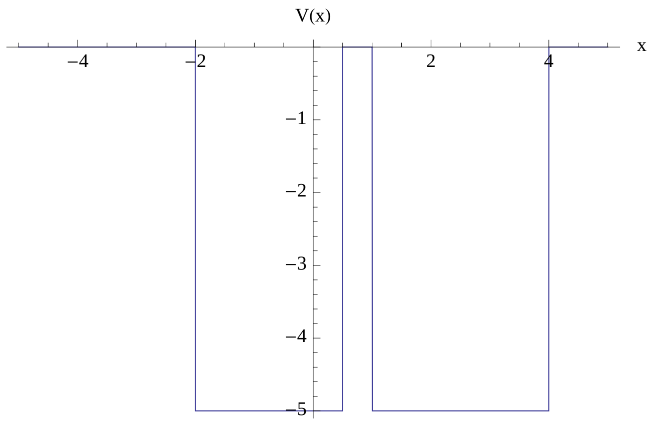
Redo the above animation for the well shown below.



You will get a warning message from NDSolve. Devise and execute a strategy for deciding if the warning message is serious. If it is, fix the problem.

### Charge oscillations

A harder but very interesting problem is charge oscillation in multiple quantum wells. To see charge oscillation you make a multiple quantum well system such as the one shown below. You then make a wave packet that sits in one of the wells. Since the wave packet is not an eigenstate of the total well system (although it may be in an eigenstate one of the wells) the wave packet will oscillate back and forth between the wells. The first experimental work on charge oscillation was done by Loe, Shah, Göbel, Damen, Schmitt-Rink, Schäfer and Köhler [11].
.
Consider the multiple well shown below. The first step is to create a wave packet which is an eigenstate (or a superposition of several eigenstates) of say the right hand well. Experimentally the wave packet is often a superposition of several states but for simplicity we will start with a wave packets that is in a definite energy eigenstate.



Multiple quantum well structure suitable for observing charge oscillations.

The well shown above is given by

```
Clear[V]
V[x_] = Piecewise[{{0, x < -2}, {-5, -2 < x < 1 / 2}, {0, 1 / 2 < x < 1}, {-5, 1 < x < 4}}]
```

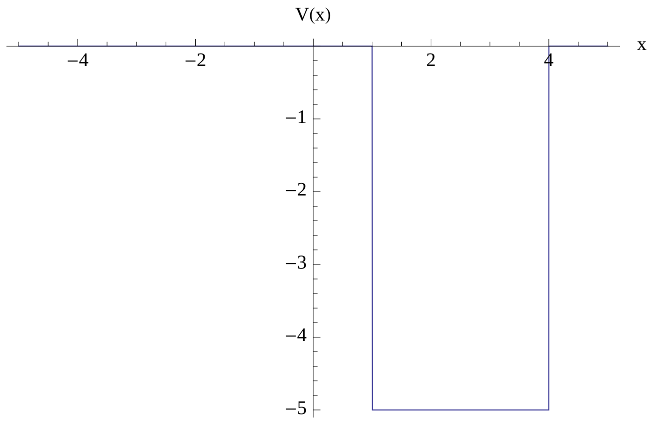
$$\begin{cases} 0 & x < -2 \\ -5 & -2 < x < \frac{1}{2} \\ 0 & \frac{1}{2} < x < 1 \\ -5 & 1 < x < 4 \end{cases}$$

The first step is to specify the initial wave packet. We want this to be an energy eigenstate of the right-hand well. This well is given by

```
Clear[VRight]
VRight[x_] = Piecewise[{{0, x < 1}, {-5, 1 < x < 4}}]
```

$$\begin{cases} 0 & x < 1 \\ -5 & 1 < x < 4 \end{cases}$$

```
Plot[VRight[x], {x, -5, 5}, Exclusions → None, AxesLabel → {"x", "V(x)"}]
```



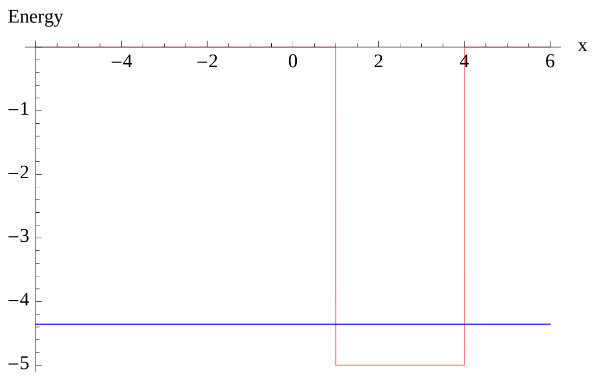
We can use the numerical code that we developed earlier to find the ground state of this well. Of course since this is a finite square well, we could also find the ground state just by solving a set of transcendental equations (see for example Phillips[4]). However, the purely numerical approach will allow us to easily generalize our method to coupled wells of arbitrary shape. For convenience I have bundled all the code we developed for finding bound states into a single function called EigenSolver. For input the function takes the potential, the range over which you want to find the wave function, the point at which you want to match the left and right wave functions, and a initial guess for the energy. The function returns the energy, a plot of the potential with the energy of the bound state drawn as a blue line and a plot of the probability distribution. A tooltip shows the equation for the potential upon mouse over. The wave function is stored as an global variable called "wave function."

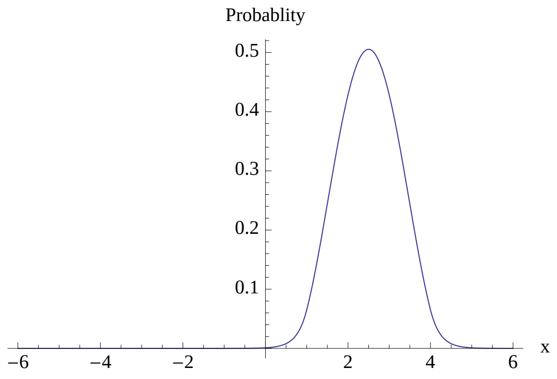
```
Developer`SetSystemOptions["EvaluateNumericalFunctionArgument" → False];
EigenSolver[V_, {q_, qmin_, qmax_}, matchPoint_, EnergyGuess_] :=
 Module[{MatchingPoint, leftψ, rightψ, scaleLeft,
   scaleRight, DRight, DLeft, result, normalization, plot1, plot2, ψ},
  MatchingPoint = Rule[q, matchPoint];
  leftψ[ϵ_, q] :=
   First[NDSolve[{-D[ψ[q], {q, 2}] + V ψ[q] == ϵ ψ[q], ψ'[qmin] == 0.0001, ψ[qmin] == 0},
      ψ[q], {q, qmin, q /. MatchingPoint}]][[1, 2]];
rightψ[ϵ_, q] := First[NDSolve[{-D[ψ[q], {q, 2}] + V ψ[q] == ϵ ψ[q], ψ'[qmax] == 0.0001,
       ψ[qmax] == 0}, ψ[q], {q, qmax, q /. MatchingPoint}]][[1, 2]];
  scaleLeft[ϵ_] := leftψ[ϵ, q] /. MatchingPoint;
scaleRight[ϵ_] := rightψ[ϵ, q] /. MatchingPoint;
scaledLeft[ϵ_, q] := leftψ[ϵ, q] scaleRight[ϵ] / scaleLeft[ϵ];
DRight[ϵ_, q] := D[rightψ[ϵ, q], q];
DLeft[ϵ_, q] := D[scaledLeft[ϵ, q], q];
  Energy = ϵ /. FindRoot[(DLeft[ϵ, q] /. MatchingPoint) == (DRight[ϵ, q] /. MatchingPoint),
     {ϵ, EnergyGuess, EnergyGuess + EnergyGuess / 10.0}];
  result = First[ψ[q] /. NDSolve[{-D[ψ[q], {q, 2}] + V ψ[q] == Energy ψ[q],
       ψ'[qmin] == 0.0001, ψ[qmin] == 0}, ψ[q], {q, qmin, qmax}]];
  normalization = 1 / √(NIntegrate[result^2, {q, qmin, qmax}]) ;
  wavefunction := normalization result;
  plot1 = Show[Plot[Tooltip[V, ToString[TraditionalForm[V]]], {q, qmin, qmax},
     PlotPoints -> 100, Exclusions → None, PlotStyle -> {RGBColor[1, 0, 0], Opacity[.5]},
     AxesOrigin -> {qmin, 0}, AxesLabel → {"x", "Energy"}],
    Graphics[{RGBColor[0, 0, 1], Line[{{qmin, Energy}, {qmax, Energy}}]}]];
  plot2 = Plot[normalization^2 result^2, {q, qmin, qmax}, PlotRange -> All,
    AxesLabel -> {"x", "Probablity"}, RotateLabel -> True];
  Print[StringJoin["Energy=", ToString[Energy]]];
  GraphicsArray[{{plot1}, {plot2}}]]
```

We can now run our code on the right-hand well to find the ground state.

```
EigenSolver[VRight[x], {x, -6, 6}, 1, -4]
```

```
Energy=-4.35595
```





There is one small complication. The function EigenSolver has returned the wave function only over the interval $-6 < x < 6$ but we will want to solve the time-dependent Schrö dingequation over the larger interval since we have two wells. The method used for finding the wave function breaks down if we try to solve on intervals which are too large compared to the extent of the well. You should try this for yourself! However we know that for bound states the wave function must vanish at infinity, so we can define an initial wave by simply setting the wave function to zero ousidet the interval $-6 < x < 6$. You should check the value of the wave function at $x = 6$ to convince yourself that this is legitimate.

```
initialShape = Piecewise[{{0, x < -6}, {wavefunction, -6 < x < 6}, {0, x > 6}}]
```

```
⎡ 0                                                              x < -6
⎣ 0.00481173 InterpolatingFunction[{{-6., 6.}}, <>][x]   -6 < x < 6
```

We are now ready to solve the time-dependent Schrö dingequation. Just as before we will force the wave function to zero at the ends of a box. The box length should be "large" compared to the region occupied by the wells.

```
eqn = ⅈ ℏ D[ψ[x, t], t] == -(ℏ^2 / 2 m) D[ψ[x, t], {x, 2}] + V[x] ψ[x, t]
```

$$i\,\psi^{(0,1)}[x,t] == \begin{cases} 0 & x < -2 \\ -5 & -2 < x < \frac{1}{2} \\ 0 & \frac{1}{2} < x < 1 \\ -5 & 1 < x < 4 \end{cases} \psi[x,t] - \frac{1}{2}\psi^{(2,0)}[x,t]$$

