Calculating a Wave Function from an Asymptotic Solution

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1 Obtaining the Asymptotic Solution

We begin with the energy eigenvalue equation,

$$\hat{H}\psi = E\psi. \tag{1}$$

For a one dimensional system, the equation becomes

$$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x) = E\psi(x). \tag{2}$$

Inserting the given potential, $V(x) = Ax$, into the energy eigenvalue equation and rearranging terms gives

$$\frac{\partial^2}{\partial x^2}\psi(x) = \frac{2m}{\hbar^2}(Ax - E)\psi(x). \tag{3}$$

To simplify things, we set the total energy E to 0. This gives

$$\frac{\partial^2}{\partial x^2}\psi(x) = \frac{2m}{\hbar^2}Ax\psi(x). \tag{4}$$

Now we define $R \equiv \frac{2m}{\hbar^2}A$, so that our equation becomes

$$\frac{\partial^2}{\partial x^2}\psi(x) = Rx\psi(x). \tag{5}$$

We are now ready to guess at an asymptotic solution to this equation. The region x > 0 is the classically forbidden region and, although we know there is a finite probability of finding the particle here, the solution in this region must be a decaying exponential that goes to 0 as x approaches infinity. By treating x as a constant in the differential equation above we obtain an asymptotic solution for x > 0:

$$\psi(x) = e^{-cx^{\frac{3}{2}}}. \tag{6}$$

To find the constant c we simply take two derivatives and match it with the energy eigenvalue equation for large x:

$$\frac{\partial}{\partial x}\psi(x) = -\frac{3c\sqrt{x}}{2}\psi(x) \qquad \frac{\partial^2}{\partial x^2}\psi(x) = (-\frac{3c}{4\sqrt{x}} + \frac{9}{4}c^2 x)\psi(x).$$

As $x \to \infty$,

$$\frac{\partial^2}{\partial x^2}\psi(x) = \frac{9}{4}c^2 x\psi(x) = Rx\psi(x). \tag{7}$$

Since this matches the exact form of the energy eigenvalue equation we can be confident that our wave function is valid for large x. Now we can find an expression for c and the final form of the asymptotic solution:

$$\psi(x) = e^{-\frac{2\sqrt{R}}{3}x^{\frac{3}{2}}}. \tag{8}$$

2 The Taylor Expansion

A functional value for a deviation from a known functional value can be found from the Taylor expansion:

$$\psi(x + \Delta) = \psi(x) + \Delta\frac{\partial}{\partial x}\psi(x) + \frac{\Delta^2}{2!}\frac{\partial^2}{\partial x^2}\psi(x) + \ldots \tag{9}$$

For reasons of convenience that will be seen shortly, we define $\Delta \equiv 2d$. If d is sufficiently small, the previous equation can be written with good approximation as

$$\psi(x + 2d) \approx \psi(x) + 2d\frac{\partial}{\partial x}\psi(x) + 2d^2\frac{\partial^2}{\partial x^2}\psi(x). \tag{10}$$

Now we use the definition of the derivative,

$$\frac{\partial}{\partial x}\psi(x) = \lim_{d \to 0}\frac{\psi(x + d) - \psi(x - d)}{2d},$$

and Eq.(7) to obtain

$$\psi(x + 2d) \approx \psi(x) + \psi(x + d) - \psi(x - d) + 2d^2 Rx\psi(x). \tag{11}$$

Notice the limit is removed since we will use a sufficiently small value for the step, d. This equation says that given three adjacent points, we can obtain the next adjacent point. One can see that after doing many iterations of this, we can obtain the entire function. But where does one get the first three points? From the asymptotic solution, of course!

3 The Specific Problem

For the specific problem statement given, we have A = 1, m = 1, and $\hbar = 1$. This gives us the form of the asymptotic solution that will actually be implemented in the program:

$$\psi(x) = e^{-\frac{2\sqrt{2}}{3}x^{\frac{3}{2}}}, \tag{12}$$

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where we have used $R \equiv \frac{2m}{\hbar^2} A = 2$. $\psi(x_0 - d)$, $\psi(x_0)$, and $\psi(x_0 + d)$ give the first three points, where $x_0 > 0$ and $|d| << 1$. These three points will allow, after many iterations, the entire form of the wave function to be constructed. The Fortran 77 code to do this is now presented.

```
------------------------------------------------------------------
PROGRAM QUANTUM

REAL d, n, x0, psi(4)
PARAMETER (d = -0.001, n=25000, x0=5)

c d = step size
c n = number of iterations
c x0 = initial x value
c psi(i) = function values

open(1,file='psi.out',status='unknown')
open(2,file='psisquared.out',status='unknown')
open(3,file='x.out',status='unknown')

c finds initial 3 adjacent points from asymptotic solution
do i = 1, 3
   psi(i) = 2.7182818**(-0.94280904*(x0+(i-2)*d)**1.5)
end do
c here psi(1)=psi(x-d); psi(2)=psi(x); psi(3)=psi(x+d)

c uses the Taylor expansion to find the wave function
do i = 0, n
   psi(4) = psi(2) + psi(3) - psi(1) + 4*d**2*(x0+i*d)*psi(2)
   psi(1)=psi(2)
   psi(2)=psi(3)
   psi(3)=psi(4)
   if (mod(i,10).eq.0) then
     write(1,*) psi(4)
     write(2,*) psi(4)**2
     write(3,*) x0+i*d
   end if
end do

end
------------------------------------------------------------------
```

