Project 1

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October 11, 2015

Contents

List of Figures

1 Question 1: Quantum Uncertainty in the Harmonic Oscillator

In this question we studied the quantum uncertainty in the harmonic oscillator.

1.1 part a: Hermite Polynomials and Wavefunctions

In this part we studied the Hermite polynomials and harmonic oscillator wave functions.

1.1.1 part a(i): Hermite Polynomials

In this part I wrote a code to calculate Hermite polynomials. The data are saved for $n = 1, 2, 3$ for the plotting and data for $n = 5, 12$ are saved to compare exact values of table of Abramowitz.
Comparison of table values and my values:

$n = 5$	$x = 3$	$x = 10$
$Tablevalue =$	(3)3.8160000	(6)3.041200000
$Myvalue =$	$3.8160000000E + 03$	$3.0412000000E + 06$

$n = 12$	$x = 3$	$x = 10$
$Tablevalue =$	(6)5.5175040	(15)2.8894199383
$Myvalue =$	$5.5175040000E + 06$	$2.8894199383E + 15$

In this code, Table values and my values are matching upto 11 significant figures.

The Hermite Polynomials were calculated using the recursion relation:

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \tag{1}$$

The first two Hermite Polynomials are:
$H_0(x) = 1$
$H_1(x) = 2x$

folder : qn1a/polynomial
outputs : n1.dat,n2.dat,n3.dat,n5.dat,n12.dat
plots : hnx123.eps

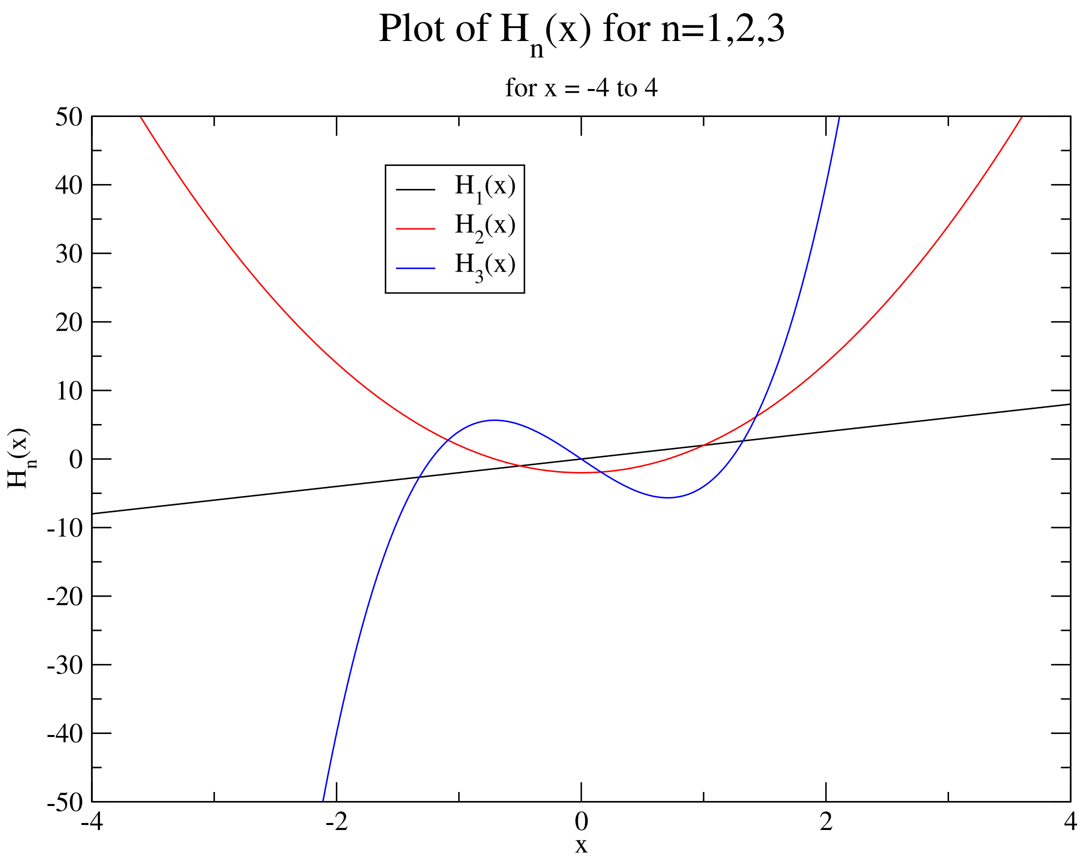

Figure 1: Hermite polynomials

1.1.2 part a (ii): Harmonic Oscillator Wave Functions

In this part we studied the harmonic oscillator wave functions. The wave function of a spinless point particle in a quadratic potential well is given by:

$$\psi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} e^{\frac{-x^2}{2}} H_n(x) \tag{2}$$

