Assignment VI: Eigensystems

Due 10/17/2016 (4 pm)

1. Testing Matrix Calls *(partially in Class)*

Before using subroutines from external libraries such as *lapack* or *linpack*, it is a good idea to test those routines with small matrices, for which you know the correct answer. In this way it will only take a short time to realize how hard it is to get the calling procedure perfectly correct.

The subroutine *dminv.f90* inverts a matrix and computes its determinant. Write a driver routine to test this subroutine with the matrix

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

(a) Verify that the inverse of A is [R.L. Eq. (15.39)]

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

(b) As a general procedure, applicable even if you do not know the analytic answer, check the your inverse in both directions, i.e. verify that

$$AA^{-1} = A^{-1}A = \mathbf{1} \tag{3}$$

(c) Compute the determinant of A and compare with your analytic answer.

(d) Consider the same matrix A as in Eq. (1), but now used to describe a system of three linear equations of the form

$$AX = B. \tag{4}$$

Here the vector B on the RHS is assumed to be known, and the problem is to solve for the vector X. Use the routine *dgesv.f* from LAPACK to solve the system for

$$B_1 = \begin{pmatrix} +4 \\ -10 \\ +22 \end{pmatrix}. \tag{5}$$

The LAPACK and BLAS libraries are available on the Suse-Linux computers under /usr/local/lib

(e) Consider the symmetric matrix

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

Use the LAPACK routine *dsyev.f* to verify that the eigenvalues are 6, -3, -3, and compute the eigenvectors. Do the same using the LAPACK routine *dgeev.f*.

(e) Consider the matrix

$$A = \begin{pmatrix} -2 & +2 & -3 \\ +2 & +1 & -6 \\ -1 & -2 & 0 \end{pmatrix}. \tag{7}$$

Use the LAPACK routine *dgeev.f* to verify that the eigenvalues are $\lambda_1 = 5$, $\lambda_2 = \lambda_3 = -3$.

Notice that double roots can cause problems. In particular, there is a uniqueness problem with their eigenvectors since any combination of these eigenvectors would also be an eigenvector.

1. Verify that the eigenvector for $\lambda_1 = 5$ is proportional to

$$X_1 = \begin{pmatrix} -1 \\ -2 \\ +1 \end{pmatrix}. \tag{8}$$

2. The eigenvalue -3 corresponds to a double root. This means that the corresponding eigenvectors are degenerate, i.e. their are not unique. Two linearly independent ones are

$$X_2 = \begin{pmatrix} -2 \\ +1 \\ 0 \end{pmatrix}, \qquad X_3 = \begin{pmatrix} 3 \\ 0 \\ 1 \end{pmatrix}. \tag{9}$$

In this case it is not clear what your eigenproblem solver will give as eigenvectors. Try to find a relationship between your computed eigenvectors to the above given ones.

2. Schrödinger Equation via Diagonalization (M.H-J_07 12.6)

Instead of solving the Schrödinger equation in coordinate space as differential equation, we will solve it through diagonalization of a large matrix. Please see Section 12.6 in the handout for details. However, you will solve the three-dimensional harmonic oscillator. Please review your quantum mechanics notes.

The radial part of the wave function, $R(r)$ is the solution to

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{l(l+1)}{r^2}\right)R(r) + V(r)R(r) = ER(r). \tag{10}$$

Then one substitutes $R(r) = (1/r)u(r)$ to obtain the differential equation for $u(r)$. Furthermore, it is convenient to introduce the dimensionless variable $\rho = (1/\alpha)r$, where α is a constant with dimension length to obtain the radial equation as

$$-\frac{\hbar^2}{2m\alpha^2}\frac{d^2}{d\rho^2}u(\rho) + \left(V(\rho) + \frac{l(l+1)}{\rho^2}\frac{\hbar^2}{2m\alpha^2}\right)u(\rho) = Eu(\rho) \tag{11}$$

Concentrate on the special case $l = 0$ and use $V(\rho) = \frac{1}{2}k\alpha^2\rho^2$, which leads to

$$-\frac{d^2}{d\rho^2}u(\rho) + \frac{mk}{\hbar^2}\alpha^4\rho^2u(\rho) = \frac{2m\alpha^2}{\hbar^2}Eu(\rho). \tag{12}$$

The constant α can now be fixed so that

$$\frac{mk}{\hbar^2}\alpha^4 = 1 \tag{13}$$

Define

$$\lambda = \frac{2m\alpha^2}{\hbar^2}E \tag{14}$$

and show that you can rewrite the Schrödinger equation as

$$-\frac{d^2}{d\rho^2}u(\rho) + \rho^2u(\rho) = \lambda u(\rho) \tag{15}$$

Include your derivation of the final equation in your write-up, and give the expression for the expected eigenvalues E_{nl} for the 3D harmonic oscillator. Here $n = 0, 1, 2, \ldots$, and $l = 0, 1, 2, \ldots$.

In your calculation use units such that $k = \hbar = m = \alpha = 1$. Using a 3-point discretization (see Homework III) for the second derivative this differential equation is turned into a matrix equation of the form $Ax = b$, Eq. (12.9).

Follow Section 12.6.1 in setting up the algorithm.

1. Define values for N_{step}, R_{min}, and R_{max}. These values then define the step-size h. Typical values for R_{min} and R_{max} should be -10 and 10 respectively for the lowest-lying eigenvalues. The number of mesh-points N_{step} should range from 100 to about 1000.

2. Construct the arrays (dimension 0 to N_{step}), which contain all values of x_k and V_k (Hint, write a small function routine to set up the potential as function of x_k).

3. Then construct the vectors d (containing the diagonal) and e (containing the off-diagonal. Note that the dimension of these two vectors runs from 1 to N_{step}-1, since the wave function u is known at both ends of the grid. Then you have everything to fill the upper or lower half of the input matrix for your diagonalization routine.

(a) Perform a series of diagonalization of the matrix for different step sizes h. You obtain a series of eigenvalues $E(h/2^k)$ with k=0,1,2 ... That will give you an array of 'x-values' h,$h/2$, $h/4$, .. and an array of 'y-values' $E(h)$, $E(h/2)$ ...
You will have such a set of values as function of h for each eigenvalue.

(b) Use these values to perform an extrapolation to obtain the energy value for $h \rightarrow 0$. You may plot the values as function of h and use *xmgrace* for the extrapolation, you you may use a function like *polint* to extrapolate to $h = 0$.

(c) Carry out this analysis for the three lowest eigenvalues and comment on the error of your calculation.

(d) Calculate and plot the radial wave function for those three lowest eigenstates.