Physics 562 - Computational Physics

Assignment 4: Eigenvalues of Simple Harmonic Oscillator

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Abstract

This paper examines the eigenvalues and eigenvectors of two one-dimensional harmonic oscillators.

1 Hamiltonian

The one dimensional harmonic oscillator is given by the differential operator

$$m\frac{\partial^2 x}{\partial t^2} = -kx. \tag{1}$$

This differential equation has the solution

$$x = x_0 sin(wt + \theta), \tag{2}$$

where

$$w = \sqrt{\frac{k}{m}}. \tag{3}$$

The total energy of the system is the same as the hamiltonian which is given by

$$E = \mathcal{H} = \frac{p^2}{2m} + \frac{mw^2x^2}{2} \tag{4}$$

Now, make the following substitutions of the form

$$\xi = x\sqrt{\frac{mw}{\hbar}}, \tag{5}$$

$$\pi = \frac{p}{\sqrt{\hbar mw}}. \tag{6}$$

This gives the equation

$$\mathcal{H} = \frac{\hbar w}{2}(\pi^2 + \xi^2). \tag{7}$$

The expression can be factorized so that it then becomes

$$\mathcal{H} = \frac{\hbar w}{2}[(\xi + i\pi)(\xi - i\pi) + (\xi - i\pi)(\xi + i\pi)]. \tag{8}$$

The following two operators can be defined in terms of the position and momentum,

$$a = \frac{\xi + i\pi}{\sqrt{2}} = \frac{1}{\sqrt{2\hbar mw}}(mwx + ip) \tag{9}$$

$$a^\dagger = \frac{\xi - i\pi}{\sqrt{2}} = \frac{1}{\sqrt{2\hbar mw}}(mwx - ip). \tag{10}$$

from the commutator relation $[i\pi, \xi] = 1$, it follows that $[a, a^\dagger] = 1$. Using this, the hamiltonian can be written in the form

$$\mathcal{H} = \hbar w(a^\dagger a + \frac{1}{2}) = \hbar w(N + \frac{1}{2}). \tag{11}$$

Note that $N = a^\dagger a$. The energy eigenvalues is given by

$$\mathcal{H}\,|n\rangle = (n + \frac{1}{2})\hbar w\,|n\rangle \tag{12}$$

The only nonzero matrix elements of $a^\dagger$ are $\langle n+1| a^\dagger |n\rangle = \sqrt{n+1}$. So, this gives the matrix

$$a^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 & \dots \\ \sqrt{1} & 0 & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

and the adjoint

$$a = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

Now, the position and momentum can be defined in terms of a and $a^\dagger$. This gives x and p in the form

$$x = \sqrt{\frac{\hbar}{2mw}}(a^\dagger + a) \tag{13}$$

$$p = i\sqrt{\frac{mw\hbar}{2}}(a^\dagger - a). \tag{14}$$

Plugging in for $a^\dagger$ and a results in

$$x = \sqrt{\frac{\hbar}{2mw}} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \dots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

and

$$p = i\sqrt{\frac{mw\hbar}{2}} \begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 & \dots \\ \sqrt{1} & 0 & -\sqrt{2} & 0 & \dots \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Now look at the hamiltonians of two different harmonic oscillators. The first harmonic oscillator has the parameters of $\hbar = 1$, $m = 1$, and $w = .5$. The second harmonic oscillator has the parameters of $\hbar = 1$, $m = 1$, and $w = 1$. If you calculate the hamiltonians using equation 11 you get

$$\mathcal{H}_1 = (N + \frac{1}{2}) \tag{15}$$

$$\mathcal{H}_2 = .5 \cdot (N + \frac{1}{2}) \tag{16}$$

writing as a 10×10 matrix we get

$$\mathcal{H}_1 = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{5}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{7}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{9}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{11}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{13}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{15}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{17}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{19}{2} \end{pmatrix}$$

and

$$\mathcal{H}_2 = \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{5}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{7}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{9}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{11}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{13}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{15}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{17}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{19}{4} \end{pmatrix}$$

In the system that we are looking at, the first harmonic oscillator is going to be in the basis of the second harmonic oscillator. The new hamiltonian will be of the form

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2 + \frac{1}{2} m \cdot (\omega_2 - \omega_1)^2 \cdot (x_2 - x_1)^2 \tag{17}$$

where w_2 and x_2 are the matrices associated with the second harmonic oscillator, and w_1 and x_1 are the matrices associated with the first harmonic oscillator. The eigenvalues and eigenvector will now be calculated for the hamiltonian given in equation 17.

2 The Fortran95 code

The code calculates the eigenvalues and eigenvectors of a matrix of any size. For this project, a 10×10 matrix is used. First a module called `NumType` is created to store all my global parameters.

Listing 1: Module `NumType`

```
1
2  module NumType
3
4      save
5      integer, parameter       ::  dp = kind(1.d0)
6      real(dp), parameter      ::  pi = 4*atan(1._dp)
7      complex(dp), parameter   ::  iic = (0._dp,1._dp),&
8                                   one = (1._dp,0._dp),&
9                                   zero = (0._dp,0._dp)
10
11 end module NumType
```