Trying the standard call to NDSolve (given below) reveals problems. The cell below has been made inactive to prevent you from accidentally evaluating it. You can change this from the Cell menu using the Cell Properties sub-menu. If you evaluate it you will find that the code takes a very long time to run, uses a huge amount of virtual memory and depending on your machine may cause the kernel to quit with an out of memory error.

```
L = 14;
m = 1;
ℏ = 1;
wavefunction2[x_, t_] = NDSolve[{eqn, ψ[x, 0] == initialShape, ψ[-L, t] == 0, ψ[L, t] == 0},
    ψ[x, t], {x, -L, L}, {t, 0, 40}, MaxSteps → 40 000][[1, 1, 2]];
```

To get a solution we must give NDSolve some help. The default method over-samples in the spatial dimension and thus breaks the PDE up into more ODE's than is necessary. However NDSolve offers the user great control over the method used and the number of points sampled. We can use the Method option to select the method that we want to use. I have chosen the Method of Lines (the only method currently implemented for this type of problem), picked a tensor product grid for the spacial discretization, and most importantly set the spacial grid to 400 points by specifying that the maximum and minimum number of grid points should be 400. I am indebted Rob Knapp of Wolfram Research for help with selecting the best method. You can read about the options available for NDSolve in the advanced documentation for NDSolve.

```
kernalTime = TimeUsed[];
nx = 400;
tend = 40;
L = 14;
m = 1;
ℏ = 1;
Clear[wavefunction]
wavefunction2[x_, t_] =
  NDSolve[{eqn, ψ[x, 0] == initialShape, ψ[-L, t] == 0, ψ[L, t] == 0}, ψ[x, t], {x, -L, L},
    {t, 0, tend}, MaxSteps → 40 000, Method → {"MethodOfLines", "SpatialDiscretization" →
       {"TensorProductGrid", "MinPoints" → nx, "MaxPoints" → nx}}][[1, 1, 2]];
TimeUsed[] -
 kernalTime
```

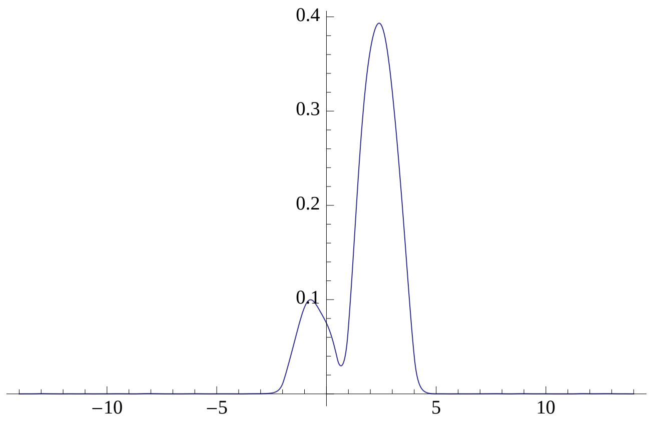
```
NDSolve::eerri : Warning: Estimated initial error on the specified spatial grid
      in the direction of independent variable x exceeds prescribed error tolerance. ≫

NDSolve::eerr :
  Warning: Scaled local spatial error estimate of 72.51237912860316` at t = 40.` in the direction
      of independent variable x is much greater than prescribed error tolerance.
      Grid spacing with 400 points may be too large to achieve the desired accuracy
      or precision.  A singularity may have formed or you may want to specify a
      smaller grid spacing using the MaxStepSize or MinPoints method options. ≫

30.3517
```

With this method the code is fairly fast but you notice that we get a warning message about the accuracy. We will have to check the accuracy of our result but first we will plot the probability distribution. We need the wave function times its complex conjugate.

```
wave[x_, t_] :=
 Chop[Times[wavefunction2[x, t], (wavefunction2[x, t] /. Complex[a_, b_] → Complex[a, -b])]]
```

Plotting this at say $t = 20$gives a result that looks reasonable.

```
Plot[wave[x, 20], {x, -L, L}, PlotRange → All]
```



To check the accuracy of the result we can double the number of grid points used by setting MaxPoints and MinPoints to 800. Not surprisingly this doubles the computation time. I have called the result HPwavefunction (for high precision wave function.)

```
kernalTime = TimeUsed[];
nx = 800;
tend = 40;
L = 14;
m = 1;
ħ = 1;
Clear[wavefunction]
HPwavefunction[x_, t_] =
  NDSolve[{eqn, ψ[x, 0] == initialShape, ψ[-L, t] == 0, ψ[L, t] == 0}, ψ[x, t], {x, -L, L},
    {t, 0, tend}, MaxSteps → 40 000, Method → {"MethodOfLines", "SpatialDiscretization" →
       {"TensorProductGrid", "MinPoints" → nx, "MaxPoints" → nx}}][[1, 1, 2]];
TimeUsed[] -
 kernalTime
```

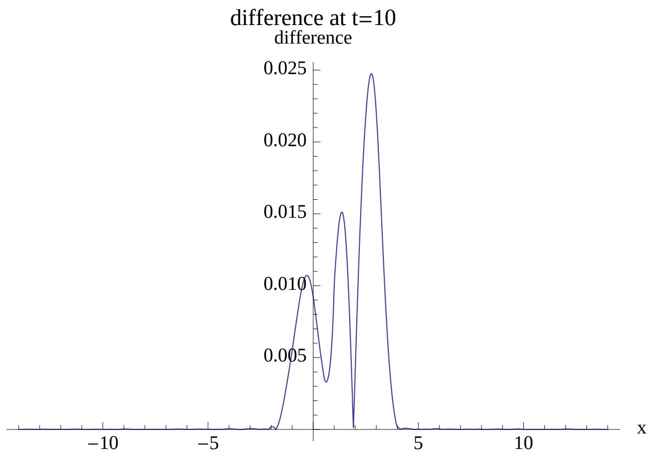
```
NDSolve::eerri : Warning: Estimated initial error on the specified spatial grid
      in the direction of independent variable x exceeds prescribed error tolerance. ≫

NDSolve::eerr :
  Warning: Scaled local spatial error estimate of 85.12360160741603` at t = 40.` in the direction
      of independent variable x is much greater than prescribed error tolerance.
      Grid spacing with 800 points may be too large to achieve the desired accuracy
      or precision.  A singularity may have formed or you may want to specify a
      smaller grid spacing using the MaxStepSize or MinPoints method options. ≫

67.3942
```

We can now form the probability distribution

```
HPwave[x_, t_] :=
 Chop[Times[HPwavefunction[x, t], (HPwavefunction[x, t] /. Complex[a_, b_] → Complex[a, -b])]]
```

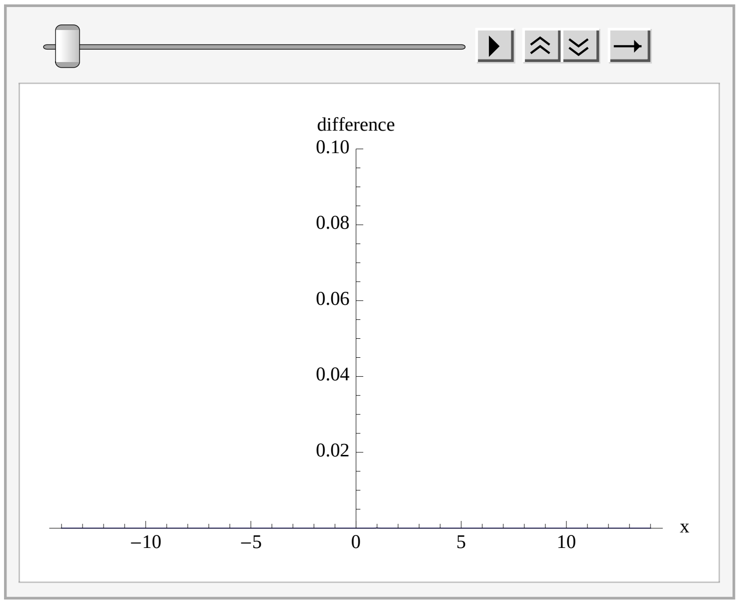
and compare the absolute value of the difference between our result with 800 grid points and the result with 400 grid points. The plot below shows the difference at $t = 10$.

```
Plot[Abs[HPwave[x, 10] - wave[x, 10]], {x, -L, L}, PlotRange → All,
 PlotLabel → "difference at t=10", AxesLabel -> {"x", "difference"}]
```



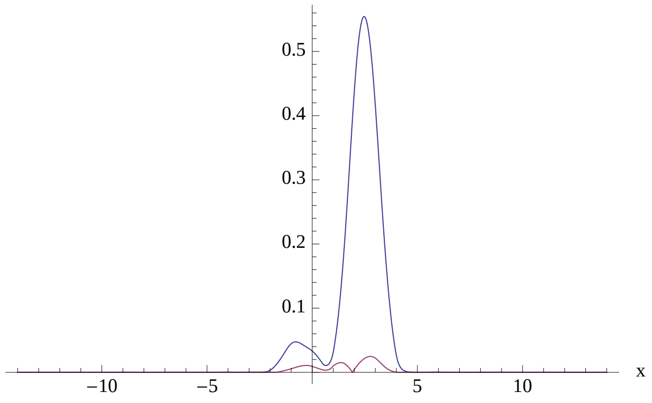
These errors look small but we are faced with the question of what to compare them to. In other word,s small compared to what? We can not compute a percent error by dividing by the probability distribution because the probability distribution is zero at several points. We also have only a snapshot in time. Maybe the errors are worse later. This question is easily answered with an animation in time.

```
ListAnimate[Table[Plot[Abs[HPwave[x, t] - wave[x, t]], {x, -L, L},
   PlotRange → {0, 0.1}, AxesLabel → {"x", "difference"}], {t, 0, 40, 1}]]
```



The hard question is small compared to what? We can compare the error to the probability distribution itself.

