Thus the two eigenvalues of $\mathbf{O}$ are

$$\omega_1 = O_{11}\cos^2\theta_0 + O_{22}\sin^2\theta_0 + O_{12}\sin 2\theta_0 \tag{1.106a}$$

and

$$\omega_2 = O_{11}\sin^2\theta_0 + O_{22}\cos^2\theta_0 - O_{12}\sin 2\theta_0 \tag{1.106b}$$

Upon comparison of Eqs. (1.104) and (1.89), we find the two eigenvectors to be

$$\begin{pmatrix} c_1^1 \\ c_2^1 \end{pmatrix} = \begin{pmatrix} \cos\theta_0 \\ \sin\theta_0 \end{pmatrix} \tag{1.107a}$$

and

$$\begin{pmatrix} c_1^2 \\ c_2^2 \end{pmatrix} = \begin{pmatrix} \sin\theta_0 \\ -\cos\theta_0 \end{pmatrix} \tag{1.107b}$$

It should be mentioned that the Jacobi method for diagonalizing $N \times N$ matrices is a generalization of the above procedure. The basic idea of this method is to eliminate iteratively the off-diagonal elements of a matrix by repeated applications of orthogonal transformations, such as the ones we have considered here.

Exercise 1.11 Consider the matrices

$$\mathbf{A} = \begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix}$$

$$\mathbf{B} = \begin{pmatrix} 3 & 1 \\ 1 & 2 \end{pmatrix}$$

Find numerical values for the eigenvalues and corresponding eigenvectors of these matrices by a) the secular determinant approach; b) the unitary transformation approach. You will see that approach (b) is much easier.

1.1.7 Functions of Matrices

Given a Hermitian matrix $\mathbf{A}$, we can define a function of $\mathbf{A}$, i.e., $f(\mathbf{A})$, in much the same way we define functions $f(x)$ of a simple variable x. For example, the square root of a matrix $\mathbf{A}$, which we denote by $\mathbf{A}^{1/2}$, is simply that matrix which when multiplied by itself gives $\mathbf{A}$, i.e.,

$$\mathbf{A}^{1/2}\mathbf{A}^{1/2} = \mathbf{A} \tag{1.108}$$

The sine or the exponential of a matrix are defined by the Taylor series of the function, e.g.,

$$\exp(\mathbf{A}) = \mathbf{1} + \frac{1}{1!}\mathbf{A} + \frac{1}{2!}\mathbf{A}^2 + \frac{1}{3!}\mathbf{A}^3 + \cdots$$

or in general

$$f(\mathbf{A}) = \sum_{n=0}^{\infty} c_n \mathbf{A}^n \tag{1.109}$$

After these definitions, we are still faced with the problem of calculating $\mathbf{A}^{1/2}$ or exp ($\mathbf{A}$). If $\mathbf{A}$ is a diagonal matrix

$$(\mathbf{A})_{ij} = a_i \delta_{ij}$$

everything is simple, since

$$(\mathbf{A})^n = \begin{pmatrix} a_1^n & & & \\ & a_2^n & & \mathbf{0} \\ & \mathbf{0} & \ddots & \\ & & & a_N^n \end{pmatrix} \tag{1.110}$$

so that

$$f(\mathbf{A}) = \sum_{n=0}^{\infty} c_n \mathbf{A}^n = \begin{pmatrix} \sum_n c_n a_1^n & & & \\ & \sum_n c_n a_2^n & & \mathbf{0} \\ & \mathbf{0} & \ddots & \\ & & & \sum_n c_n a_N^n \end{pmatrix}$$

$$= \begin{pmatrix} f(a_1) & & & \\ & f(a_2) & & \mathbf{0} \\ & \mathbf{0} & \ddots & \\ & & & f(a_N) \end{pmatrix} \tag{1.111}$$

Similarly, the square root of a diagonal matrix is

$$\mathbf{A}^{1/2} = \begin{pmatrix} a_1^{1/2} & & & \\ & a_2^{1/2} & & \mathbf{0} \\ & \mathbf{0} & \ddots & \\ & & & a_N^{1/2} \end{pmatrix} \tag{1.112}$$

