10.34 – Fall 2006

Homework #4 - Solutions

Problem 1: Problem 3.A.3 in Beers' textbook – Eigenvalue/vectors

Part A: (see page 150-151 in Beers)
We are asked is any of the matrices are known to have all real eigenvalues. Matrices A can be visually seen to have only real eigenvalues, this is because it is a real symmetric matrix. Matrix C can also be determined to have only real eigenvalues because:

Trace(C) – 4*det(C) = 24 > 0

This requires a small calculation, but not the actual calculation of the eigenvalues.

Part B: (see page 156-157 in Beers)
The bounding of the eigenvalues involves the use of Gershgorin's Theorem, which states that the eigenvalues of a matrix must lie within some range around the diagonal elements of the matrix. More specifically:

$$\left|\lambda_i - a_{kk}\right| \le \sum_{elements\ j\neq k} \left|a_{kj}\right| = \Gamma_k$$

The summation is the sum of the modulus of all the off-diagonal elements for row *k*.

Matrix A:
Doing this analysis for matrix A, we find that the Gamma value for rows 1 – 4 are: 4, 5, 2, and 5, respectively. This results in the following bounds:

$$\left.\begin{array}{lll} \left|\lambda_i\right| \le 4 & or & -4 \le \lambda_i \le 4 \\ \left|\lambda_i - 2\right| \le 5 & or & -3 \le \lambda_i \le 7 \\ \left|\lambda_i - 3\right| \le 3 & or & 0 \le \lambda_i \le 6 \\ \left|\lambda_i + 1\right| \le 5 & or & -6 \le \lambda_i \le 4 \end{array}\right\} \Rightarrow \quad \boxed{-6 \le \lambda_i \le 7}$$

Matrix C:
Similarly for matrix C, we find Gamma values of: 2 and 1.

$$\left.\begin{array}{lll} \left|\lambda_i - 3\right| \le 2 & or & 1 \le \lambda_i \le 5 \\ \left|\lambda_i + 1\right| \le 1 & or & -2 \le \lambda_i \le 0 \end{array}\right\} \Rightarrow \quad \boxed{-2 \le \lambda_i \le 5}$$

Note that in this case, the range between 0 and 1 is also excluded from the value eigenvalue space, but the problem asked for an upper and lower bound.

Part C:
For a unitary matrix, $D^{-1} = D^{T}$. So if we can calculate the inverse and show it equals the transpose, then *D* is unitary. In order to determine the inverse, we can make an augmented matrix to solve $D*D^{-1} = I$. Similar to the idea of Gaussian elimination, we want to do row operations to turn *D* into *I*, and the matrix that was formerly *I*, will be the inverse of *D*. To accomplish this, we only need to do two things: exchange rows 1 and 2; then multiply row 2 by -1. The results are shown below.

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$$\left[\begin{array}{ccc|ccc} 0 & -1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \end{array}\right] \xrightarrow{\text{Row operations}} \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \end{array}\right]$$

By visual inspection, you can see that D^{-1} does equal D^{T}.

Part D: (see page 149 in Beers)
For this part, we are asked to calculate the eigenvalue and *unit* eigenvector *by hand* (a very useful skill to have in the day and age).

To solve this, we can use the determinant of $(C - \lambda I)$. The following expression will allow for the eigenvalues to be determined:

$$\det\left(C - \lambda I\right) = 0 = \begin{vmatrix} c_{11} - \lambda & c_{12} \\ c_{21} & c_{22} - \lambda \end{vmatrix} = \left(c_{11} - \lambda\right)\left(c_{22} - \lambda\right) - c_{21}c_{12}$$

We can expand to get the following quadratic, and the resulting use of the quadratic formula will yield:

$$\lambda^2 - \left(c_{11} + c_{22}\right)\lambda + \left(c_{11}c_{22} - c_{21}c_{12}\right) = 0$$

$$\lambda_{1,2} = \frac{\left(c_{11} + c_{22}\right) \pm \sqrt{\left(c_{11} + c_{22}\right)^2 - 4\left(c_{11}c_{22} - c_{21}c_{12}\right)}}{2}$$

