Homework 7: Eigensystems

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1 Question 1: Testing Matrix Calls

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

1.1 part a: Verify the inverse of the matrix

In this part I verified the inverse of the matrix A . First i solved the matrix analytically. Then I wrote the program to calculate the inverse of the given matrix.
The given matrix is :

$$A = \begin{pmatrix} 4 & -2 & 1 \\ 3 & 6 & -4 \\ 2 & 1 & 8 \end{pmatrix}$$

The inverse of matrix A is:

$$A^{-1} = \frac{1}{263} \begin{pmatrix} 52 & 17 & 2 \\ -32 & 30 & 19 \\ -9 & -8 & 30 \end{pmatrix}$$

The solution location is :

```
location             : hw7/qn1abc
provided subroutine  : dminv.f90
source code          : dminv_test.f90
additional subroutine: print_matrix.f90
makefile             : Makefile
```

1.2 part b: verify properties of inverse matrix

In this part I verified the inverse matrix property. The source code is same as in part *a*. I got unit matrix of dimension three for single significant figures precision, however, for other significant figures I got some deviations from perfect anticipated unit matrix.

1.3 part c: comparison of determinant

In this part I compared the determinant from my analytic and computational result. They matched correctly. Source code is same as in part a.

1.4 part d: use of LAPACK subroutine *dgesv*

In this part I used the *LAPACK* library routine *dgesv* to solve the system of three linear equations of the form:

$$AX = B \tag{1}$$

Where:

$$A = \begin{pmatrix} 4 & -2 & 1 \\ 3 & 6 & -4 \\ 2 & 1 & 8 \end{pmatrix}$$

And,

$$B = \begin{pmatrix} 4 \\ -10 \\ 22 \end{pmatrix}$$

I solved this equation for X.
The solution is :

$$X = \begin{pmatrix} 0.312 \\ -0.038 \\ 2.677 \end{pmatrix}$$

```
location             : hw7/qn1d/
library used         : LAPACK
source code          : dgesv_test.f90
makefile             : Makefile
```

1.5 part e: use of LAPACK subroutines dsyev and dgeev

In this part the given matrix is symmetric. At first i used the lapack routine for symmetric matrix 'dsyev' to calculate the eigenvalues and eigenvectors. Then, i used the another lapack routine 'dgeev' to calculate the real eigenvalues and right eigenvectors.I got the same eigenvalues and proportionate eigenvectors. Note that these lapack subroutine gives normalized eigenvectors and eigenvectors are different from that in Wolfram Alpha website. The given symmetric matrix is :

$$A = \begin{pmatrix} 1 & -4 & 2 \\ -4 & 1 & -2 \\ 2 & -2 & -2 \end{pmatrix}$$

Here, I found same eigenvalues for both of the subroutines.
The eigenvector for non-degenerate eigenvalue is same.
However, for the doubly degenerate eigenvalue, the eigenvectors are different.
The solution location is :

```
location             : hw7/qn1e/dgesv and dgeev
library used         : LAPACK
source code          : dgesv_test.f90, dgeev_test.f90
output files         : dgesv.dat,dgeev.dat
makefile             : Makefile
```

1.6 part f: use of LAPACK subroutine dgeev

In this part the given input matrix is non-symmetric. I used the LAPACK subroutine dgeev to find the eigenvalues and eigenvectors. The eigenvectors are printed as columns in the same order as the eigenvalues appears in my code. The given non-symmetric matrix is :

$$A = \begin{pmatrix} -2 & 2 & -3 \\ 2 & 1 & -6 \\ -1 & -2 & 0 \end{pmatrix}$$

Here, I found that the calculated eigenvectors are proportional to exact eigenvectors.
Here, for the degenerate eigenvalue -3, the eigen vectors are:
$X_2^{'} = 0.23X_2 - 0.11X_3$
$X_3^{'} = 0.67X_2 - 0.48X_3$

The solution location is :

```
location             : hw7/qn1f/
library used         : LAPACK
source code          : dgeev_test.f90
output files         : hw7qn1f.dat
makefile             : Makefile
```

2 Question 2: Schrodinger equation via diagonalization

2.1 part a: Derivation of radial wavefunction

In this part the radial part of wave function was provided as equation 10.
I solved the further steps and derived the equation 15.
The file is $hw7qn2.pdf$.

