# APPENDIX A

# EIGENVALUE PROBLEMS

## *A.1 Summary of Matrices*

A column vector is indicated by

$$f = \begin{matrix} f_1 \\ f_2 \\ . \\ . \\ . \\ f_N \end{matrix}$$

A matrix consisting of M rows and N columns is defined by

$$A = \begin{matrix} A_{11} & A_{12} & \dots & A_{1N} \\ A_{21} & A_{22} & \dots & A_{2N} \\ A_{31} & A_{32} & \dots & A_{3N} \\ . & & & \\ . & & & \\ . & & & \\ A_{M1} & A_{M2} & \dots & A_{MN} \end{matrix}$$

A is said to be an M x N matrix which is denoted by $A_{ij}$. The vector f is considered as a M x 1 matrix.

The product of a M x N matrix with a N x K matrix gives a M x K matrix. It is obvious that matrix multiplication is not commutative, that is AB is not equal to BA. When C = AB we have

$$C_{ik} = \Sigma A_{ij} B_{jk} .$$

Matrix products are associative so that A(BC) = (AB)C.

On the basis of the rule of matrix multiplication, the product of a row vector (1 x N) and a column vector (N x 1) gives a (1 x 1) matrix, or the scalar product

$$f^t f = f_1f_1 + f_2f_2 + ... + f_Nf_N.$$

But the product of a column vector (N x 1) and a row vector (1 x N) gives a (N x N) matrix, or a vector product

$$f f^t = \begin{matrix} f_1f_1 & f_1f_2 & \dots & f_1f_N \\ f_2f_1 & f_2f_2 & \dots & f_2f_N \\ . & & & \\ . & & & \\ f_Nf_1 & f_Nf_2 & \dots & f_Nf_N \end{matrix}$$

To summarize these few properties of matrix multiplication: (a) matrix multiplication is not commutative, (b) the ji element of AB is the sum of products of elements from the jth row of A and ith column of B, and (c) the number of columns in A must equal the number of rows in B if the product AB is to make sense.

There are several matrices that are related to A. They are:

(a) $A^t$ which is the transpose of A so that $[A^t]_{ij} = [A]_{ji}$,

(b) $A^*$ which is the complex conjugate of A so that

$$[A^*]_{ij} = [A]^*_{ij},$$

(c) $A^+$ which is the adjoint of A so that $[A^+]_{ij} = [A]^*_{ji}$, and

(d) $A^{-1}$ which is the inverse of A so that $A^{-1}A = AA^{-1} = I$, where I denotes the identity matrix.

A few definitions follow:

(a) A is real if $A^* = A$,

(b) A is symmetric if $A^t = A$,

(c) A is antisymmetric if $A^t = -A$,

(d) A is Hermitian if $A^+ = A$,

(e) A is orthogonal if $A^{-1} = A^t$, and

(f) A is unitary if $A^{-1} = A^+$.

## *A.2 Eigenvalue Problems*

To understand some of the techniques for solving the radiative transfer equation it is necessary to review solutions to eigenvalue problems. When a operator A acts on a vector x, the resulting vector Ax is in general distinct from x. However there may exist certain non-zero vectors for which Ax is just a multiple of x. That is

$$A\,x = \lambda\,x$$

or written out explicitly

$$\Sigma\, A_{ij}\, x_j = \lambda\, x_i \quad I=1,...,n \;.$$

Such a vector is called an eigenvector of the operator A, and the constant λ is called an eigenvalue. The eigenvector is said to belong to the eigenvalue. Consider an example where the operator A is given by

$$\begin{matrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{matrix} = A \quad ; \quad \begin{matrix} x_1 \\ x_2 \\ x_3 \end{matrix} = x \, .$$

So we are trying to solve

$$x_1 + 2x_2 + 3x_3 = \lambda x_1$$

$$4x1 + 5x_2 + 6x_3 = \lambda x_2$$

$$7x_1 + 8x_2 + 9x_3 = \lambda x_3$$

For a nontrivial solution the determinant of coefficients must vanish

$$\begin{matrix} 1-\lambda & 2 & 3 \\ 4 & 5-\lambda & 6 \\ 7 & 8 & 9-\lambda \end{matrix} = 0$$

This produces a third order polynomial in λ whose three roots are the eigenvalues $\lambda_i$.

There are several characteristics of the operator A that determine the character of the eigenvalue. Briefly summarized they are (a) if A is hermitian, then the eigenvalues are real and the eigenvectors are orthogonal (eigenvectors of identical or degenerate eigenvalues can be made orthogonal through the Gram Schmidt process) and (b) if A is a linear operator, then the eigenvalues and eigenvectors are independent of the coordinate system. A proof of (b) is quickly apparent.

$$A\,x = \lambda\,x$$

Let Q represent an arbitrary coordinate transformation, then

$$\gamma^{-1} A\,x = \lambda\,\gamma^{-1} x$$

$$\gamma^{-1} A\,\gamma\,\gamma^{-1} x = \lambda\,\gamma^{-1} x$$

$$A'\,x' = \lambda\,x' \, .$$

Thus if x is an eigenvector of the linear operator A, its transform

$$x' = \gamma^{-1} x$$

is an eigenvector of the transformed matrix

$$A' = \gamma^{-1} A \gamma,$$

and the eigenvalues are the same.

It is often desirable to make a transformation to a coordinate system in which A' is a diagonal matrix and the diagonal elements are the eigenvalues. The desired transformation matrix consists of the eigenvectors of the original matrix A.

$$\gamma = \begin{array}{ccc} e_1 & e_2 & e_n \\ \downarrow & \downarrow & \downarrow \end{array}$$

where the $j^{th}$ col consists of components of eigenvector $e_j$. For the transformation to be unitary, the eigenvectors must be orthonormal (orthogonal and normalized).