Listing 2: `mtest.f95`

```
1
2  module setup
3
4      use NumType
5      implicit none
6      integer,     parameter   ::  ndim=10,lwork=5*ndim
7      real(dp),    parameter   ::  mass=1.0_dp, &
8                                   hbar=1.0_dp,&
9                                   omega1=0.5_dp,&
10                                  omega2=1._dp
11
12 end module setup
13
```

```
14 program matrix
15
16     use setup
17     implicit none
18
19     complex(dp), dimension(ndim,ndim)    :: A,B,E,H1,H2,H3
20     real(dp),    dimension(ndim)         :: w
21     integer                              :: i, nn, info
22     complex(dp)                          :: work(lwork)
23     real(dp)                             :: rwork(lwork)
24
25     A(1:10,1:10) = reshape((/                                  &
26             zero, sqrt(1*one), zero, zero, zero,               &
27             zero, zero, zero, zero, zero,                      &
28             sqrt(1*one), zero, sqrt(2*one), zero, zero,        &
29             zero, zero, zero, zero, zero,                      &
30             zero, sqrt(2*one), zero, sqrt(3*one), zero,        &
31             zero, zero, zero, zero, zero,                      &
32             zero, zero, sqrt(3*one), zero, sqrt(4*one),        &
33             zero, zero, zero, zero, zero,                      &
34             zero, zero, zero, sqrt(4*one), zero,               &
35             sqrt(5*one), zero, zero, zero, zero,               &
36             zero, zero, zero, zero, sqrt(5*one),               &
37             zero, sqrt(6*one), zero, zero, zero,               &
38             zero, zero, zero, zero, zero,                      &
39             sqrt(6*one), zero, sqrt(7*one), zero, zero,        &
40             zero, zero, zero, zero, zero,                      &
41             zero, sqrt(7*one), zero, sqrt(8*one), zero,        &
42             zero, zero, zero, zero, zero,                      &
43             zero, zero, sqrt(8*one), zero, sqrt(9*one),        &
44             zero, zero, zero, zero, zero,                      &
45             zero, zero, zero, sqrt(9*one), zero                &
46     /),                                                        &
47     (/10,10/))
48
49     H1(1:10,1:10) = reshape((/                                 &
50             1/2._dp*one, zero, zero, zero, zero,               &
51             zero, zero, zero, zero, zero,                      &
52             zero, 3/2._dp*one, zero, zero, zero,               &
53             zero, zero, zero, zero, zero,                      &
```

```
54              zero, zero, 5/2._dp*one, zero, zero,          &
55              zero, zero, zero, zero, zero,                 &
56              zero, zero, zero, 7/2._dp*one, zero,          &
57              zero, zero, zero, zero, zero,                 &
58              zero, zero, zero, zero, 9/2._dp*one,          &
59              zero, zero, zero, zero, zero,                 &
60              zero, zero, zero, zero, zero,                 &
61              11/2._dp*one, zero, zero, zero, zero,         &
62              zero, zero, zero, zero, zero,                 &
63              zero, 13/2._dp*one, zero, zero, zero,         &
64              zero, zero, zero, zero, zero,                 &
65              zero, zero, 15/2._dp*one, zero, zero,         &
66              zero, zero, zero, zero, zero,                 &
67              zero, zero, zero, 17/2._dp*one, zero,         &
68              zero, zero, zero, zero, zero,                 &
69              zero, zero, zero, zero, 19/2._dp*one          &
70      /),                                                   &
71      (/10,10/))
72
73      H2(1:10,1:10) = reshape((/                            &
74              1/4._dp*one, zero, zero, zero, zero,          &
75              zero, zero, zero, zero, zero,                 &
76              zero, 3/4._dp*one, zero, zero, zero,          &
77              zero, zero, zero, zero, zero,                 &
78              zero, zero, 5/4._dp*one, zero, zero,          &
79              zero, zero, zero, zero, zero,                 &
80              zero, zero, zero, 7/4._dp*one, zero,          &
81              zero, zero, zero, zero, zero,                 &
82              zero, zero, zero, zero, 9/4._dp*one,          &
83              zero, zero, zero, zero, zero,                 &
84              zero, zero, zero, zero, zero,                 &
85              11/4._dp*one, zero, zero, zero, zero,         &
86              zero, zero, zero, zero, zero,                 &
87              zero, 13/4._dp*one, zero, zero, zero,         &
88              zero, zero, zero, zero, zero,                 &
89              zero, zero, 15/4._dp*one, zero, zero,         &
90              zero, zero, zero, zero, zero,                 &
91              zero, zero, zero, 17/4._dp*one, zero,         &
92              zero, zero, zero, zero, zero,                 &
93              zero, zero, zero, zero, 19/4._dp*one          &
```

```
94      /),                                                          &
95      (/10,10/))
96
97      A(1:10,1:10)= sqrt(hbar/(2*mass*omega1))*A(1:10,1:10)
98      B(1:10,1:10)= sqrt(hbar/(2*mass*omega2))*A(1:10,1:10)
99      H3(1:10,1:10)= H1 + H2 + 1/2._dp*mass*&
100                     (omega2-omega1)**2*(B-A)**2
101
102     nn = 10
103     info = 0
104     E(1:nn,1:nn) = H3(1:nn,1:nn)
105
106     call zheev('v','u',nn,E,ndim,w,work,lwork,rwork,info)
107
108     print *, 'info=', info
109
110     do i = 1,10
111         print '(a,f15.8,a,20f6.0)','eigenvalues',w(i),&
112         'vector', dble(e(1:nn,i))
113     end do
114
115 end program matrix
```

The code is run by typing `./mat`. The resulting eigenvalues and eigenvectors are printed out to the terminal.

3 Results

The eigenvalues are not the same as the eigenvalues of the individual harmonic oscillators.

	eigenvalue(eV)
ground state	$\frac{3}{4}$
1st excited	$\frac{9}{4}$
2nd excited	$\frac{15}{4}$
3rd excited	$\frac{21}{4}$
4th excited	$\frac{27}{4}$
5th excited	$\frac{33}{4}$
6th excited	$\frac{39}{4}$
7th excited	$\frac{45}{4}$
8th excited	$\frac{51}{4}$
9th excited	$\frac{57}{4}$

References

[1] M. Metcalf, J. Reid and M. Cohen, *Fortran 95/2003 explained*. Oxford University Press, 2004.