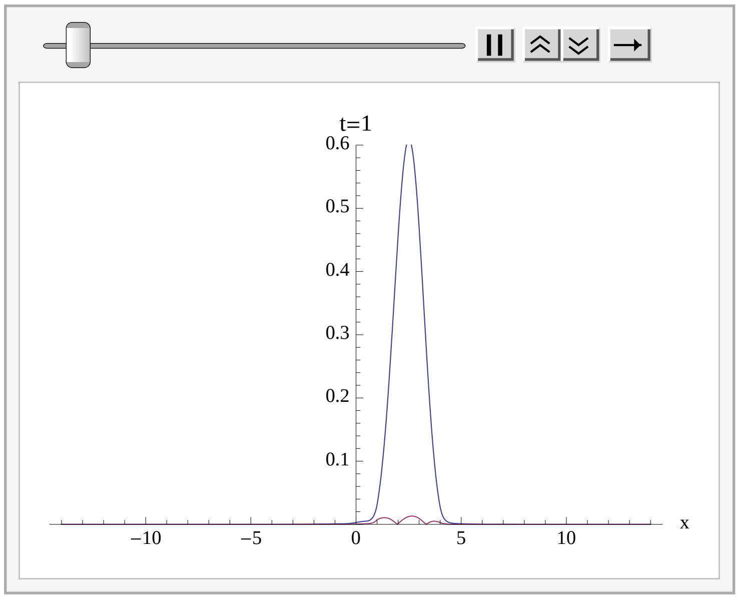
```
Plot[{HPwave[x, 10], Abs[HPwave[x, 10] - wave[x, 10]]},
  {x, -L, L}, PlotRange → All, AxesLabel → {"x", None}]
```



The error in the probability distribution is shown in purple. The probability distribution itself is in blue.

This still looks good but what about at other times? If we animate the result

```
ListAnimate[
 Table[Plot[{HPwave[x, t], Abs[HPwave[x, t] - wave[x, t]]}, {x, -L, L}, PlotRange → {0, .6},
   AxesLabel → {"x", None}, PlotLabel → StringJoin["t=", ToString[t]]], {t, 0, 40, 1}]]
```



The error in the probability distribution is shown in purple. The probability distribution itself is in blue.

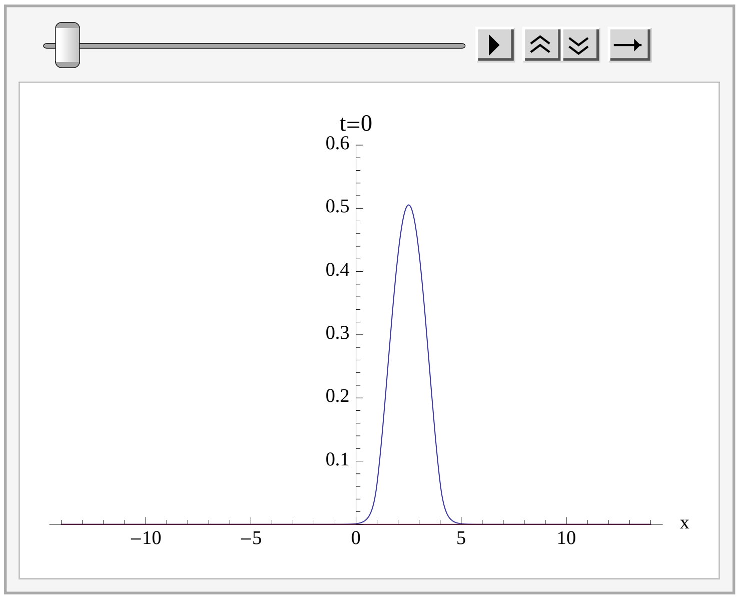
we see that although the results are good overall, at $t = 36$ the error in the region $x < 0$ is almost as large as the function itself. This should not be too surprising since the overall value of the function is small in that region. When the absolute value of a function is small even a small absolute error is a large relative error. The solution as it stands may well be good enough. It all depends on what you want it for. If you really need a high accuracy solution for all $x$ and $t$ you can always double the number of grid points again. Of course you pay a price in both memory and CPU time. This is done below.

```
kernalTime = TimeUsed[];
nx = 1600;
tend = 40;
L = 14;
m = 1;
ℏ = 1;
Clear[wavefunction]
VHPwavefunction[x_, t_] =
  NDSolve[{eqn, ψ[x, 0] == initialShape, ψ[-L, t] == 0, ψ[L, t] == 0}, ψ[x, t], {x, -L, L},
    {t, 0, tend}, MaxSteps → 40 000, Method → {"MethodOfLines", "SpatialDiscretization" →
       {"TensorProductGrid", "MinPoints" → nx, "MaxPoints" → nx}}][[1, 1, 2]];
TimeUsed[] -
 kernalTime
```

```
NDSolve::eerri : Warning: Estimated initial error on the specified spatial grid
      in the direction of independent variable x exceeds prescribed error tolerance. ≫

NDSolve::eerr :
  Warning: Scaled local spatial error estimate of 86.06675379188026` at t = 40.` in the direction
      of independent variable x is much greater than prescribed error tolerance. Grid
      spacing with 1600 points may be too large to achieve the desired accuracy
      or precision.  A singularity may have formed or you may want to specify a
      smaller grid spacing using the MaxStepSize or MinPoints method options. ≫

155.107
```

```
VHPwave[x_, t_] := Chop[
  Times[VHPwavefunction[x, t], (VHPwavefunction[x, t] /. Complex[a_, b_] → Complex[a, -b])]]
```

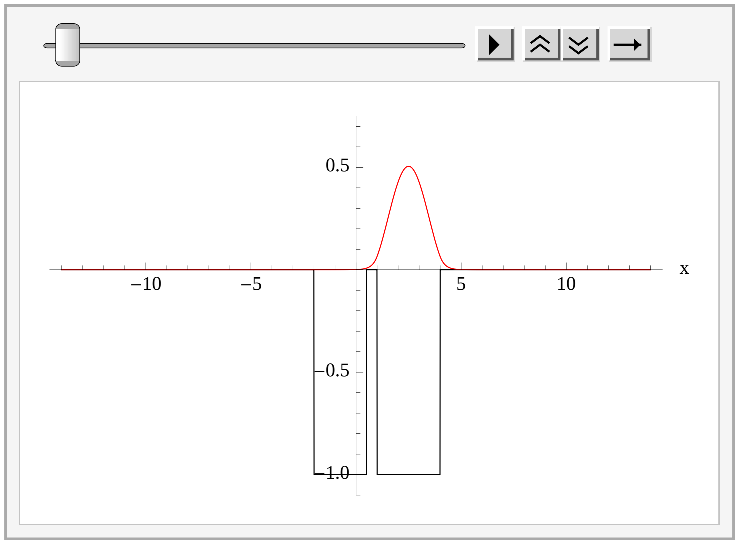
```
ListAnimate[
 Table[Plot[{VHPwave[x, t], Abs[VHPwave[x, t] - HPwave[x, t]]}, {x, -L, L}, PlotRange → {0, .6},
   AxesLabel → {"x", None}, PlotLabel → StringJoin["t=", ToString[t]]], {t, 0, 40, 1}]]
```



The error in the probability distribution is shown in purple. The error is the absolute value of the difference between using 800 grid points and 1600 grid points.The probability distribution itself is in blue.

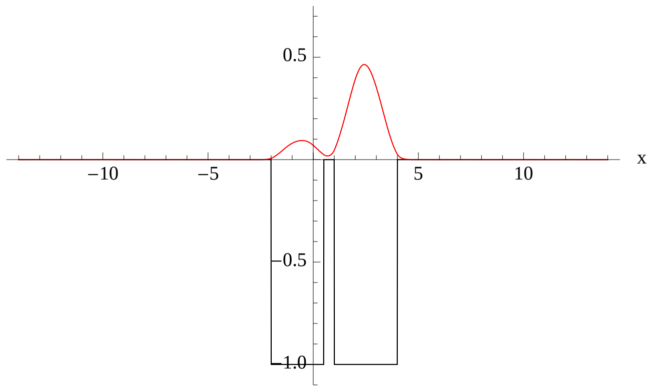
Now that we have confidence that we understand the accuracy of our solution, we should plot it and the well structure on the same plot. I have scaled the well by 1/5 for visual clarity.

```
wavePlot = ListAnimate[Table[
   Plot[{.2 V[x], VHPwave[x, t]}, {x, -L, L}, PlotStyle → {RGBColor[0, 0, 0], RGBColor[1, 0, 0]},
    PlotRange → {-1.1, .75}, Exclusions → None, AxesLabel → {"x", None}], {t, 0, 40, 1}]]
```



The time dependent probability density is shown in red. The upper *y*-axis shows the probability of finding the particle. The lower *y* axis gives the well depth. Well depths are scaled by a factor of 1/5 so -1 on the figure corresponds to -5. The well structure is shown in black.

Looking at the animation we see that probability of finding the particle is always higher in the righ- hand well, but that we get some oscillation into the left-hand well.  If we look at a time when there is a significant probability of finding the wave packet in the left well we see that the distances between the nodes in the left and right wells are the same. Since the energy of the packet is proportional to the distance between the nodes, this tells us that our solution conservers energy which is reassuring.



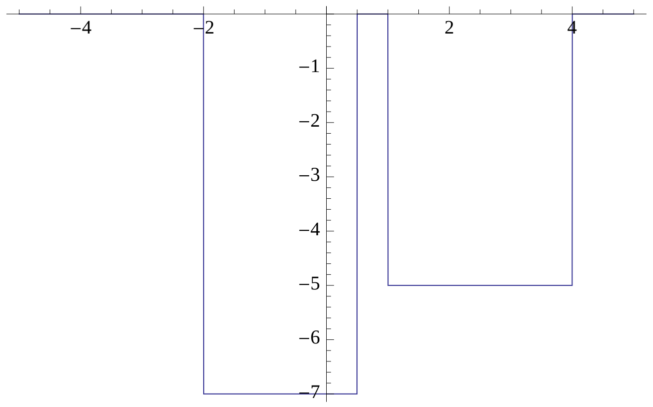
Oscillation into the second well. Note the wavelength of the left peak.