I wrote a code to calculate wave functions for $n = 0, 1, 2, 3$ in the range $x = -4, 4$

folder : qn1a/wavefunction
outputs : n0.dat,n1.dat,n2.dat,n3.dat
plots : pr1qn1a.eps

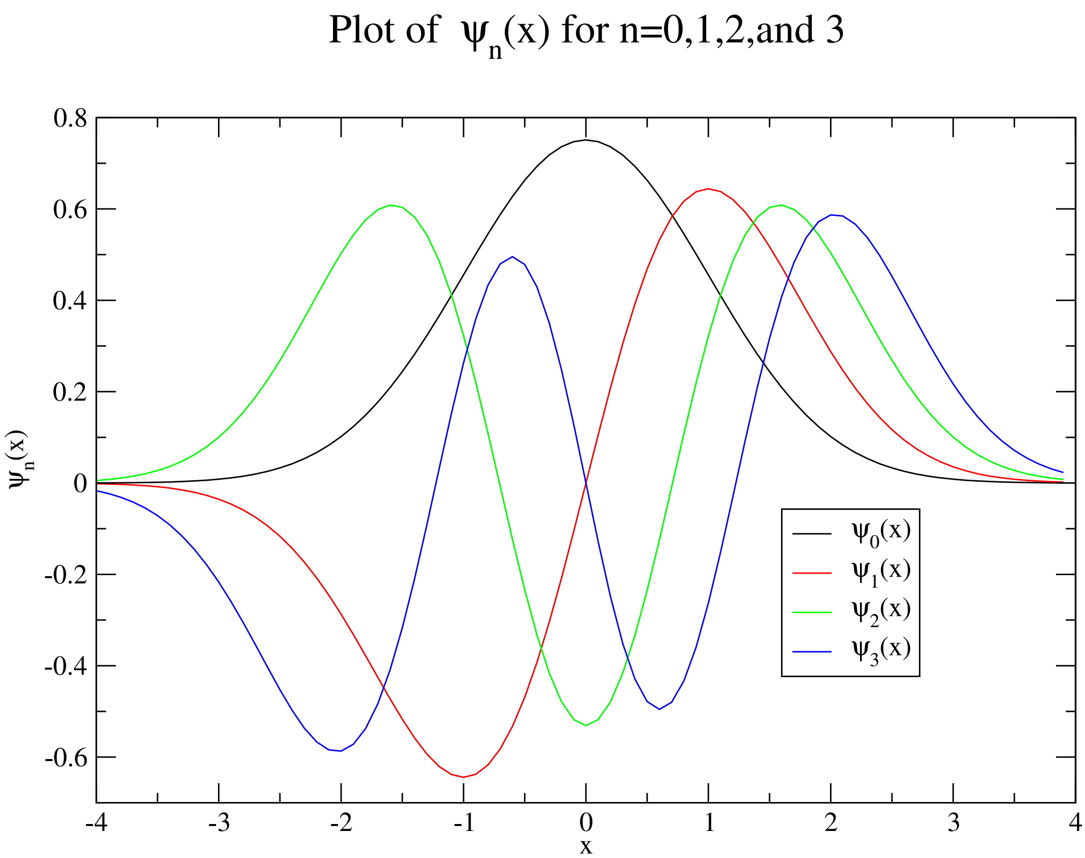

Figure 2: Hermite Wave functions

1.2 part b: Wavefunction for $n = 30$

In this part I plotted the wave function for $n = 30$ from $x = -10, 10$. I also calculated the time of run for the code using bash command 'time'. The code is not too slow, in fact it is fast.
command is : $time \quad f90 \quad pr1qn1b.f90 \quad \&\& \quad ./a.out$
result is:

$$\begin{aligned} real &= 0m0.078s \\ user &= 0m0.062s \\ sys &= 0m0.016s \end{aligned}$$