## *A.3 $CO_2$ Vibration Example*

Consider the problem of molecular vibrations in $CO_2$, which is shown schematically as a simple linear triatomic molecule system consisting of three masses connected by springs of spring constant k. Let $x_i$ represent deviations from the equilibrium position.

| | | |
|---|---|---|
| $x_1$ | $x_2$ | $x_3$ |
| m | M | m |
| O | C | O |

The kinetic energy of this system can be written

$$T = \frac{1}{2} \sum_i m_i v_i^2 = \frac{1}{2} v^t \, M \, v$$

where v represents dx/dt. The potential energy is given by

$$P = \frac{1}{2} \sum_{ij} P_{ij} x_i x_j = \frac{1}{2} x^t \, P \, x$$

where

$$P = P_o + \sum_i \left(\frac{\partial P}{\partial x_i}\right)_o x_i + \frac{1}{2} \sum_{ij} \left(\frac{\partial^2 P}{\partial x_i \partial x_j}\right)_o x_i x_j$$

and without loss of generality let $P_o = 0$ and use the fact that $\partial P/\partial x = 0$ at equilibrium. Then Lagrange's equation:

$$\frac{d}{\phantom{dt}} \frac{\partial T}{\phantom{\partial v}} + \frac{\partial P}{\phantom{\partial x}}$$

dt $\partial v$ $\partial x$

with

$$T = \frac{1}{2} mv^2 \text{ and } P = \frac{1}{2} kx^2,$$

becomes

$$mv = - kx .$$

This suggests a solution of the form $x_i = a_i \sin(\omega_i t + \delta_i)$, so that

$$\sum_j P_{ij} a_j - \omega^2 T_{ij} a_j = 0 .$$

Now the potential energy is written

$$P = \frac{1}{2} k (x_2 - x_1)^2 + \frac{1}{2} k (x_3 - x_2)^2$$

$$= \frac{1}{2} k (x_1^2 + 2x_2^2 + x_3^2 - 2x_1x_2 - 2x_2x_3) ,$$

so the matrix operator is,

$$P = \begin{matrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{matrix}$$

which is real and symmetric. And the kinetic energy is written

$$T = \frac{1}{2} m (x_1^2 + x_3^2) + \frac{1}{2} Mx_2^2 ,$$

so the matrix operator is

$$T = \begin{matrix} m & o & o \\ o & M & o \\ o & o & m \end{matrix}$$

which is diagonal. So, we find $| P - \omega^2 T | = 0$ implies

$$\det A = [\begin{matrix} k-\omega^2 m & -k & o \\ -k & 2k-\omega^2 M & -k \end{matrix}] = 0$$

$$\begin{matrix} o & -k & k-\omega^2 m \end{matrix}$$

and direct evaluation of the determinant leads to the cubic equation

$$\omega^2(k-\omega^2 m)(kM + 2km - \omega^2 Mm) = 0 .$$

This yields the three roots

$$\omega_1 = 0 ,\ \omega_2 = [k/m]^{1/2} ,\ \omega_3 = [(k/m)(1+2m/M)]^{1/2}.$$

Now solve for the eigenvectors. For $\omega_1 = 0$

$$\begin{matrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{matrix} \quad \begin{matrix} a_{11} \\ a_{12} \\ a_{13} \end{matrix} \quad = 0 \quad \Rightarrow a_{11} = a_{12} = a_{13}$$

which represents a translation since the centre of mass doesn't move $mx_1 + Mx_2 + mx_3 = 0$.

For $\omega_2 = [k/m]^{1/2}$

$$\begin{matrix} 0 & -k & 0 \\ -k & 2k-kM/m & -k \\ 0 & -k & 0 \end{matrix} \quad \begin{matrix} a_{21} \\ a_{22} \\ a_{23} \end{matrix} \quad = 0 \Rightarrow \ a_{22} = 0,\ a_{21} = -a_{23}$$

which represents a vibration in the breathing mode with the carbon molecule stationary and the oxygen molecules moving in opposite directions.
For $\omega_3 = [(k/m)(1+2m/M)]^{½}$

$$\begin{matrix} -2mk/M & -k & 0 \\ -k & -kM/m & -k \\ 0 & -k & -2mk/M \end{matrix} \quad \begin{matrix} a_{31} \\ a_{32} \\ a_{33} \end{matrix} \quad = 0 \ \Rightarrow a_{31} = a_{33} ,\ a_{32} = -(2m/M)a_{31}$$

which represents the carbon molecule motion offset by the combined motion of the oxygen molecules.

Recalling that the mass of the proton is given by $m_p = 1.67\text{x}10^{-27}$ Kg, that the spring constant for the $CO_2$ is roughly $k \sim 1.4\text{x}10^3$ J/m2 (from the second derivative of the potential curves), and that $m = 16m_p$ while $M = 12m_p$, then

$$\omega_3 = [\frac{1.4\text{x}10^3}{16\text{x}1.67\text{x}10^{-27}} \ (1 \ + \frac{32}{12})\ ]^{½} = [.192 \text{ x } 10^{30}]^2 = .438 \text{ x}10^{15} ,$$

and

$$\lambda = \frac{2\pi c}{\omega} = \frac{2\pi\ 3x10^{8}}{.438x10^{15}} \sim 4.3 \times 10^{-6}\ \text{m} = 4.3\ \mu\text{m}$$

This simple one dimensional model of the $CO_2$ molecular motions yields the absorption wavelength of 4.3 micron observed in the spectra. Considering two dimensional vibrations yields the solution at 15 micron.