If we make the left well some what deeper we will get more oscillation into the left well.  Suppose we have the following well.

```
Clear[V]
V[x_] = Piecewise[{{0, x < -2}, {-7, -2 < x < 1/2}, {0, 1/2 < x < 1}, {-5, 1 < x < 4}}]
```

$$\begin{cases} 0 & x < -2 \\ -7 & -2 < x < \frac{1}{2} \\ 0 & \frac{1}{2} < x < 1 \\ -5 & 1 < x < 4 \end{cases}$$

```
Plot[V[x], {x, -5, 5}, Exclusions → None]
```



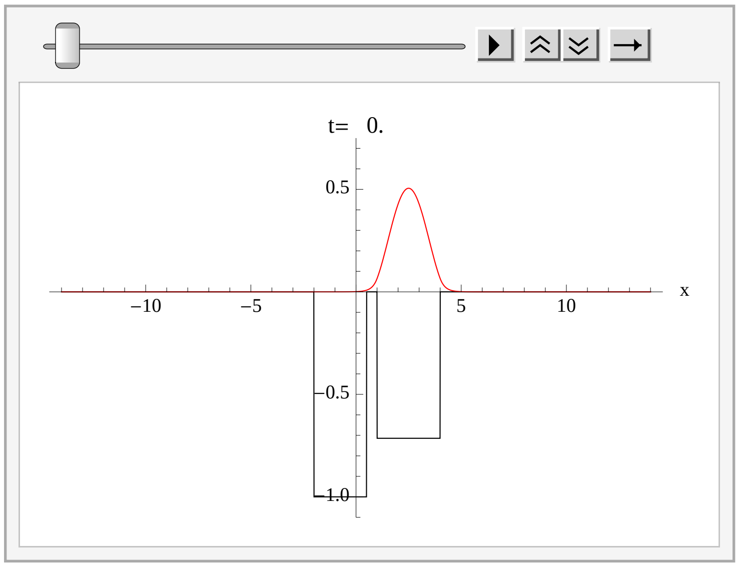
Since the right hand well is unchanged we can use the same initial shape as before and simply repeat the calculation with the new potential.

```
nx = 400;
tend = 40;
L = 14;
m = 1;
ℏ = 1;
Clear[wavefunction]
wavefunction[x_, t_] =
  NDSolve[{eqn, ψ[x, 0] == initialShape, ψ[-L, t] == 0, ψ[L, t] == 0}, ψ[x, t], {x, -L, L},
    {t, 0, tend}, MaxSteps → 40 000, Method → {"MethodOfLines", "SpatialDiscretization" →
      {"TensorProductGrid", "MinPoints" → nx, "MaxPoints" → nx}}][[1, 1, 2]];
```

```
NDSolve::eerri : Warning: Estimated initial error on the specified spatial grid
     in the direction of independent variable x exceeds prescribed error tolerance. ≫

NDSolve::eerr :
  Warning: Scaled local spatial error estimate of 72.51237912860316` at t = 40.` in the direction
     of independent variable x is much greater than prescribed error tolerance.
     Grid spacing with 400 points may be too large to achieve the desired accuracy
     or precision.  A singularity may have formed or you may want to specify a
     smaller grid spacing using the MaxStepSize or MinPoints method options. ≫
```

```
wave[x_, t_] :=
 Chop[Times[wavefunction[x, t], (wavefunction[x, t] /. Complex[a_, b_] → Complex[a, -b])]]
```

```
wavePlot = ListAnimate[Table[Plot[{(1 / 7) V[x], wave[x, t]},
    {x, -L, L}, PlotStyle → {RGBColor[0, 0, 0], RGBColor[1, 0, 0]},
    PlotRange → {-1.1, .75}, Exclusions → None, AxesLabel → {"x", None},
    PlotLabel → StringJoin["t=", ToString[PaddedForm[t, 3]]]], {t, 0, 40, .5}]]
```



The time dependent probability density is shown in red. The upper *y*-axis shows the probability of finding the particle. The lower *y* axis gives the well depth. Well depths are scaled by a factor of 1/7 so -1 on the figure corresponds to -7. The well structure is shown in black.

In experiments what is detected is not the oscillation of the wave packet, but rather the electromagnetic radiation emitted due to the acceleration of the charge density. The experiments [11,12,13] measure the emitted power which is propositional to the square of the acceleration. An accurate calculation of the emitted radiation is a hard problem that is beyond the scope of this module. However we can see the qualitative features of the radiation by just computing the acceleration of the wave packet. The major flaw in this approach is that it does not take into account the energy the wave packet loses due to the radiation. The first step is to compute $< x >$. We can then differentiate the result to get the average acceleration. Since $< x > = \int \psi^* \, x \, \psi \, dx$ we can compute it with the code below.

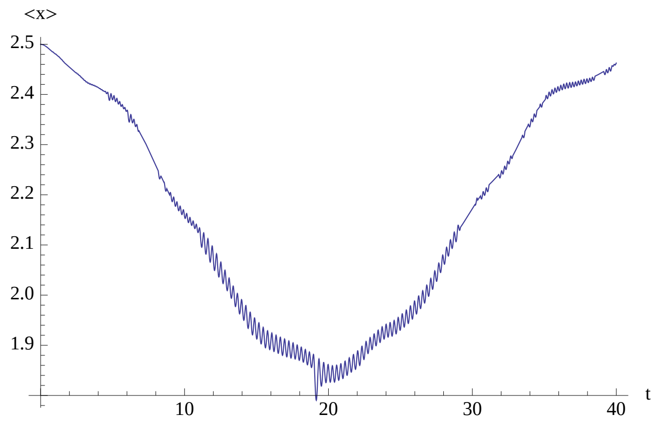
```
integrand[x_, t_] :=
 Chop[(wavefunction[x, t] /. Complex[a_, b_] → Complex[a, -b]) x wavefunction[x, t]]
```

Version 6.0 can not do the integral analytically and so we must resort to numerical integration.

```
Clear[xAverage]
xAverage[t_] := NIntegrate[integrand[x, t], {x, -14, 14}]
```

Plotting the result shows that there maybe a problem.

```
xAveragePlot = Plot[xAverage[t], {t, 0, 40}, AxesLabel → {"t", "<x>"}]
```



The function does not look very smooth and we need to take two time derivatives of it. Taking a derivative always gives a result that is less smooth then the original function. The first question to ask is our solution accurate enough to give an accurate value for $<x>$? We can answer this question by computing a solution with more grid points and comparing the answers. The solution from which the plot of xAverage was generated was computed using 400 grid points. Let's try 800. I have called the result HPwavefunction (for high precision wave function).

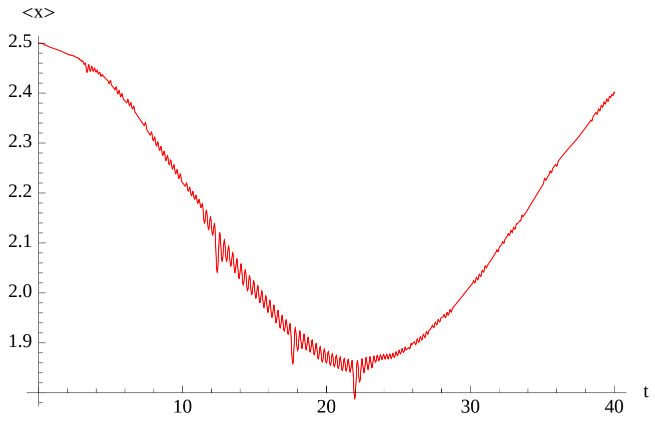
```
nx = 800;
tend = 40;
L = 14;
m = 1;
ℏ = 1;
Clear[HPwavefunction]
HPwavefunction[x_, t_] =
  NDSolve[{eqn, ψ[x, 0] == initialShape, ψ[-L, t] == 0, ψ[L, t] == 0}, ψ[x, t], {x, -L, L},
    {t, 0, tend}, MaxSteps → 100 000, Method → {"MethodOfLines", "SpatialDiscretization" →
      {"TensorProductGrid", "MinPoints" → nx, "MaxPoints" → nx}}][[1, 1, 2]];
```

```
NDSolve::eerri : Warning: Estimated initial error on the specified spatial grid
     in the direction of independent variable x exceeds prescribed error tolerance. ≫

NDSolve::eerr :
  Warning: Scaled local spatial error estimate of 85.12360160741603` at t = 40.` in the direction
     of independent variable x is much greater than prescribed error tolerance.
     Grid spacing with 800 points may be too large to achieve the desired accuracy
     or precision.  A singularity may have formed or you may want to specify a
     smaller grid spacing using the MaxStepSize or MinPoints method options. ≫
```

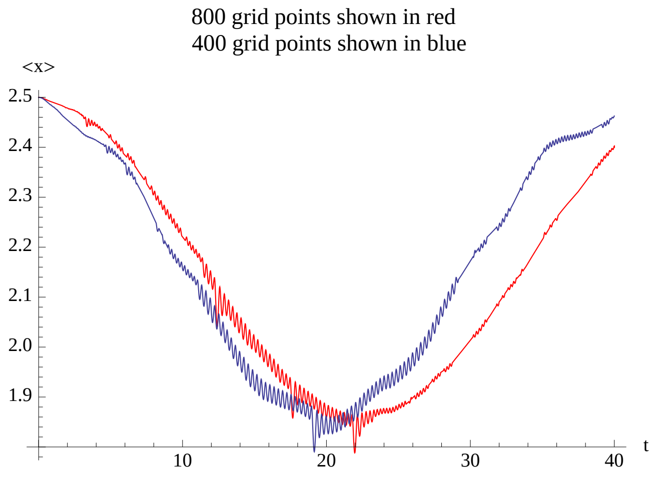
We now form the probability density and the integrand we need to compute $<x>$ just as before. The variables have all been renamed with an HP as the first two letters.

```
HPwave[x_, t_] :=
 Chop[Times[HPwavefunction[x, t], (HPwavefunction[x, t] /. Complex[a_, b_] → Complex[a, -b])]]

HPintegrand[x_, t_] :=
 Chop[(HPwavefunction[x, t] /. Complex[a_, b_] → Complex[a, -b]) x HPwavefunction[x, t]]

Clear[HPxAverage]
HPxAverage[t_] := NIntegrate[HPintegrand[x, t], {x, -14, 14}]
```

```
HPxAveragePlot = Plot[HPxAverage[t], {t, 0, 40}, PlotStyle → Red, AxesLabel → {"t", "<x>"}]
```



```
Show[HPxAveragePlot, xAveragePlot,
 PlotLabel → "800 grid points shown in red \n 400 grid points shown in blue",
 AxesLabel → {"t", "<x>"}]
```



The two plots don't look very much alike so we should try using a still finer grid, say 1200 points and 2400 points. Here I have tagged the variable names with VHP (for very-high precision) for the 1200 point grid and UH (for ultra-high precision) for the 2400 point grid. Notice that this example shows that the degree of accuracy needed depends on what we want to do with the data. The two grid spacings will yield  wave packet oscillations that look very much the same but will give significantly different accelerations.

```
nx = 1200;
tend = 40;
L = 14;
m = 1;
ℏ = 1;
Clear[VHPwavefunction]
VHPwavefunction[x_, t_] =
  NDSolve[{eqn, ψ[x, 0] == initialShape, ψ[-L, t] == 0, ψ[L, t] == 0}, ψ[x, t], {x, -L, L},
    {t, 0, tend}, MaxSteps → 100 000, Method → {"MethodOfLines", "SpatialDiscretization" →
       {"TensorProductGrid", "MinPoints" → nx, "MaxPoints" → nx}}][[1, 1, 2]];
```

```
NDSolve::eerri : Warning: Estimated initial error on the specified spatial grid
      in the direction of independent variable x exceeds prescribed error tolerance. ≫
```