Plugging into the matrix elements, we find that the eigenvalues are:

$$\boxed{\lambda_1 = 3.4495 \qquad \lambda_2 = -1.4495}$$

To solve for the unit eigenvector, you can solve the following equations with the constraint of unit length:

$$\left(\underline{\underline{C}} - \lambda_j \underline{\underline{I}}\right) \cdot \underline{w}_j = \begin{bmatrix} c_{11} - \lambda_j & c_{12} \\ c_{21} & c_{22} - \lambda_j \end{bmatrix} \cdot \begin{bmatrix} w_{1,j} \\ w_{2,j} \end{bmatrix} = \underline{0}$$

Since the two equations are dependent (the matrix is singular), you can only use one equation, and then an arbitrary equation to determine the vector length (unit in our case).

$$\left(c_{11} - \lambda_j\right) w_{1,j} + c_{12} w_{2,j} = 0 \qquad \textit{and} \qquad w_{1,j}^2 + w_{2,j}^2 = 1$$

To solve this, solve the first equation for $w_{2,j}$, and insert in the second equation. The following are the solutions:

$$w_{1,j} = \pm\left\{1 + \left[\frac{-\left(c_{11} - \lambda_j\right)}{c_{12}}\right]^2\right\}^{-1/2} \qquad \textit{and} \qquad w_{2,j} = \frac{-\left(c_{11} - \lambda_j\right)}{c_{12}} \cdot w_{1,j}$$

Insert the appropriate values for each eigenvalue, one will find the following vectors:

$$\underline{w}_1 = \begin{bmatrix} 0.97566 \\ 0.21928 \end{bmatrix} \qquad \textit{and} \qquad \underline{w}_2 = \begin{bmatrix} -0.40998 \\ 0.91210 \end{bmatrix}$$

Note that these eigenvectors can be multiplied by -1 and still be correct.

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Homework 4

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1 Problem 2

(a) To solve the schrodinger equation we use the basis set $b_m(\phi) = \exp(im\phi)$. For our particular case we can convert the operator $\hat{H}$ from function space into an matrix H by using the formula

$$H_{k,l} = \frac{1}{2\pi}\int_0^{2\pi} b_k^*(\phi)\hat{H}b_l(\phi)d\phi$$

Here $H_{k,l}$ is the k, l element of the matrix H and the operator $\hat{H}$ is given by the equation

$$\hat{H} = -\frac{h^2}{8\pi^2 I}\frac{d^2}{d\phi^2} + V(\phi)$$

Lets first calculate the matrix elements of the differential operator

$$\begin{aligned}
\frac{1}{2\pi}\int_0^{2\pi} b_k^*(\phi)\frac{-h^2}{8\pi^2 I}\frac{d^2}{d\phi^2}b_l(\phi)d\phi &= -\frac{h^2}{16\pi^3 I}\int_0^{2\pi}\exp(-ik\phi)\frac{d^2\exp(il\phi)}{d\phi^2}d\phi \\
&= \frac{h^2 l^2}{16\pi^3 I}\int_0^{2\pi}\exp(-ik\phi)\exp(il\phi)d\phi \\
&= \frac{h^2 l^2}{16\pi^3 I}(2\pi\delta_{lk}) \\
&= \frac{h^2 l^2}{8\pi^2 I}\delta_{lk}
\end{aligned}$$

In the above equation δ_{lk} is the kronecker-delta function which is 1 when $l = k$ or 0 when $l \neq k$. This kronecker-delta function ensures that for the differntial operator only the diagonal elements are non-zero, the rest of the elements are 0.

