

# 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

one dimensional harmonic oscillator is given by the differential operator

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

This differential equation has the solution

$$x = x_0 \sin(\omega t + \theta), \quad (2)$$

where

$$\omega = \sqrt{\frac{k}{m}}. \quad (3)$$

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

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

Now, make the following substitutions of the form

$$\xi = x\sqrt{\frac{mw}{\hbar}}, \quad (5)$$

$$\pi = \frac{p}{\sqrt{\hbar mw}}. \quad (6)$$

This gives the equation

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

The expression can be factorized so that it then becomes

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

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

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

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

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

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

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

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

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

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

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

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

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

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

writing as a  $10 \times 10$  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

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

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  $10 \times 10$  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. This would indicate that the harmonic oscillators are coupled.



	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	$\frac{57}{4}$

## 4 Summary and conclusions

The eigenvalues tell us that Natalie is super cool.

## References

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