I chose a step size here of -0.001. It must be negative because we need to go backwards in the function. This value gives great accuracy. Starting from a value of x=5, and doing 25000 iterations takes us to about x=-20. Notice that the statement "`if (mod(i,10).eq.0) then...`" allows one to put in the data files only every other point or every tenth point, etc. which makes it easier to organize very precise data (i.e. tiny step size with a huge number of iterations) into an Excel or other type of spreadsheet. The x value, $\psi(x)$ and $[\psi(x)]^2$ are all put into their own data file which makes putting the numbers into a data sheet a simple cut and paste exercise. The graphs obtained from the particular program I wrote are as follows.

Psi(x) vs. x

[Psi(x)]^2 vs. x
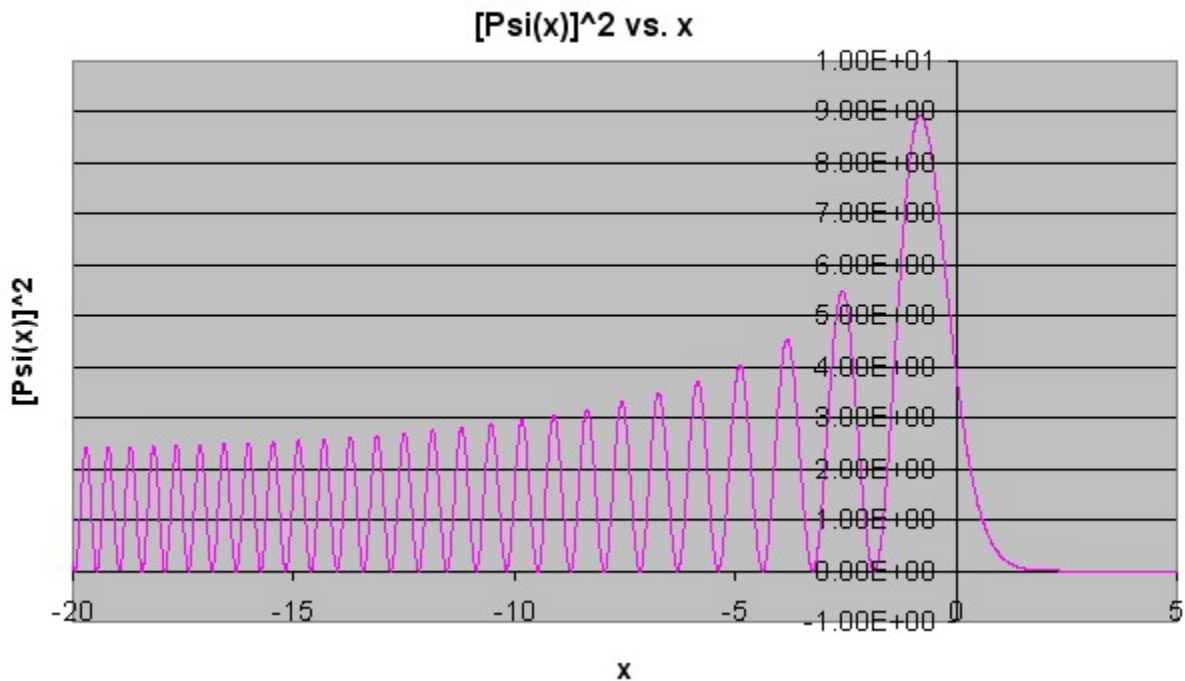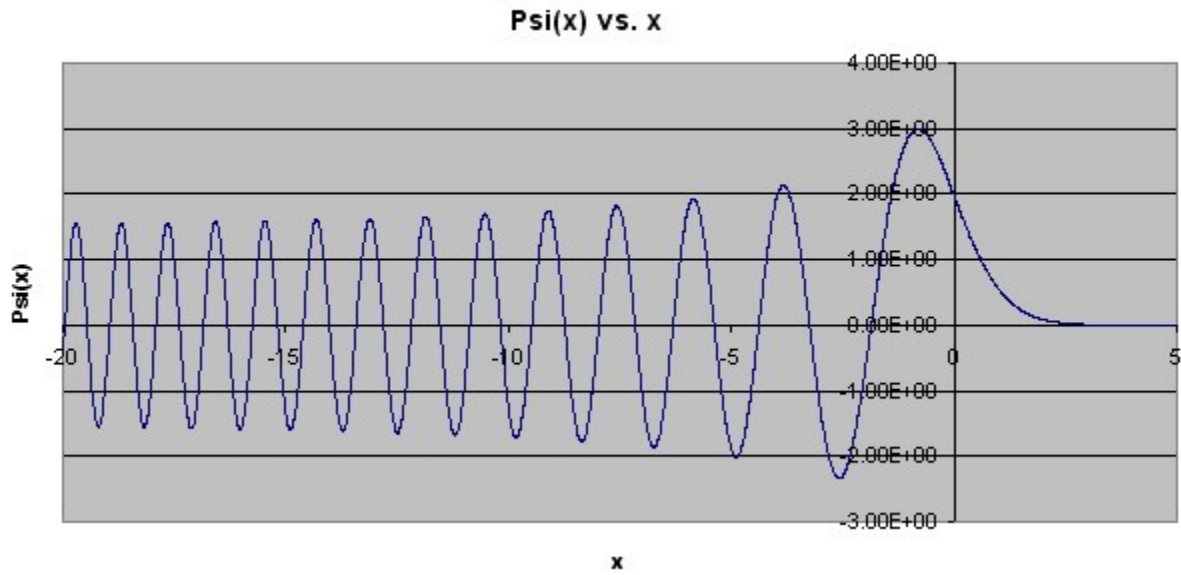
Here, both graphs are plotted together to see exactly how ψ and its square compare.