folder : qn1b
outputs : n30.dat
plots : pr1qn1b.eps

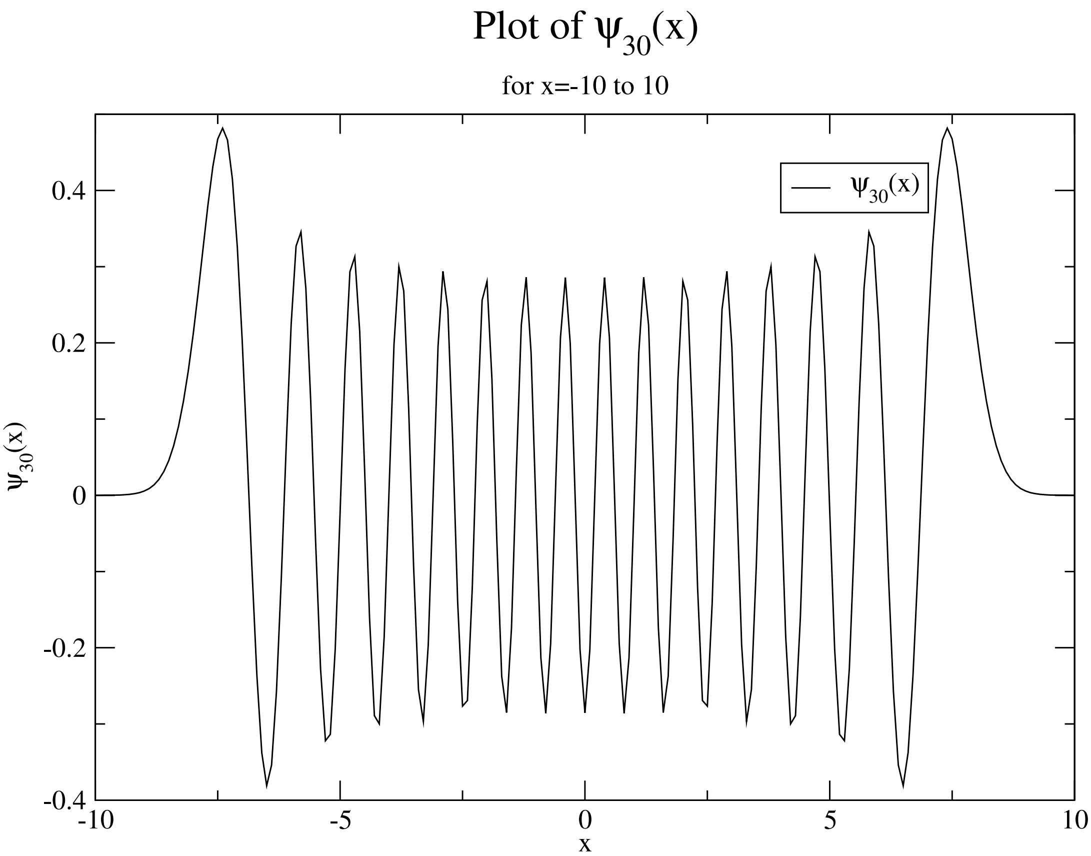

Figure 3: Hermite Wave function for $n = 30$

1.3 part c: Mean Square Position

In this part I wrote a code to calculate mean square position.
The mean square position is given by:

$$< x^2 >= \int_{-\infty}^{\infty} x^2 |\psi_n(x)|^2 \, dx \tag{3}$$

Where $\psi_n(x)$ is given by eq.(2)

For Hermite polynomial of degree $n = 5$, i got the converging result:
$< x^2 >= 5.50000$
Then, root mean square value is:
$\sqrt{< x^2 >} = 2.3452$
The result is correct upto five significant figures.

folder : qn1c
source code : gaulag.f90 (it was provided)
source code : pr1qn1c.f90
outputs : pr1qn1c.dat

2 Question 2: High Energy Scattering Cross Section

In this problem we studied the high energy scattering of electron by alpha particle.

2.1 part a: Yukawa Potential

In this part I wrote a code to calculate the ionic potential.
The given values are:
$Z = 2$
$a_0 = 0.5292A^0$
$r_0 = a_0/4 = 0.1323A^0$
$\frac{e^2}{4\pi\epsilon_0} = 14.4A^0eV$

$$
\begin{aligned}
V(r) &= \frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r}e^{-r/r_0} && (4)\\
&= Z\frac{e^2}{4\pi\epsilon_0}\frac{e^{-r/r_0}}{r}\\
&= 2 * 14.40 * \frac{e^{-r/r_0}}{r}\\
&= 28.8 * \frac{e^{-r/0.1323}}{r}\\
&= 28.8 * \frac{e^{-7.559r}}{r} \qquad (eV)\\
& && (5)
\end{aligned}
$$

folder : qn2/potential
source code : pr1qn2pot.f90
outputs : pr1qn2pot.dat
plots : pr1qn2pot.eps