2.2 part b: solving radial equation using diagonalizing routine dsyev

In this part I solved the radial part of schrodinger equation using diagonalization method. I followed the process of Morten's Computational Physics 2014 Fall notes section 7.8. The given potential of the harmonic oscillator is :

$$V(x) = \frac{1}{2}kx^2 \text{ where, k=1} \tag{2}$$

The step size is given by:

$$\begin{aligned} h &= \frac{R_{max} - R_{min}}{N_{step}} \\ &= \frac{10 - (-10)}{100} \\ &= 0.1 \end{aligned} \tag{3}$$

Then i created arrays of dimension 0 to nstep for x_i and V_i.
where,

$$x(i) = R_{min} + i * h \tag{4}$$

where, i = 1,2,3,...,nstep-1

$$V(i) = x(i) * x(i) \tag{5}$$

The diagonal elements d(i) has dimension 1 to $nstep - 1$.
Then, the diagonal matrix elements are given by:

$$d(i) = \frac{2}{h^2} + V(i) \tag{6}$$

The non-vanishing non-diagonal elements e(i) has dimension 1 to $nstep - 1$.
The all non-vanishing non-diagonal matrix elements are given by:

$$e(i) = \frac{-1}{h^2} \tag{7}$$

And, all the rest elements are zero.
Then i constructed the symmetric matrix A such that:

$$Au = 2Eu$$

Here, A is symmetric matrix of dimension (nstep * nstep).
u is column eigenvector of dimension (1 to $nstep - 1$).
The matrix A looks like this:

$$A = \begin{pmatrix} d_1 & e_1 & 0 & 0 & \cdots & 0 & 0 \\ e_1 & d_2 & e2 & 0 & \cdots & 0 & 0 \\ 0 & e_2 & d_3 & e_3 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & \cdots & \cdots & \cdots & d_{nstep-2} & e_{nstep-1} \\ 0 & \cdots & \cdots & \cdots & \cdots & e_{nstep-1} & d_{nstep-1} \end{pmatrix}$$

The matrix u looks like this:

$$u = \begin{pmatrix} u_1 \\ u_2 \\ \cdots \\ \cdots \\ \cdots \\ u_{nstep-1} \end{pmatrix}$$

Diagonalizing the matrix will yield the twice of the energy values.
For three dimensional harmonic oscillator the energy eigenvalues are given by:

$$E_{n,l} = (2k + l + \frac{3}{2})\hbar\omega \tag{8}$$

$$n = 2k + l \tag{9}$$

where k is no. of nodes in a wavefunction.
Here, I found k from the plot of wavefunction which was zero, one and two for ground state, first excited, and second excited state respectively.
Also, here $l = 0$ for all the cases.
Hence,

ground state

$$E_0 = 3/2 \quad \hbar\omega$$

first excited state

$$E_1 = 7/2 \quad \hbar\omega$$

second excited state

$$E_2 = 11/2 \quad \hbar\omega$$

For simplicity, i have plotted the graph for one dimensional case.
I have plotted eigenvalue versus value of h.
The nature of the plot will be same and energy values will be changed.
Here, each of my energy eigenvalue are in terms of $\frac{\hbar\omega}{2}$.
Also, no. of nodes are 1,2,3 for ground,first,and second excited states.
for ground state:
1d value = 1 so, 3d value = $1 + (1/2) = 3/2$
for first excited state:
1d value = 3 so, 3d value = $2 + (3/2) = 7/2$
for second excited state:
1d value = 5 so, 3d value = $3 + (5/2) = 11/2$

The solution and source code directory is :

```
location             : hw7/qn2/
library used         : LAPACK ( dsyev)
source code          : hw7qn2.f90, hw7qn2plot.f90
output data files    : first.dat, second.dat,third.dat ( for three lowest eigenvalue
output data file     : u123.dat ( for lowest three eigenvectors)
plots                : e0.eps,e1.eps,e2.eps (for three energy eigenvalues)
plot                 : u123.eps (for radial wavefunctions)
makefile             : Makefile
```

The figures are shown below:

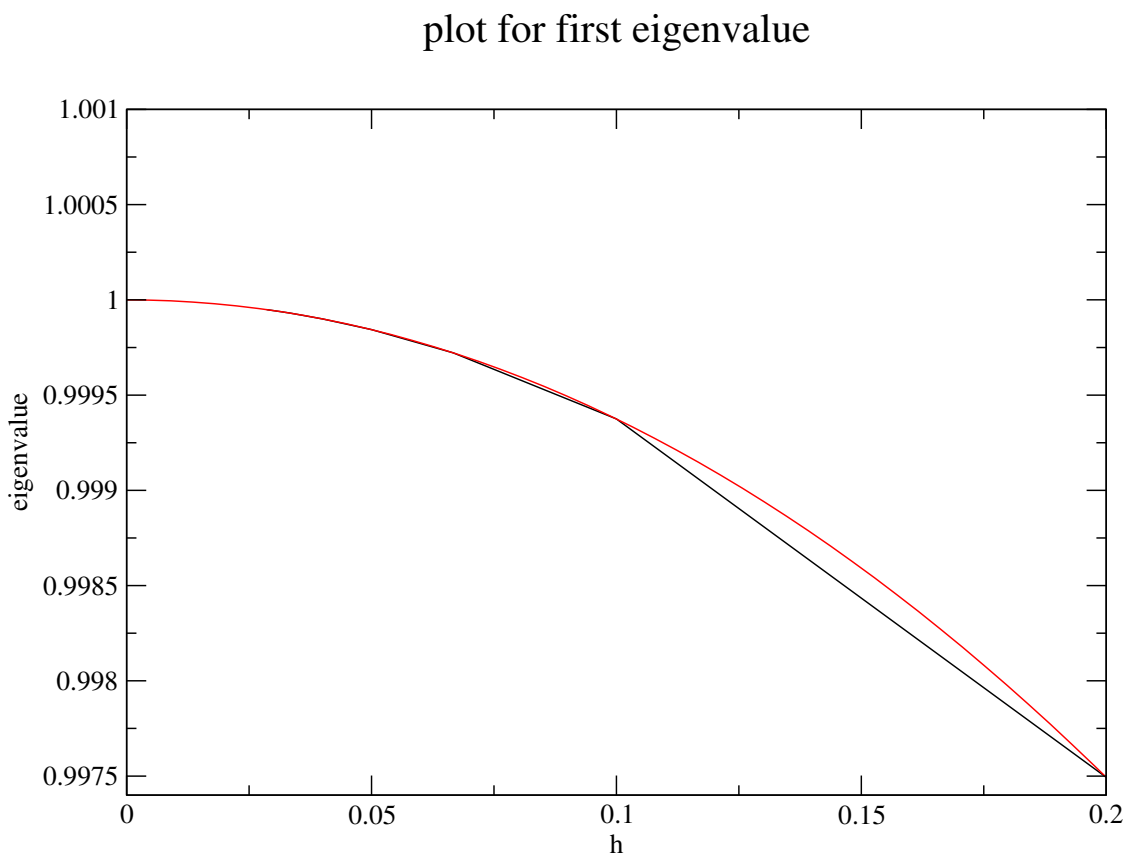

Figure 1: Energy eigenvalue for ground state

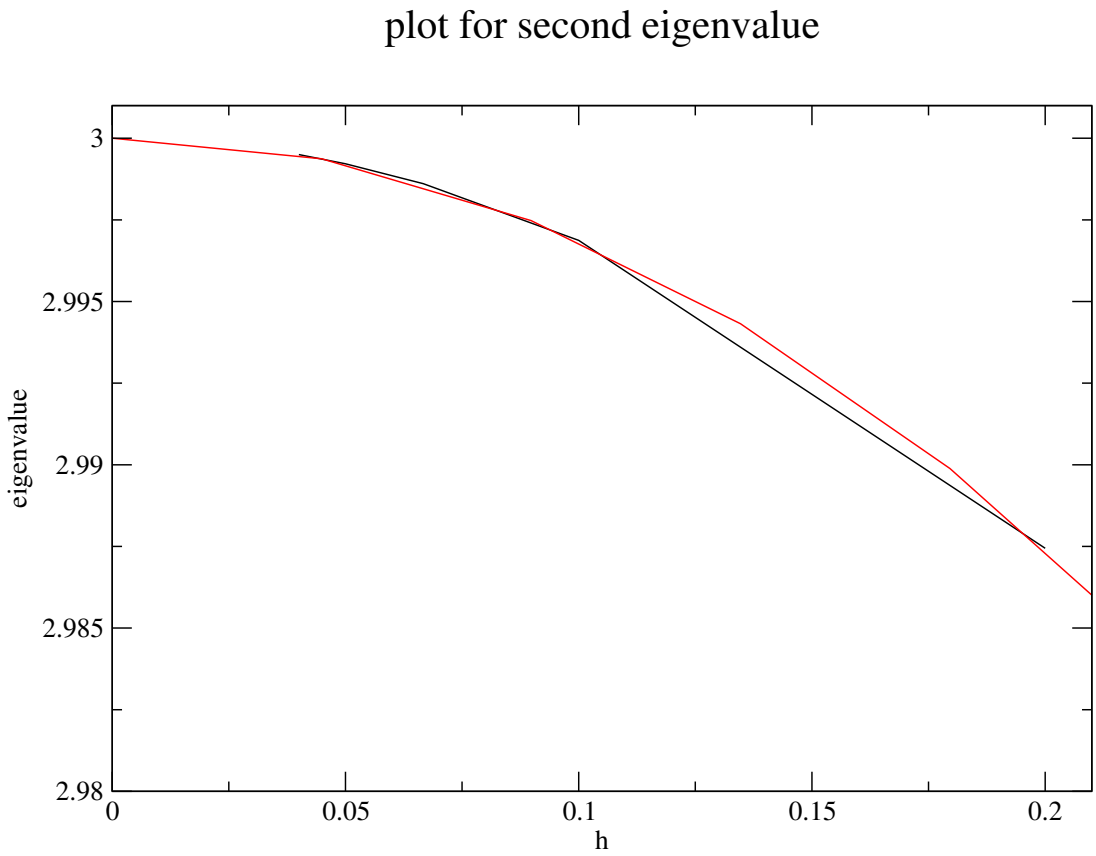

Figure 2: Energy eigenvalue for first excited state

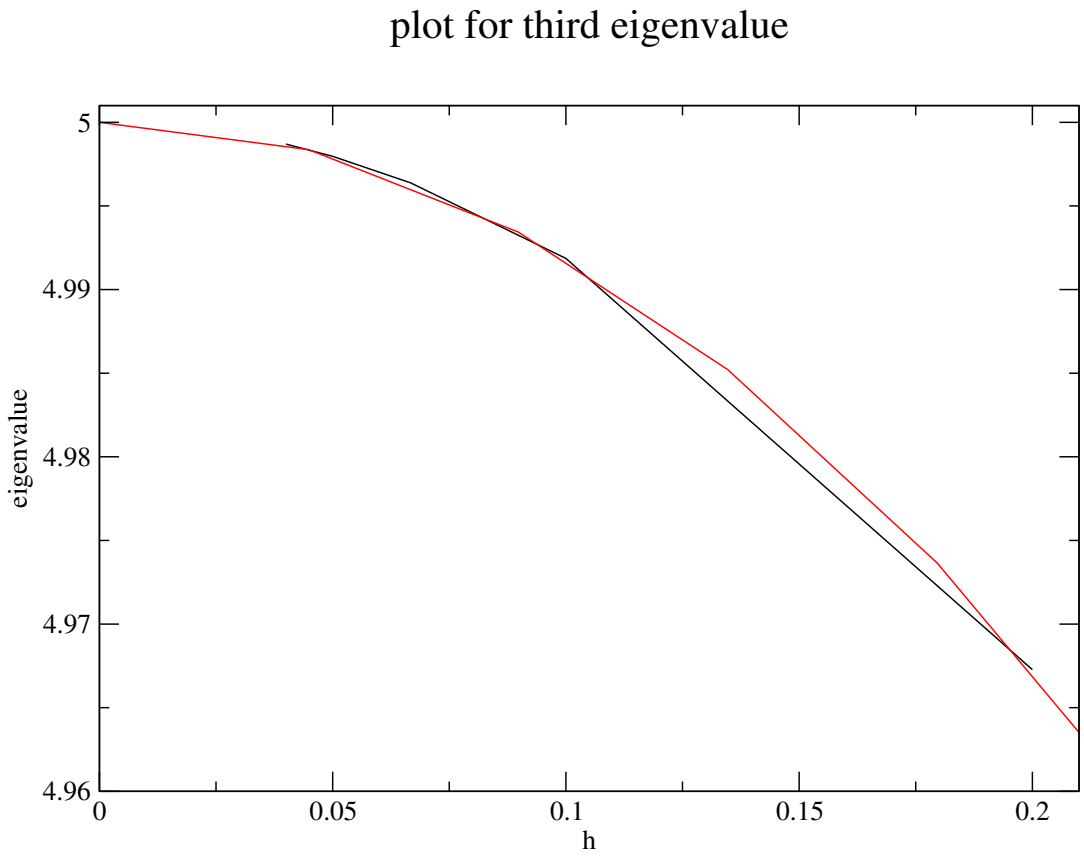

Figure 3: Energy eigenvalue for second excited state

2.3 part c: extrapolation to get energy value when h tends to zero

