

Mathematical Physics II

PHYS 502

Solution to Problem Set # 2

In the first two problems you will learn (hopefully) how to use numerical computations to suggest analytic results to you.

1. Fixed BC: Tridiagonal matrices of the form $K = 2\delta_{ij} - \delta_{i,i-1} - \delta_{i,i+1}$ always occur in problems involving coupled harmonic oscillators in one dimension with fixed boundary conditions, as well as lots of other places. In the 5×5 case they have the form shown on the left in the equation below:

$$K_{\text{fixed}} = \begin{bmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}, \quad K_{\text{free}} = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \quad (1)$$

- Choose a convenient value for n (the size of the matrix you will have to diagonalize).
- Create a matrix with the structure shown on the left above.
- Diagonalize this matrix.
- Sort the output from “bottom to top”, that is, from smallest to largest eigenvalue.
- Plot the lowest couple of eigenvectors (if you don’t understand what that means, ask in class).
- Do the plots suggest that the components of the eigenvectors have some analytic form in terms of functions you are aware of? (The answer is yes.)
- Guess this form.
- Test this guess by doing some simple paper-and-pencil calculations.
- When you get this right you will find an analytic expression for the eigenvalues also.
- Plot your analytic expression for the eigenvalues and compare with a plot of the numerically computed eigenvalues.
- Announce EURIKA! when everything works as suggested.

Solution: A code was written to diagonalize tridiagonal matrices. The subroutine `tqli` from *Numerical Recipes* was used. The input to this subroutine were two arrays of length n , $d(n)$ defining the matrix elements on the diagonal, and $e(n)$ defining those on the sub/super diagonal. In the code n is easy to

change. A second subroutine, `eigsrt`, was used to sort the output eigenvectors according to the size of the eigenvalues.

For debugging purposes n was set to 5 and all input and output were written to screen. After a while the output looked OK, so n was set to 2, where eigenvalues/vectors could be computed by hand. When that checked, n was reset to 5 and the output compared with the output of a comparable code in Maple.

For the ‘production run’ n was set to 50 and the lowest 5 eigenvectors plotted. For the first, the i^{th} component of the first eigenvector was plotted (vertical) above position i in the plot. Same deal for all the others. The plot runs from 1 to 50. The axis has been extended to the left and right, and is shown running from 0 to 51. The plot is shown in Fig. 1 on the left. With a little imagination you can extend ‘by hand’ the curves on the left to 0, where they go through the origin, and on the right to 51, where they go through the origin. The physical basis for this intuition is that you can imagine a particle at the anchor point 0, nailed to the brick wall, and another at 51, anchored to the other brick wall. Their displacements must be zero.

The plots look like the sine function. The k^{th} eigenvector has $k - 1$ zero crossings. To check this leap of imagination we guess (in published papers wild guesses like this are called ‘ansatz’ because it sounds more professional) that the i^{th} component of the k^{th} eigenvector, with $1 \leq i \leq 50, 1 \leq k \leq 50$, is $\sin \frac{ki\pi}{n+1}$, since these functions vanish at $i = 0$ and $i = n + 1$.

Now we have to check this guess. For the i^{th} row we find

$$-\sin \frac{k(i-1)\pi}{n+1} + 2 \sin \frac{k(i)\pi}{n+1} - \sin \frac{k(i+1)\pi}{n+1} \stackrel{\text{some algebra}}{=} E(k) \sin \frac{k(i)\pi}{n+1} \quad (2)$$

This result is valid for the first row ($i = 1$) also, since the first term on the left automatically vanishes. It is also valid for the last row ($i = n$) since the last term on the right is zero. Algebra gives $E(k) = 2 - 2 \cos \frac{k\pi}{n+1}$. A plot of the numerically computed eigenvalues (for $n = 50$, in black) is compared with this analytic expression (in cyan) in Fig. 1 on the right. The two curves appear as a single curve, so you could suspect I only plotted one of these two curves. The usual way to compare results that are identical is to shift one of the curves a bit, so the two can be seen and compared. This is done in the plot.

2. Free BC: For free boundary conditions (*e.g.*, an organ pipe with open ends) the matrices that arise have +1 instead of +2 at the corners (top left and bottom right). In the 5×5 case they have the form shown on the right in the equation above.

a. Choose a convenient value for n (the size of the matrix you will have to diagonalize).

b. Create a matrix with the structure shown on the right above.

c. Diagonalize this matrix.

d. Sort the output from “bottom to top”.

e. Plot the lowest couple of eigenvectors.

f. Do the plots suggest that the components of the eigenvectors have some analytic form in terms of functions you are aware of? (The answer is still yes.)

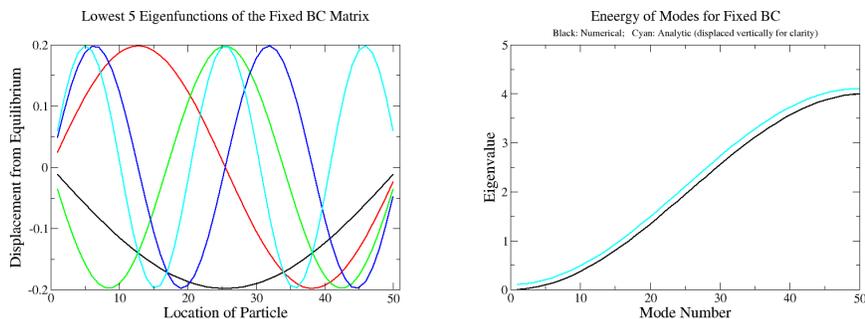


Figure 1: (Left) Plots of the five eigenvectors with the smallest eigenvalues of the ‘fixed boundary condition matrix’. The energy increases with the number of zero crossings. (Right) Plot of the numerically computed energy (black) and that computed using an analytic expression $E(k) = 2 - 2 \cos \frac{k\pi}{n+1}$ (cyan). The latter is shifted up slightly for comparison purposes.