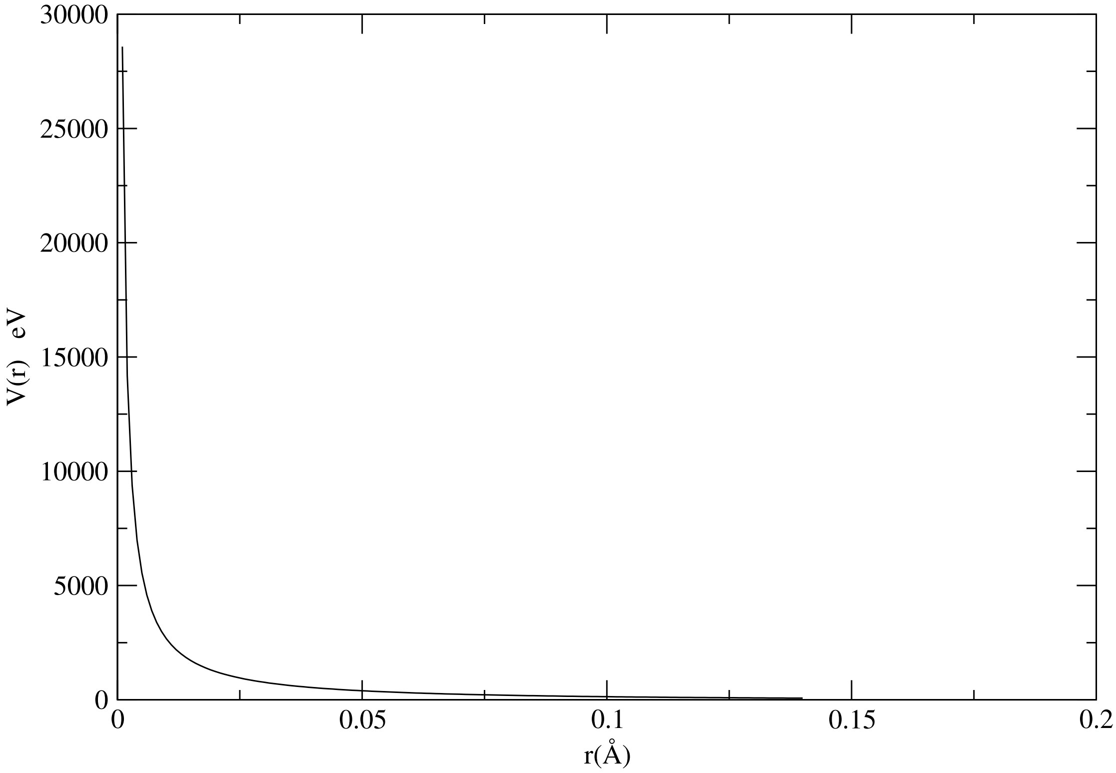

Figure 4: Yukawa Potential

2.2 part b: Scattering Amplitude

In this question I have used following values:
$mc^2 = 0.5110 Mev$
$k = 8(A^0)^{-1}$
$\hbar c = 197.33 Mevfm$
Using Born approximation, the scattering amplitude is given by:

$$f(\theta) = -\frac{2m}{q\hbar^2}\int_0^\infty rV(r)sin(qr)\,dr \tag{6}$$

Where, $q = 2ksin(\theta/2)$ where, k is initial or final magnitude of momentum. For low energy scattering $kr_0 << 1$. For high energy scattering I have chosen $kr_0 = 1$ then we get $k = 8(A^0)^{-1}$.

$$\begin{aligned} f(\theta) &= -\frac{2m}{q\hbar^2}\int_0^\infty rV(r)sin(qr)\,dr & (7)\\ &= -\frac{2mc^2}{(2ksin(\theta/2)\hbar^2c^2}\int_0^\infty r(28.80)\frac{e^{-7.559r}}{r}sin(2krsin(\theta/2))\,dr \\ &= -\frac{0.4726}{sin(\theta/2)}\int_0^\infty sin(16rsin(\theta/2))e^{-7.559r}\,dr \\ & & (8)\end{aligned}$$

Comparing to the standard format for generalized Gauss-Laguerre quadrature:

$$I = \int_0^\infty e^{-r}r^\alpha f(r)\,dr$$

we get: $\alpha = 0$ and

$$f(r) = -\frac{0.4726}{sin(\theta/2)}sin(16rsin(\theta/2))e^{r-7.559r}$$

I also compared my calculation of scattering amplitude with value from Wolfram Alpha.
From Wolfram alpha for $\theta = 3.139$ i got that:

$$\int_0^\infty -0.4726 sin(16rsin(\theta/2))\frac{e^{-7.559r}}{sin(\theta/2)}\,dr = -0.0241 \quad 478 \tag{9}$$