Here, I used xmgrace to extrapolate the energy value.
The values found are 1,3,and 5.
The plots are shown above.

2.4 part d: plot of radial wavefunction

In this part I plotted the first three eigenvectors from the code 'hw7qn2.f90'.

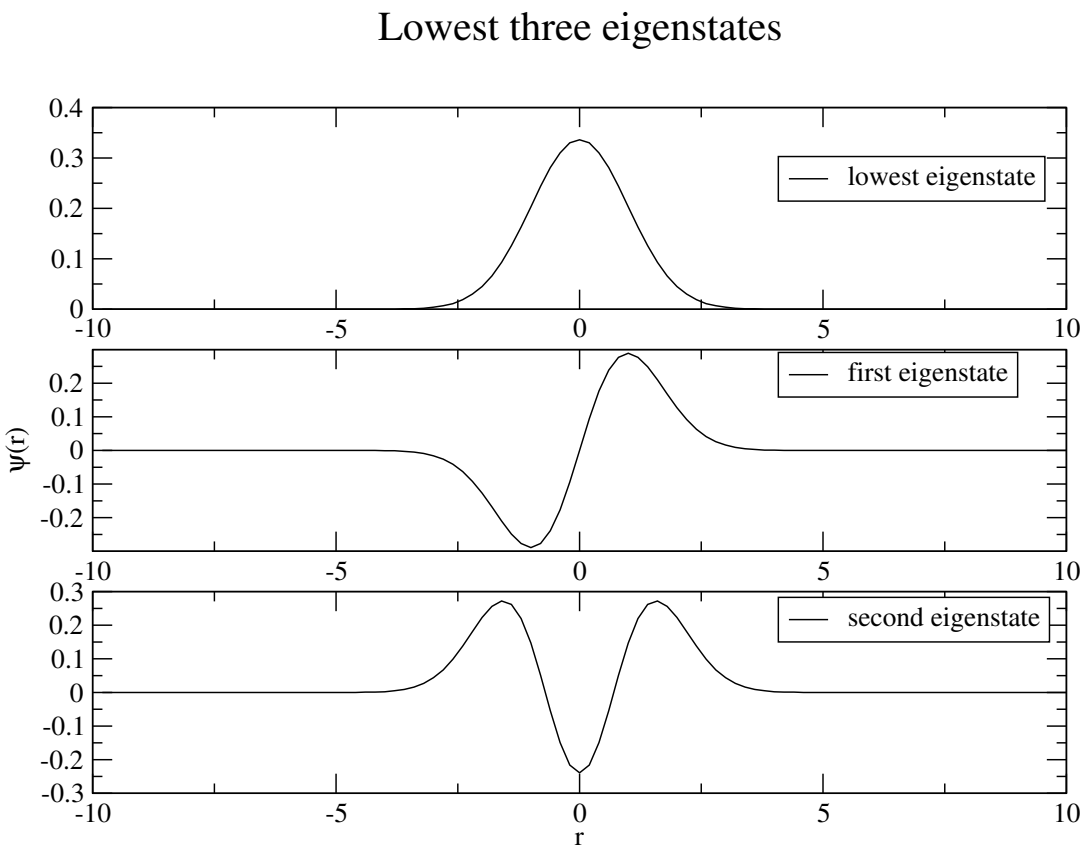

Figure 4: Radial wave functions for three lowest eigenstates

The solution location is :

```
location             : hw7/qn2
library              : LAPACK (dsyev subroutine)
source code          : hw7qn2.f90
output data file     : u123.dat
plot                 : u123.eps
makefile             : Makefile
handsout             : hw7qn2a.pdf
```