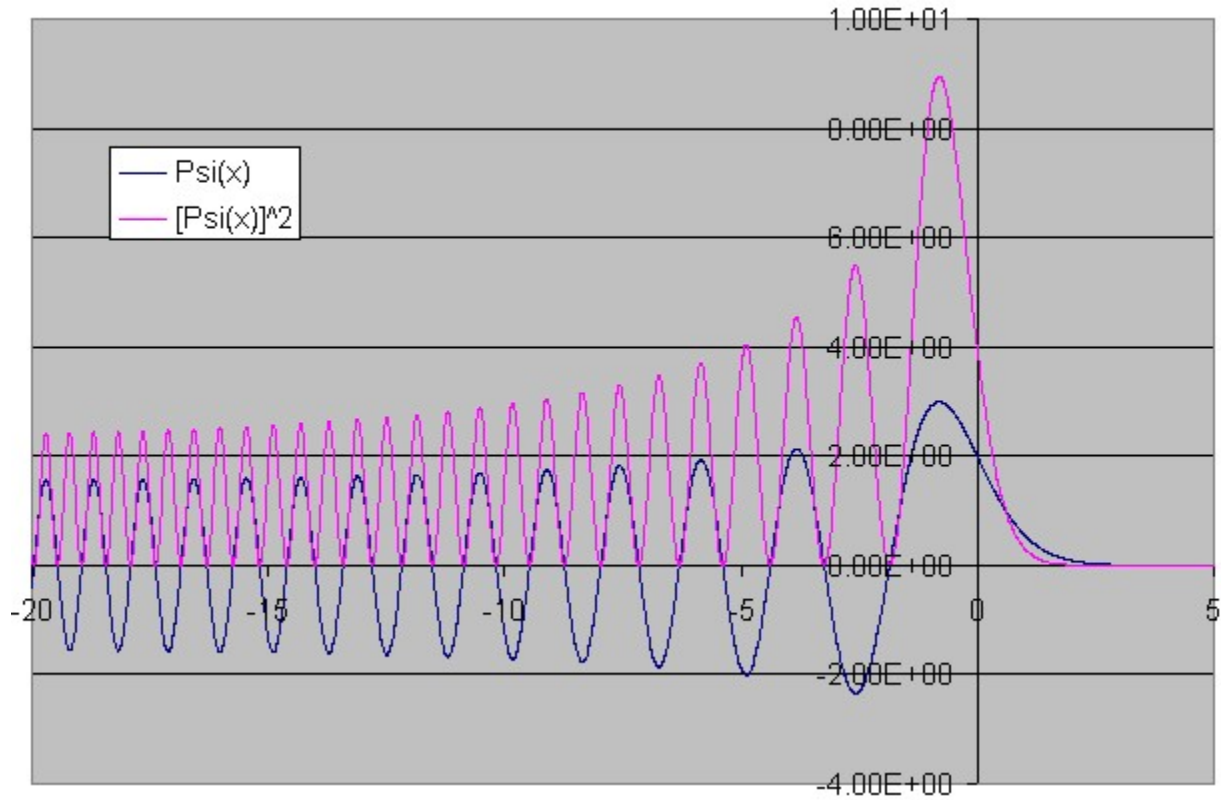
For the range I had chosen to compute and plot, my step size was quite adequate. However, since the frequency keeps on increasing as x gets smaller and smaller, the plot will eventually diverge for any step size as the frequency gets comparable to the stepsize. This is an important consideration to keep in mind. Something to notice from the graph is that the probability of finding the particle peaks near the classical turning point and decays exponentially in the classically forbidden region. Also, the probability of finding the particle as x gets smaller also gets smaller because one can think classically of the particle going down the potential hill (thus moving faster) and therefore spending less time in a given region, hence the probability decreasing. In conclusion, one can see that from a few fairly simple steps and derivations, one can reconstruct the wave function without actually solving the differential equation.