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Now let us calculate the matrix elements of $V(\phi)$ part of the $\hat{H}$ operator. But before we do that we will first write $V(\phi)$ in a more convenient form

$$\begin{aligned} V(\phi) &= \sum_0^4 y_n \cos(n\phi) \\ &= \sum_0^4 y_n \frac{\exp(in\phi) + \exp(-in\phi)}{2} \end{aligned}$$

This form of writing the potential function is much more convenient when we are integrating it between the basis functions to calculate the matrix elements. Now let us proceed to calculation of the matrix elements of the potential $V(\phi)$.

$$\begin{aligned} V_{kl} &= \frac{1}{2\pi}\int_0^{2\pi} b_k^*(\phi) V(\phi) b_l(\phi) d\phi \\ &= \frac{1}{2\pi}\int_0^{2\pi} \exp(-ik\phi)\left(\sum_0^4 y_n \frac{\exp(in\phi) + \exp(-in\phi)}{2}\right)\exp(il\phi)d\phi \\ &= \frac{1}{2\pi}\sum_0^4 y_n \int_0^{2\pi} \exp(-ik\phi)\frac{\exp(in\phi) + \exp(-in\phi)}{2}\exp(il\phi)d\phi \\ &= \sum_0^4 \frac{y_n}{2}(\delta_{k(n+l)} + \delta_{(k+n)l}) \end{aligned}$$

Again the kronecker-delta function appears in the expression. The potential function populates the non-diagonal elements and the diagonal elements of the matrix H.

Based on the values of k, l element of the differential and the V operator we realize can write the the elements of H matrix as follows

$$H_{lm} = \frac{h^2 l^2}{8\pi^2 I}\delta_{lk} + \sum_0^4 \frac{y_n}{2}(\delta_{k(n+l)} + \delta_{(k+n)l})$$

The overall size of the matrix H is dependent on the number of basis functions used. For $2M+1$ basis functions the size of the matrix will be $2M+1 \times 2M+1$. The accuracy of the solution will improve with the increase in the basis functions. The solution will be perfect when M becomes infinity.

In the matrix space the schrodinger equation just boils down to solving the eigenvalue problem of the system. Each eigenvalue of the system corresponds to a energy state of the system.

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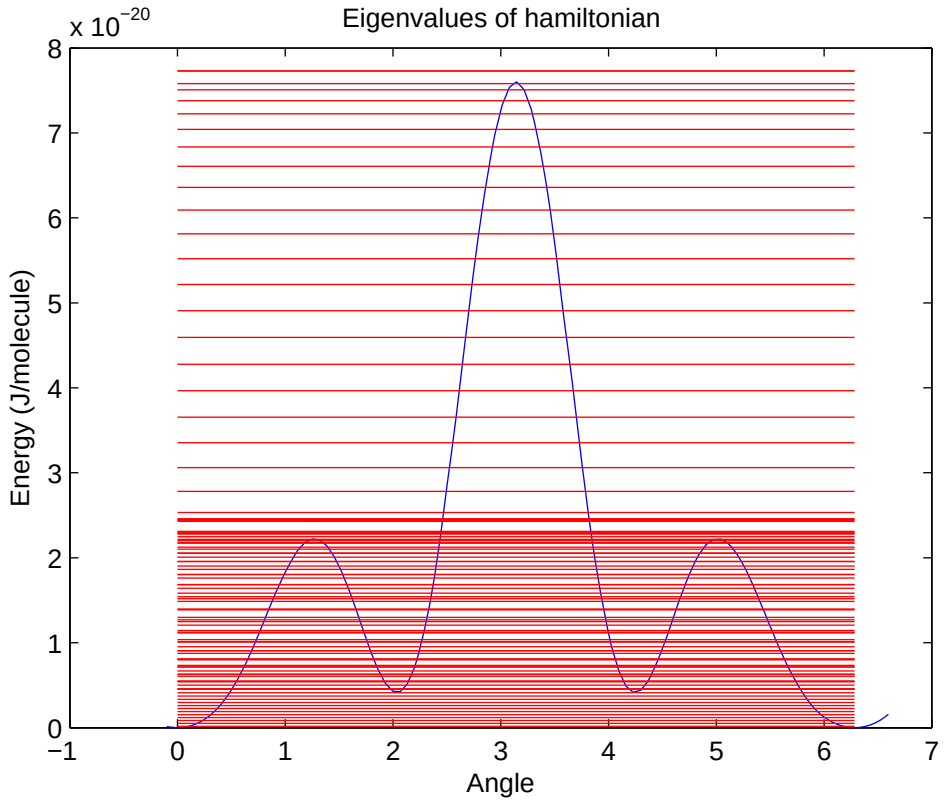