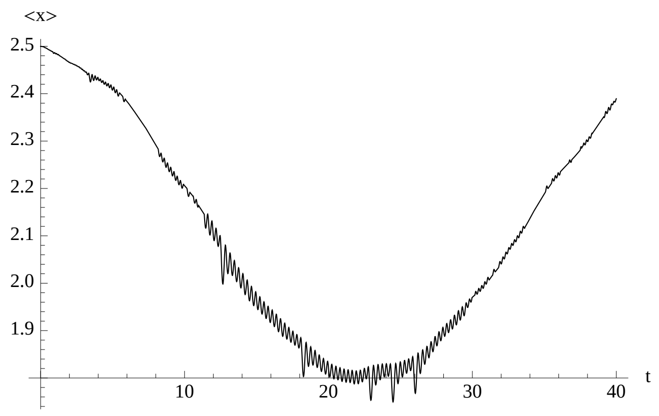
```
NDSolve::eerr :
  Warning: Scaled local spatial error estimate of 88.69468009444732` at t = 40.` in the direction
      of independent variable x is much greater than prescribed error tolerance. Grid
      spacing with 1200 points may be too large to achieve the desired accuracy
      or precision.  A singularity may have formed or you may want to specify a
      smaller grid spacing using the MaxStepSize or MinPoints method options. ≫
```

```
VHPwave[x_, t_] := Chop[
  Times[VHPwavefunction[x, t], (VHPwavefunction[x, t] /. Complex[a_, b_] → Complex[a, -b])]]
```

```
VHPintegrand[x_, t_] :=
 Chop[(VHPwavefunction[x, t] /. Complex[a_, b_] → Complex[a, -b]) x VHPwavefunction[x, t]]
```

```
Clear[VHPxAverage]
VHPxAverage[t_] := NIntegrate[VHPintegrand[x, t], {x, -14, 14}]
```

```
VHPxAveragePlot = Plot[VHPxAverage[t], {t, 0, 40}, AxesLabel → {"t", "<x>"}, PlotStyle → Black]
```



```
nx = 2400;
tend = 40;
L = 14;
m = 1;
ℏ = 1;
Clear[UHwavefunction]
UHwavefunction[x_, t_] =
  NDSolve[{eqn, ψ[x, 0] == initialShape, ψ[-L, t] == 0, ψ[L, t] == 0}, ψ[x, t], {x, -L, L},
    {t, 0, tend}, MaxSteps → 100 000, Method → {"MethodOfLines", "SpatialDiscretization" →
       {"TensorProductGrid", "MinPoints" → nx, "MaxPoints" → nx}}][[1, 1, 2]];
```

```
NDSolve::eerri : Warning: Estimated initial error on the specified spatial grid
      in the direction of independent variable x exceeds prescribed error tolerance. ≫
```

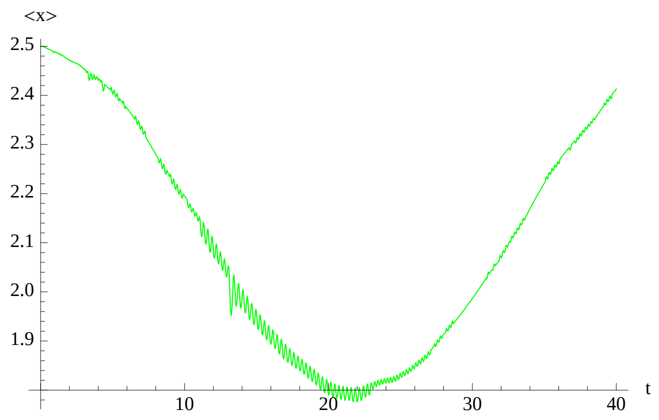
```
NDSolve::eerr :
  Warning: Scaled local spatial error estimate of 83.77951047058218` at t = 40.` in the direction
      of independent variable x is much greater than prescribed error tolerance. Grid
      spacing with 2400 points may be too large to achieve the desired accuracy
      or precision.  A singularity may have formed or you may want to specify a
      smaller grid spacing using the MaxStepSize or MinPoints method options. ≫
```

```
UHwave[x_, t_] :=
 Chop[Times[UHwavefunction[x, t], (UHwavefunction[x, t] /. Complex[a_, b_] → Complex[a, -b])]]
```

```
UPintegrand[x_, t_] :=
 Chop[(UHwavefunction[x, t] /. Complex[a_, b_] → Complex[a, -b]) x UHwavefunction[x, t]]
```

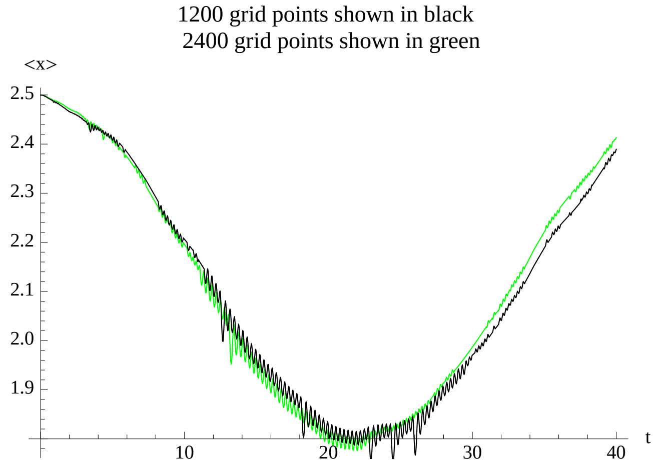
```
Clear[UPxAverage]
UPxAverage[t_] := NIntegrate[UPintegrand[x, t], {x, -14, 14}]
```

```
UPxAveragePlot = Plot[UPxAverage[t], {t, 0, 40}, PlotStyle → Green, AxesLabel → {"t", "<x>"}]
```



Comparison of the two plots shows that they are still not quite the same.

```
Show[UPxAveragePlot, VHPxAveragePlot,
 PlotLabel → "1200 grid points shown in black \n 2400 grid points shown in green"]
```



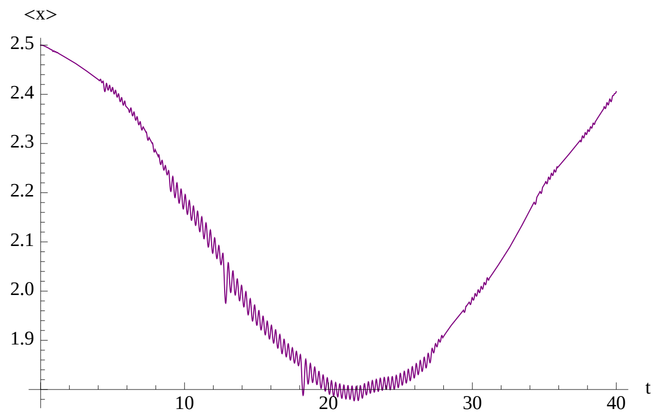
If we try a still finer grid say with 3600 grid points we see that we have finely converged. For the 3600 point grid I have tagged the variables with the letters EH (extremely high).

```
nx = 3600;
tend = 40;
L = 14;
m = 1;
ℏ = 1;
Clear[EHwavefunction]
EHwavefunction[x_, t_] =
  NDSolve[{eqn, ψ[x, 0] == initialShape, ψ[-L, t] == 0, ψ[L, t] == 0}, ψ[x, t], {x, -L, L},
    {t, 0, tend}, MaxSteps → 100 000, Method → {"MethodOfLines", "SpatialDiscretization" →
       {"TensorProductGrid", "MinPoints" → nx, "MaxPoints" → nx}}][[1, 1, 2]];
```

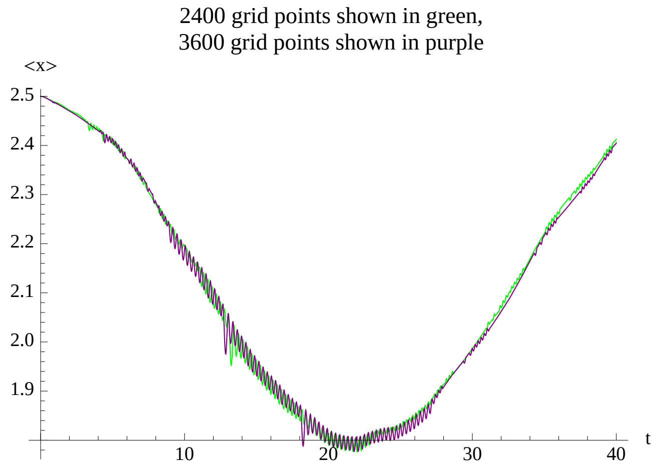
```
NDSolve::eerri : Warning: Estimated initial error on the specified spatial grid
      in the direction of independent variable x exceeds prescribed error tolerance. ≫

NDSolve::eerr :
  Warning: Scaled local spatial error estimate of 86.65895768806968` at t = 40.` in the direction
      of independent variable x is much greater than prescribed error tolerance. Grid
      spacing with 3600 points may be too large to achieve the desired accuracy
      or precision.  A singularity may have formed or you may want to specify a
      smaller grid spacing using the MaxStepSize or MinPoints method options. ≫
```

```
EHwave[x_, t_] :=
 Chop[Times[EHwavefunction[x, t], (EHwavefunction[x, t] /. Complex[a_, b_] → Complex[a, -b])]]

EHintegrand[x_, t_] :=
 Chop[(EHwavefunction[x, t] /. Complex[a_, b_] → Complex[a, -b]) x EHwavefunction[x, t]]

Clear[EHxAverage]
EHxAverage[t_] := NIntegrate[EHintegrand[x, t], {x, -14, 14}]
```

```
EHPxAveragePlot = Plot[EHxAverage[t], {t, 0, 40}, AxesLabel → {"t", "<x>"}, PlotStyle → Purple]
```



```
Show[UPxAveragePlot, EHPxAveragePlot,
 PlotLabel → " 2400 grid points shown in green,\n 3600 grid points shown in purple"]
```

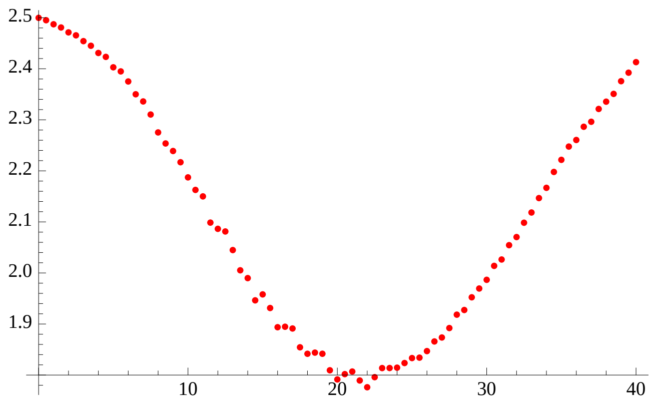


Notice that the two plots overlay one another.  Since we now have confidence in our 2400 grid point result we can, and should, use it rather than the more computationaly intensive 3600 grid point result. Although the overall shape of the curve is fine you can see that there is some jitter and this will defeat an attempt to directly take a derivative. We could data smooth but we can also sample the curve and then fit a function to it.