- g. Guess this form.
- h. Test this guess by doing some simple paper-and-pencil calculations.
- i. When you get this right you will find an analytic expression for the eigenvalues also.
- j. Plot your analytic expression for the eigenvalues and compare with a plot of the numerically computed eigenvalues.
- k. Announce EURIKA! when everything works as suggested.

Solution: The code used to solve the first problem was recycled by changing the input array $d(n)$ so that the first and last elements were +1 instead of +2. Self-consistency checks were carried out as described above. Then n was set to 50 as before and the eigenvectors and eigenvalues computed. The eigenvectors are displayed on the left in Fig. 2.

In Freshman Physics you learn that the sound waves in a organ pipe closed at both ends are sine waves. In an organ pipe open at both ends they are cosine waves. So we expect the eigenvectors to behave like cosines. So for the k^{th} eigenvectors we assume the components have the form $\cos(\alpha i + \beta)$, where the parameter α will depend on the mode index and the number of particles n , and similarly for β .

We test this ansatz for the rows $i = 2, 3, \dots, n - 1$ and find

$$-\cos(\alpha(i-1) + \beta) + 2\cos(\alpha i + \beta) - \cos(\alpha(i+1) + \beta) = 2(1 - \cos(\alpha)) \cos(\alpha i + \beta) \quad (3)$$

This gives us the eigenvalue. We use this in the first equation:

$$\cos(\alpha(1) + \beta) - \cos(\alpha(1+1) + \beta) = 2(1 - \cos(\alpha)) \cos(\alpha(1) + \beta) \quad (4)$$

A little bit of trigonometry gives us $\alpha + 2\beta = 0$. Next we look at the last equation, the equation for row n :

$$-\cos(\alpha(n-1) + \beta) + \cos(\alpha(n) + \beta) = 2(1 - \cos(\alpha)) \cos(\alpha(n) + \beta) \quad (5)$$

Somewhat more algebra gives us $(2n+1)\alpha + 2\beta = 2k\pi$, where k is an integer that will turn out to be a mode index. Solving these simultaneous linear equations we find $\alpha = k\pi/n$ and $\beta = -k\pi/2n$. Then the i^{th} component of the k^{th} mode is $\cos\left(\frac{k\pi}{n}\left(i - \frac{1}{2}\right)\right)$. This expression was plugged back into the equation for free boundary conditions and verified. The eigenvalue spectrum for the free boundary condition case is plotted on the right in Fig. 2.

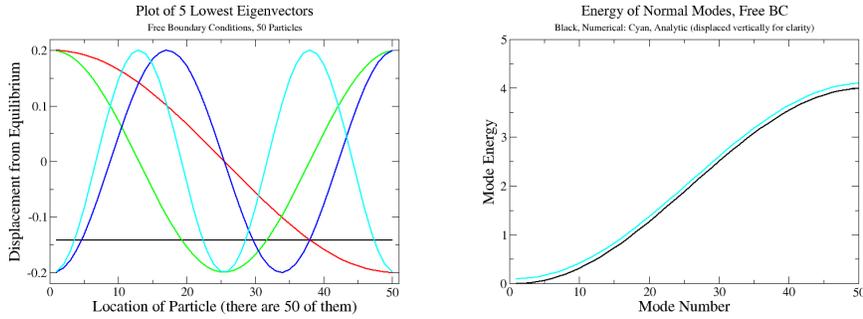


Figure 2: (Left) Plots of the five eigenvectors with the smallest eigenvalues of the ‘free boundary condition matrix’. The energy increases with the number of zero crossings. (Right) Plot of the numerically computed energy (black) and that computed using an analytic expression $E(k) = 2 - 2 \cos\left(\frac{k\pi}{n}\right)$ (cyan). The latter is shifted up slightly for comparison purposes.

3. Feynman’s Favorite Slick Trick: is “completing the square”. Here are two gaussian functions: $f_1 = \exp[-(x - a_1)^2 - (y - b_1)^2]$ and $f_2 = \exp[-(x - a_2)^2 - (y - b_2)^2]$. Write $f_1 \times f_2$ as a gaussian f_3 multiplied by a prefactor, where f_3 has the same form as f_1 and f_2 .

Solution: Take the product, take the negative log, and find

$$(x - a_1)^2 + (y - b_1)^2 + (x - a_2)^2 + (y - b_2)^2 \quad (6)$$

Expand out, collect similar terms, and find

$$2 \left[\left(x - \frac{a_1 + a_2}{2}\right)^2 + \left(\frac{a_1 - a_2}{2}\right)^2 \right] + 2 \left[\left(y - \frac{b_1 + b_2}{2}\right)^2 + \left(\frac{b_1 - b_2}{2}\right)^2 \right] \quad (7)$$

Now take the negative and exponentiate back up. The result is a narrower Gaussian centered at the midpoint, multiplied by a factor that depends exponentially on the distance between the points. In vector notation:

$$e^{-(\mathbf{x}-\mathbf{a})^2} e^{-(\mathbf{x}-\mathbf{b})^2} = e^{-(\mathbf{a}-\mathbf{b})^2/2} e^{-2(\mathbf{x}-(\mathbf{a}+\mathbf{b})/2)^2} \quad (8)$$