(b) Using the above derived rule to calculate the elements of the matix H, we generate the matrix and then calculate its eigenvalues using the command `eig` to calculate the eigenvalues of the system. Look at the commmented code pset4problem2b to see how the code is implemented. The sample input and output from the code is

```
>>
The zero point energy of the system =1.7463e-022 J
>>  pset4problem2b ( 100, 3e-45) ;
```

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(c) In this problem we make use of the code pset4problem2b to calculate the energy states of the system. Once the energies of the system are evaluated we can calculate the heat capacity without much difficulty using the formula given in the problem statement. Please look at the code pset4problem2c. to see how it is implemented. A sample input and output is given below

```
>> c = pset4problem2c (300, 100) ;
>> c

c =

9.8953

>>
```

(c) Once we have written the program that calculates the heat capacities of the system, we can loop over the program to calculate the heat capacities for at various temperatures and values of M. (Please note, for a given value of M the energy states of the system do not change. Thus to calculate the heat capacities at different temperatures for a given value of M, we only need to solve the eigenvalue problem once. Calculating the eigenvalues of the H matrix is the slowest step of the system and should be avoided as much as possible). Look at the implementation of code `problem3d`. A sample input and output is given below and the graph is also presented at the end of the solution.

```
 >> problem2d
>>
```

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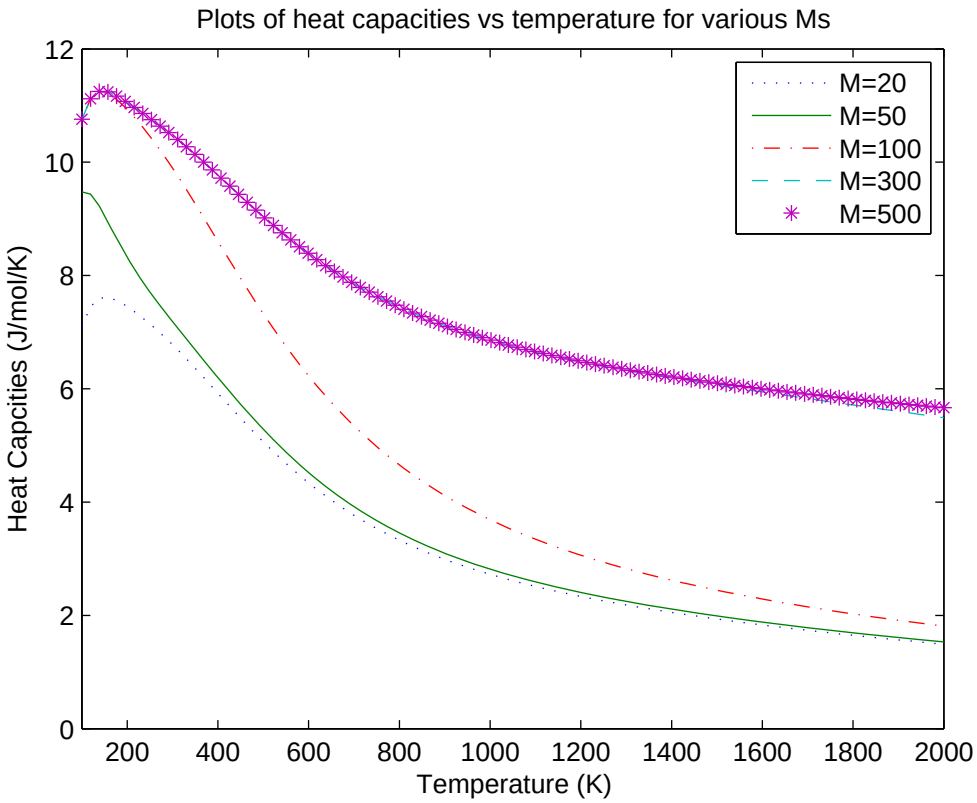

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