The trick is to fit $< x >$ to a smooth function and then differentiate the result. The question is how to fit xAverage. If we look at the plot xAverage, a polynomial fit does not look promising. However we could try fitting it with a sum of cosine functions. In fact Fourier analysis [14] guarantees that this will work.
The first step is to sample the function.

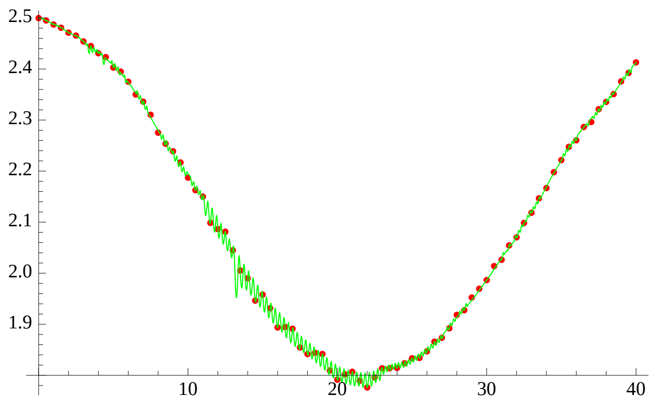
```
data = Table[{t, UPxAverage[t]}, {t, 0., 40., .5}];
```

```
dataPlot = ListPlot[data, PlotStyle → Red]
```



Comparing this to the plot of the function shows that we have accurately recreated the function.

```
Show[dataPlot, UPxAveragePlot]
```



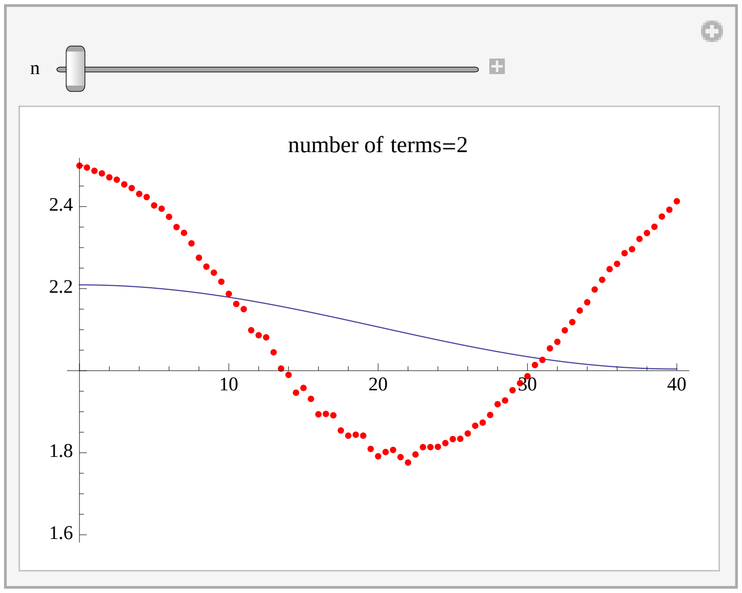
We want to fit the sampled points with a function of the form

$$f(t) = \sum_{n=0}^{N} a(n)\ \cos(n\,\pi\,t/40)$$

where $N + 1$ is the number of terms. Note that the argument to the cosine is $n\,\pi\,t/40$. The reason for the factor of 40 is that we are interested in the interval $[0, 40]$ and on this interval $t/40$ runs from zero to one. Once we have our function we can use **FindFit** to find the coefficients $a(n)$. How many terms should we take? There is no easy way to know this ahead of time. It's best just to try it and see if you get a good fit. The module below shows what happens as we increase the number of terms.

```
Clear[fit]
fit[terms_] := Module[{},
  model = Sum[a[n] Cos[n π t / 40], {n, 0, terms}];
par = Table[a[n], {n, 0, terms}];
results = Chop[FindFit[data, model, par, t]];
  resultPlot = Plot[model /. results, {t, 0, 40},
    PlotLabel → StringJoin["number of terms=", ToString[terms + 1]]];
  Show[resultPlot, ListPlot[data, PlotStyle → Red], PlotRange → {{0, 40}, {1.6, 2.5}}]]
```

```
Manipulate[fit[n], {n, 1, 30, 1}, SaveDefinitions → True]
```



From the interactive graphic it looks like an upper limit of $N = 30$ does an excellent job of fitting the data.

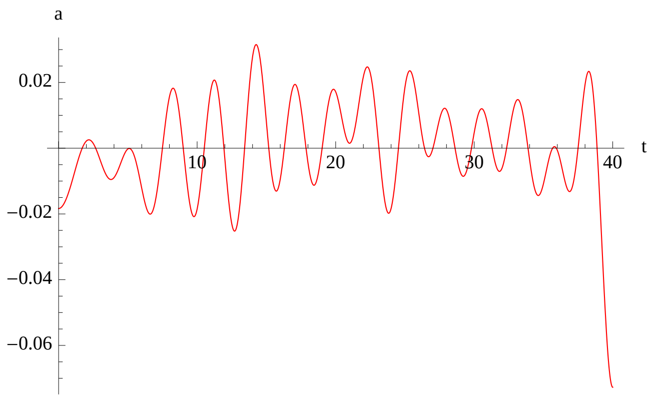
```
terms = 30;
model = Sum[a[n] Cos[n π t / 40], {n, 0, terms}];
par = Table[a[n], {n, 0, terms}];
results = Chop[FindFit[data, model, par, t]]
```

```
{a[0] → 2.10235, a[1] → 0.103967, a[2] → 0.30637, a[3] → -0.0311438,
 a[4] → 0.0165002, a[5] → -0.0118941, a[6] → 0.00685848, a[7] → -0.00473662,
 a[8] → 0.00323911, a[9] → -0.00157718, a[10] → 0.00228773, a[11] → -0.00232288,
 a[12] → 0.0012952, a[13] → 0.00116812, a[14] → 0.0046133, a[15] → -0.00255447,
 a[16] → 0.00211248, a[17] → -0.000683228, a[18] → 0.00129506, a[19] → -0.0015791,
 a[20] → 0.00193505, a[21] → -0.00121645, a[22] → -0.000205692,
 a[23] → -0.000475125, a[24] → 0.00166685, a[25] → 0.000650837, a[26] → 0.00161351,
 a[27] → -0.000129236, a[28] → -0.000806813, a[29] → -0.00198954, a[30] → 0.00118449}
```

It is now easy to take the second derivative of $< x >$ with respect to time and plot the resulting acceleration.

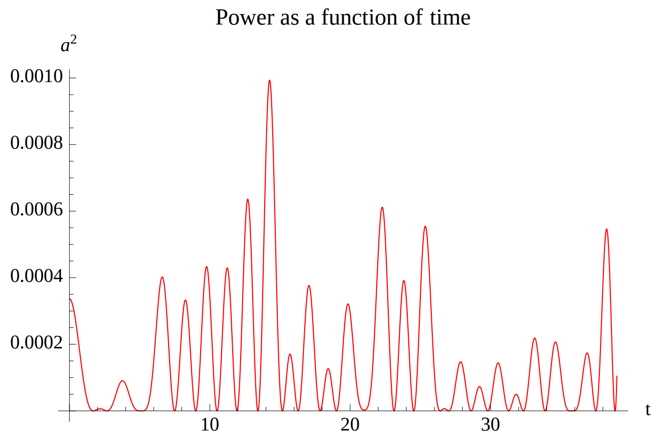
```
aBar = D[(model /. results), {t, 2}];
```

```
newabarPlot = Plot[aBar, {t, 0, 40}, AxesLabel → {"t", "a"}, PlotStyle → Red]
```



You should of course be deeply suspicious of the result at $t = 40$ which is an artifact of the Fourier fit. The power emitted by a moving charge is given for the non-relativistic case by Larmor's formula [15] and is $P = \frac{2 e^2}{3 c^3} |\mathbf{a}|^2$. So the power is proportional to the square of the acceleration.

```
Plot[aBar^2, {t, 0, 39}, AxesLabel -> {"t", "a^2"}, PlotStyle -> Red,
 PlotRange → All, PlotLabel → "Power as a function of time"]
```



Data for the radiation emitted in charge oscillations is given in [12,13]. The exact shape of the signal depends strongly on the experimental set-up.  The signal dies off quickly in the experimental data due to energy loss from the emitted radiation. This effect is not modeled by our code.

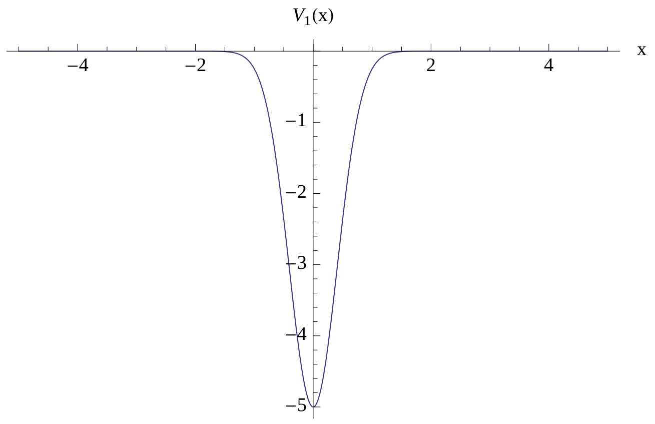
**Wave packet splitting**

An interesting wave packet phenomena of current interest is wave packet splitting. A simple method for splitting a wave packet was recently proposed by Zhang *et. al.* [16]. Wave packet splitting using a double well has recently been experimentally realized by Hall *et. al.*  [17] . We can fairly easily numerically simulate wave packet splitting.