The screen shot from Wolfram Alpha is ampWolfram.png.
From my code for the last value of $\theta = 3.139$ in the output data file 'pr1qn2amp.dat' the value is -0.0241. So I can say my calculation of scattering amplitude is accurate upto four significant figures.

folder : qn2/amplitude
source code : gaulag.f90 (obtained from Numerical Recipe)
to compare : ampWolfram.png(screenshot from Wolfram alpha)
source code : pr1qn2amp.f90
outputs : pr1qn2amp.dat
plots : pr1qn2amp.eps

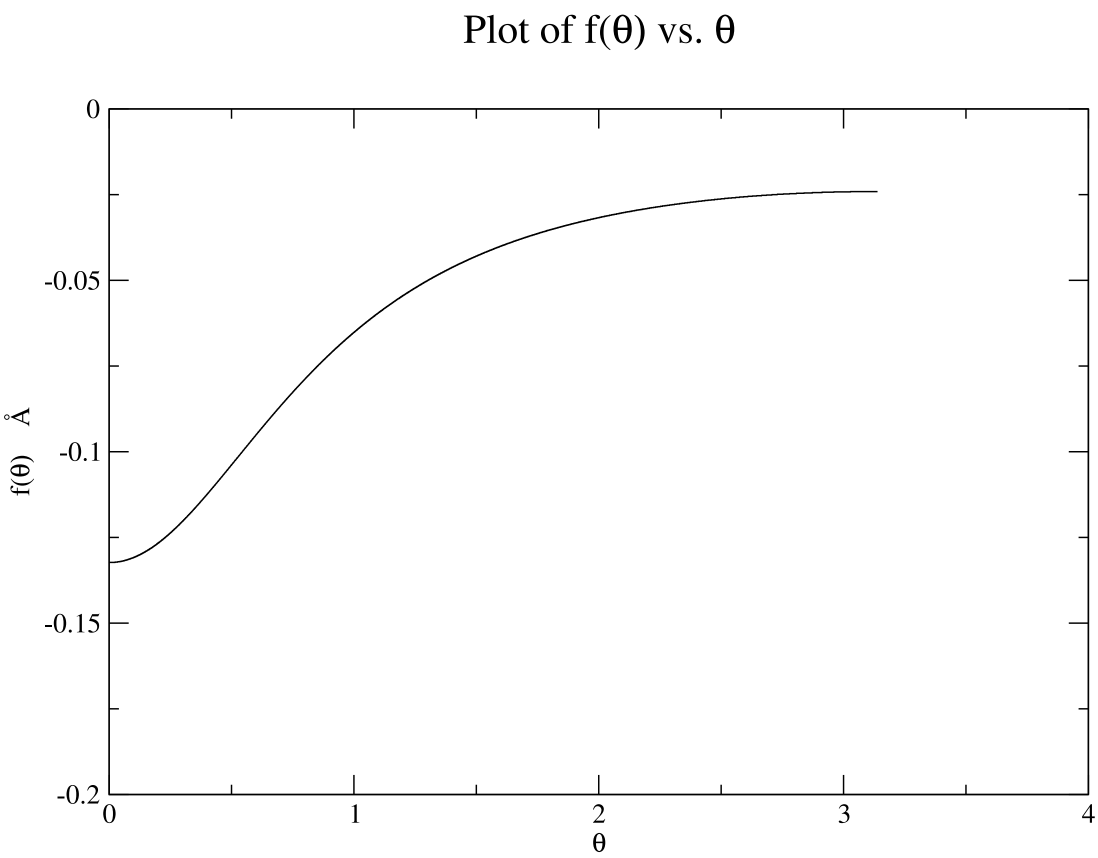

Figure 5: Scattering Amplitude

2.3 part c: Total Scattering Cross Section

In this part I calculated the total cross section area.
The total cross section area is given by:

$$\sigma = 2\pi \quad \int_0^{\pi} sin\theta |f(\theta)|^2 \, d\theta$$

Here i used the program for scattering amplitude as a subroutine to find $f(\theta)$ and used Gauss-Legendre quadrature to integrate the integral.
In the code i used do loop from 0 to 20 gauss points and obtained the converging result $0.4015E - 01(A^0)^2$.
The value obtained for scattering amplitude '$f(\theta)$' was accurate upto four significant figures, so I can say that my final value for total scattering cross section is accurate upto four significant figures.
folder : qn2/cross-section
source code : gauleg.f90 (from Numerical Recipe)
source code : pr1qn2cross.f90
outputs : pr1qn2cross.dat