We first define a static potential.

```
V₁[x_] := V₀ Exp[-3 x^2]
V₀ = -5;
```

```
Plot[V₁[x], {x, -5, 5}, PlotRange → All, AxesLabel → {"x", "V₁(x)"}]
```

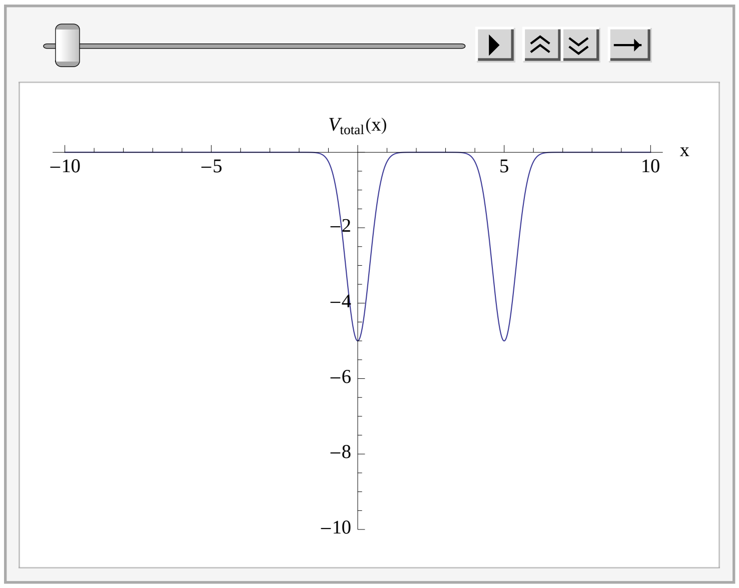


We now define a second potential which is time-dependent. This potential is left moving and its speed is controlled by $\omega$. At $t = 0$ the potential is centered around $x = 5$ so that the two potentials are distinct at $t = 0$.

```
V₂[x_, t_] := V₀ Exp[-3 (x - 5 + ω t)^2]
```

The full potential is $V_1 + V_2$ which I have plotted below for $\omega = 1$.

```
ω = 1;
ListAnimate[Table[Plot[V1[x] + V2[x, t], {x, -10, 10},
   PlotRange → {0, -10}, AxesLabel → {"x", "Vtotal(x)"}], {t, 0, 10, 0.5}]]
```



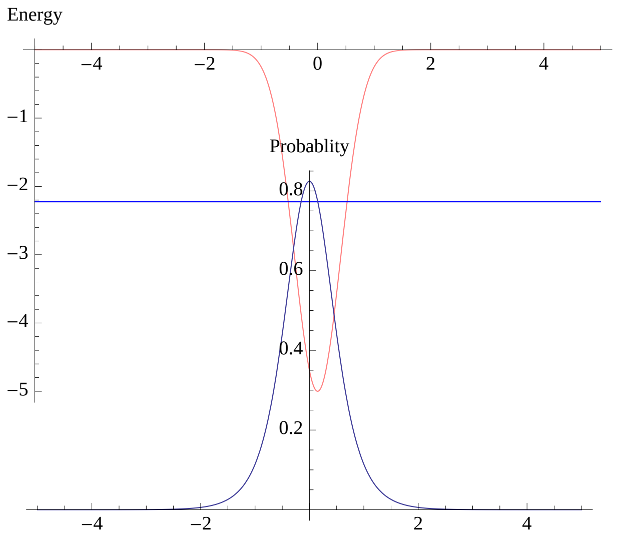
We start our wave packet in an eigenstate of $V_1$, the stationary well. To find the eigenstates we use the module EigenSolver which we have used before. The code is repeated below for convenience.

```
Developer`SetSystemOptions["EvaluateNumericalFunctionArgument" → False];
EigenSolver[V_, {q_, qmin_, qmax_}, matchPoint_, EnergyGuess_] := Module[{},
  MatchingPoint = Rule[q, matchPoint];
  leftψ[ϵ_, q] :=
   First[NDSolve[{-D[ψ[q], {q, 2}] + V ψ[q] == ϵ ψ[q], ψ'[qmin] == 0.0001, ψ[qmin] == 0},
      ψ[q], {q, qmin, q /. MatchingPoint}]][[1, 2]];
rightψ[ϵ_, q] := First[NDSolve[{-D[ψ[q], {q, 2}] + V ψ[q] == ϵ ψ[q], ψ'[qmax] == 0.0001,
       ψ[qmax] == 0}, ψ[q], {q, qmax, q /. MatchingPoint}]][[1, 2]];
  scaleLeft[ϵ_] := leftψ[ϵ, q] /. MatchingPoint;
scaleRight[ϵ_] := rightψ[ϵ, q] /. MatchingPoint;
scaledLeft[ϵ_, q] := leftψ[ϵ, q] scaleRight[ϵ] / scaleLeft[ϵ];
DRight[ϵ_, q] := D[rightψ[ϵ, q], q];
DLeft[ϵ_, q] := D[scaledLeft[ϵ, q], q];
  Energy = ϵ /. FindRoot[(DLeft[ϵ, q] /. MatchingPoint) == (DRight[ϵ, q] /. MatchingPoint),
     {ϵ, EnergyGuess, EnergyGuess + EnergyGuess / 10.0}];
  result = First[ψ[q] /. NDSolve[{-D[ψ[q], {q, 2}] + V ψ[q] == Energy ψ[q],
       ψ'[qmin] == 0.0001, ψ[qmin] == 0}, ψ[q], {q, qmin, qmax}]];
  normalization = 1 / Sqrt[NIntegrate[result^2, {q, qmin, qmax}]];
  plot1 = Show[Plot[Tooltip[V, ToString[TraditionalForm[V]]], {q, qmin, qmax},
     PlotPoints -> 100, PlotRange → All, PlotStyle -> {RGBColor[1, 0, 0], Opacity[.5]},
     AxesOrigin -> {qmin, 0}, AxesLabel -> "Energy"],
    Graphics[{RGBColor[0, 0, 1], Line[{{qmin, Energy}, {qmax, Energy}}]}]];
  plot2 = Plot[normalization^2 result^2, {q, qmin, qmax}, PlotRange -> All,
    AxesLabel -> {None, "Probablity"}, RotateLabel -> True];
  Print[StringJoin["Energy=", ToString[Energy]]];
  GraphicsArray[{{plot1}, {plot2}}, GraphicsSpacing -> -1]]
```

Using EigenSolver we can easily find the ground state. The wave function is returned as the variable normalization result.

```
EigenSolver[V1[x], {x, -5, 5}, 1, -4.5]
```

```
Energy=-2.22519
```



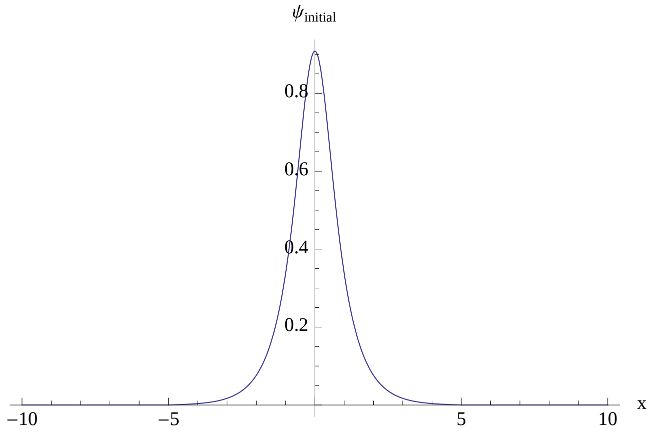
Once again we need the wave function over a larger interval than is returned by EigenSolver, but the value of the wave function is so small outside of the interval $-5 < x < 5$ that we can just set it to zero.

```
ψinitial[x_] = Piecewise[{{0, x < -5}, {normalization result, -5 ≤ x ≤ 5}, {0, x > 5}}]
```

```
⎡ 0                                                        x < -5
⎨
⎣ 25.9053 InterpolatingFunction[{{-5., 5.}}, <>][x]   -5 ≤ x ≤ 5
```

The initial wave function is plotted below.

```
Plot[ψinitial[x], {x, -10, 10}, PlotRange → All, AxesLabel → {"x", ψinitial}]
```



Now that we have the initial wave function we can solve the wave equation with the full time-dependent potential.

```
Clear[ℏ, m, ψ, V]
eqn = ⅈ ℏ D[ψ[x, t], t] == -(ℏ^2 / 2 m) D[ψ[x, t], {x, 2}] + V[x, t] ψ[x, t]
```

$$i\hbar\,\psi^{(0,1)}[x,t] == V[x,t]\,\psi[x,t] - \frac{1}{2}\,m\,\hbar^2\,\psi^{(2,0)}[x,t]$$

As usual we will solve the equation in a box and force the wave function to zero at the box boundaries. The box runs from $-L$ to $L$ and I have taken $L = 8$ in units in which $m = 1$ and $\hbar = 1$.

```
m = 1;
ℏ = 1;
L = 8;
V[x_, t_] := V₁[x] + V₂[x, t]
```

Since we don't want the wave packet to hit the boundaries of the box I have tracked the solution only until *t* = 8. I have also used AccuracyGoal → 2. This gives a low accuracy solution (the default to AccuracyGoal → 6) but it's fast and does not take much memory. We will have to check to see if our low accuracy solution is good enough.

```
Clear[packet]
packet[x_, t_] =
 NDSolve[{eqn, ψ[x, 0] == ψinitial[x], ψ[-L, t] == 0, ψ[L, t] == 0}, ψ[x, t], {x, -L, L},
    {t, 0, 10}, MaxSteps → 100 000, AccuracyGoal → 2][[1, 1, 2]] // Timing
```

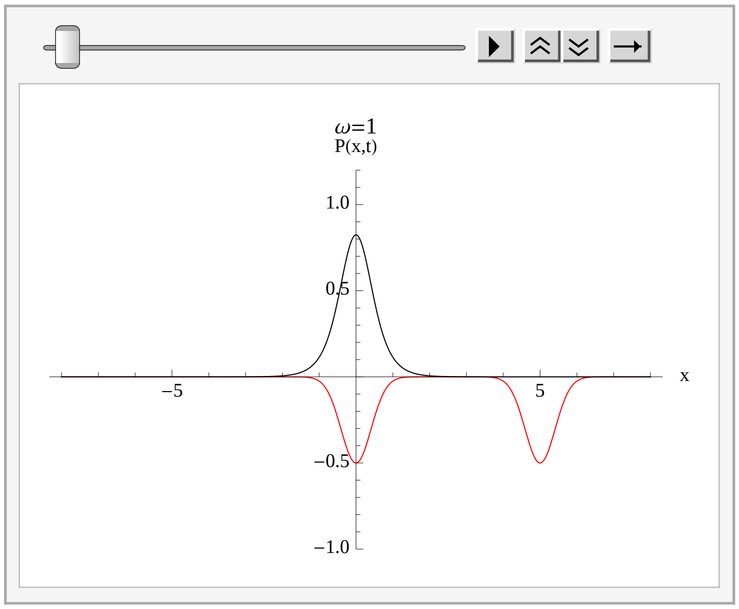
```
{0.366307, InterpolatingFunction[{{-8., 8.}, {0., 10.}}, <>][x, t]}
```

We can now form the wave packet

```
wave[x_, t_] := Chop[Times[packet[x, t][[2]], Conjugate[packet[x, t][[2]]]]]
```

and plot the time evolution.

```
ListAnimate[Table[Plot[Evaluate[{V[x, t] / 10, wave[x, t]}], {x, -L, L}, PlotRange → {-1, 1.2},
   PlotLabel → "ω=1", PlotStyle → {RGBColor[1, 0, 0], RGBColor[0, 0, 0]},
   AxesLabel → {"x", "P(x,t)"}], {t, 0, 10, .1}]]
```



Wave packet splitting. The wave packet is shown in black. The potential is shown in red.

It is important to understanding what the animation really means. Remember that we are looking at a probability distribution so we don't split the wave packet. We split the probability distribution. There is a chance that the wave packet stays in the stationary well and a chance that it moves off with the moving potential. Notice that for our potential, the probability of moving the wave packet is not very high.

To check the accuracy of our solution we can re-solve the equation with an accuracy goal of 3 and compare the solutions.

```
Clear[HPpacket]
HPpacket[x_, t_] =
 NDSolve[{eqn, ψ[x, 0] == ψinitial[x], ψ[-L, t] == 0, ψ[L, t] == 0}, ψ[x, t], {x, -L, L},
    {t, 0, 10}, MaxSteps → 100 000, AccuracyGoal → 3][[1, 1, 2]] // Timing
```

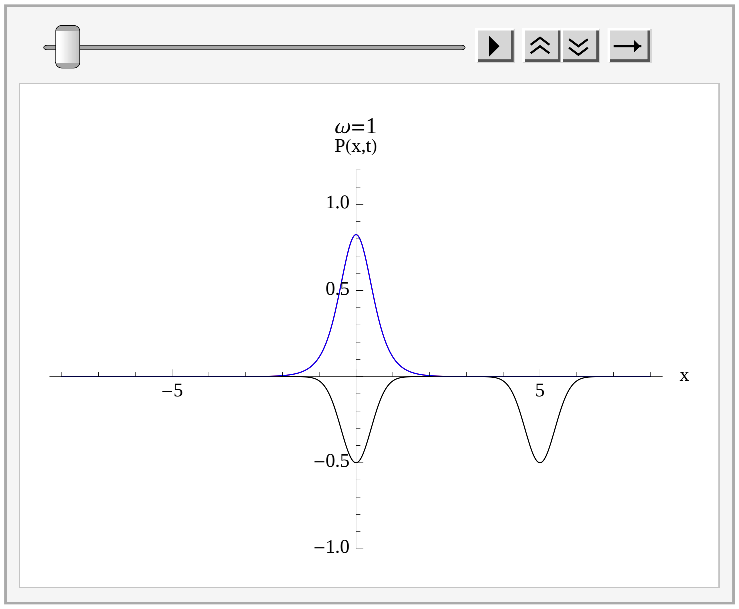
```
NDSolve::mxsst : Using maximum number of grid points 10000
    allowed by the MaxPoints or MinStepSize options for independent variable x. ≫
```

```
{30.2128, InterpolatingFunction[{{-8., 8.}, {0., 10.}}, <>][x, t]}
```

```
HPwave[x_, t_] := Chop[Times[HPpacket[x, t][[2]], Conjugate[HPpacket[x, t][[2]]]]]
```

Plotting shows that the two solutions are very similar. You can barely see the difference between the two curves.

```
ListAnimate[Table[Plot[Evaluate[{V[x, t] / 10, HPwave[x, t], wave[x, t]}],
   {x, -L, L}, PlotRange → {-1, 1.2}, PlotLabel → "ω=1",
   PlotStyle → {Black, Red, Blue}, AxesLabel → {"x", "P(x,t)"}], {t, 0, 10, .1}]]
```



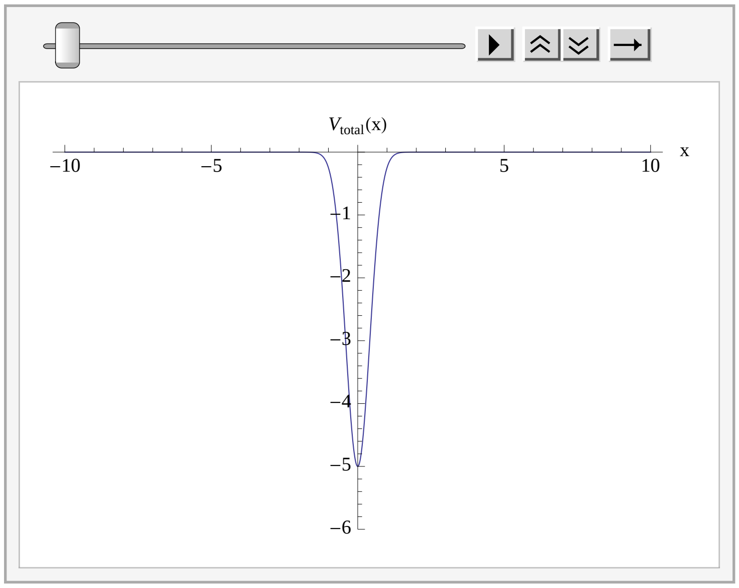
Comparing our two solutions. The two wave packet solutions are shown in red (AccuracyGoal→3) and blue (AccuracyGoal→2). Note that there is little difference between them. The potential is shown in black.

Another way to split a wave packet into two is to start from a single well and split it into two wells. This has not yet been done experimentally but it allows you to split the packet with equal probability.  Suppose we have the following potential

```
V[x_, t_] := (V0 / 2) Exp[-3 (x + ω t)^2] + (V0 / 2) Exp[-3 (x - ω t)^2]
```

This potential is centered at $x = 0$ at $t = 0$ and is composed of equal parts of a left moving and right moving wave. The potential's time-dependence is plotted below for $V_0 = -5$ and $\omega = 1$.

```
ω = 1;
V0 = -5;
ListAnimate[Table[Plot[V[x, t], {x, -10, 10},
   PlotRange → {0, -6}, AxesLabel → {"x", "Vtotal(x)"}], {t, 0, 10, 0.5}]]
```



Notice that at $t = 0$ the potential is the same as our original static potential so that we can use the same initial wave shape. This makes it easy to re-solve the wave equation.

```
Clear[packet]
packet[x_, t_] =
 NDSolve[{eqn, ψ[x, 0] == ψinitial[x], ψ[-L, t] == 0, ψ[L, t] == 0}, ψ[x, t], {x, -L, L},
    {t, 0, 10}, MaxSteps → 100 000, AccuracyGoal → 2][[1, 1, 2]] // Timing
```

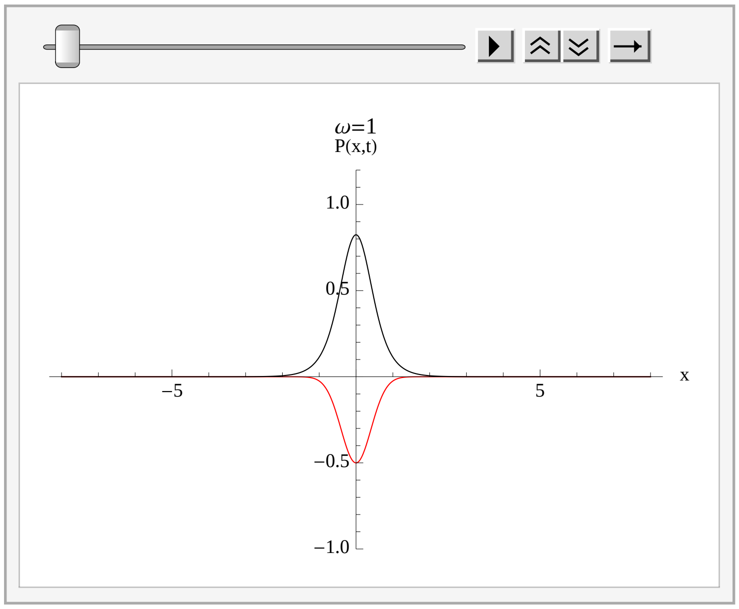
```
{0.352077, InterpolatingFunction[{{-8., 8.}, {0., 10.}}, <>][x, t]}
```

We now form the probability density

```
wave[x_, t_] := Chop[Times[packet[x, t][[2]], Conjugate[packet[x, t][[2]]]]]
```

and plot the result. To avoid effects from the box boundary we plot only until $t = 5$.

```
ListAnimate[Table[Plot[Evaluate[{V[x, t] / 10, wave[x, t]}], {x, -L, L}, PlotRange → {-1, 1.2},
   PlotLabel → "ω=1", PlotStyle → {RGBColor[1, 0, 0], RGBColor[0, 0, 0]},
   AxesLabel → {"x", "P(x,t)"}], {t, 0, 5, .1}]]
```



Wave packet splitting with equal probabilities. The wave packet is shown in black. The potential is shown in red.

Notice that we get equal probabilities of moving the wave packet to the right or the left.

## Projects

### Charge Oscillations

In real experiments the initial state of the wave packet is not a single energy eigenstate but rather a mixture of eigenstates. Investigate what happens when you start the system in a mixture of eigenstates of the right-hand well. Look up the experimental papers [11,12,13] so that you start with realistic well parameters.

### Wave Packet Splitting

Make a quantum tram. Your tram (moving wave packet) should pick-up a passenger (wave packet) with some probability $P_1$ and drop them off at second station (well) with a second probability $P_2$. Investigate how $P_1$ and $P_2$ depend on the speed of your tram and the width and depth of your wells.

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