What do we do if $\mathbf{A}$ is not diagonal? Since $\mathbf{A}$ is Hermitian, we can always find a unitary transformation that diagonalizes it, i.e.,

$$\mathbf{U}^\dagger \mathbf{A} \mathbf{U} = \mathbf{a} \tag{1.113a}$$

The reverse transformation that "undiagonalizes" $\mathbf{a}$ is

$$\mathbf{A} = \mathbf{U} \mathbf{a} \mathbf{U}^\dagger \tag{1.113b}$$

Now notice that

$$\mathbf{A}^2 = \mathbf{U}\mathbf{a}\mathbf{U}^\dagger \mathbf{U}\mathbf{a}\mathbf{U}^\dagger = \mathbf{U}\mathbf{a}^2\mathbf{U}^\dagger$$

or in general

$$\mathbf{A}^n = \mathbf{U}\mathbf{a}^n\mathbf{U}^\dagger \tag{1.114}$$

so that

$$f(\mathbf{A}) = \sum_n c_n \mathbf{A}^n = \mathbf{U}\left(\sum_n c_n \mathbf{a}^n\right)\mathbf{U}^\dagger = \mathbf{U}f(\mathbf{a})\mathbf{U}^\dagger$$

$$= \mathbf{U}\begin{pmatrix} f(a_1) & & & \\ & f(a_2) & & \mathbf{0} \\ & \mathbf{0} & \ddots & \\ & & & f(a_N) \end{pmatrix}\mathbf{U}^\dagger \tag{1.115}$$

Thus to calculate any function of a Hermitian matrix $\mathbf{A}$, we first diagonalize $\mathbf{A}$ to obtain $\mathbf{a}$, the diagonal matrix containing all the eigenvalues of $\mathbf{A}$. We then calculate $f(\mathbf{a})$, which is easy because $\mathbf{a}$ is diagonal. Finally we "undiagonalize" $f(\mathbf{a})$ using (1.113b) to obtain (1.115). For example, we can find the square root of a matrix $\mathbf{A}$ as

$$\mathbf{A}^{1/2} = \mathbf{U}\mathbf{a}^{1/2}\mathbf{U}^\dagger$$

since

$$\mathbf{A}^{1/2}\mathbf{A}^{1/2} = \mathbf{U}\mathbf{a}^{1/2}\mathbf{U}^\dagger\mathbf{U}\mathbf{a}^{1/2}\mathbf{U}^\dagger = \mathbf{U}\mathbf{a}^{1/2}\mathbf{a}^{1/2}\mathbf{U}^\dagger = \mathbf{U}\mathbf{a}\mathbf{U}^\dagger = \mathbf{A}$$

If the above procedure were to yield a result for $f(\mathbf{A})$ that was infinite, then $f(\mathbf{A})$ does not exist. For example, if we try to calculate the inverse of a matrix $\mathbf{A}$ that has a zero eigenvalue (say $a_i = 0$), then $f(a_i) = 1/a_i = \infty$ and so $\mathbf{A}^{-1}$ does not exist. As Exercise 1.12(a) shows, the determinant of a matrix is just the product of its eigenvalues. Thus if one of the eigenvalues of $\mathbf{A}$ is zero, $\det(\mathbf{A})$ is zero and the above argument shows that $\mathbf{A}^{-1}$ does not exist This same result was obtained in a different way in Exercise 1.7.

Exercise 1.12 Given that

$$\mathbf{U}^\dagger\mathbf{A}\mathbf{U} = \mathbf{a} = \begin{pmatrix} a_1 & & & \\ & a_2 & & \mathbf{0} \\ & \mathbf{0} & \ddots & \\ & & & a_N \end{pmatrix} \quad \text{or} \quad \mathbf{A}\mathbf{c}^\alpha = a_\alpha \mathbf{c}^\alpha \qquad \alpha = 1, 2, \ldots, N$$

Show that

a. $\det(\mathbf{A}^n) = a_1^n a_2^n \cdots a_N^n$.

b. $\operatorname{tr} \mathbf{A}^n = \sum_{\alpha=1}^{N} a_\alpha^n$.

c. If $\mathbf{G}(\omega) = (\omega\mathbf{1} - \mathbf{A})^{-1}$ then

$$(\mathbf{G}(\omega))_{ij} = \sum_{\alpha=1}^{N} \frac{U_{i\alpha}U_{j\alpha}^*}{\omega - a_\alpha} = \sum_{\alpha=1}^{N} \frac{c_i^\alpha c_j^{\alpha*}}{\omega - a_\alpha}.$$

Show that using Dirac notation this can be rewritten as

$$(\mathbf{G}(\omega))_{ij} \equiv \langle i|\mathscr{G}(\omega)|j\rangle = \sum_\alpha \frac{\langle i|\alpha\rangle\langle\alpha|j\rangle}{\omega - a_\alpha}$$

As an interesting application of this relation consider the problem of solving the following set of inhomogeneous linear equations

$$(\omega\mathbf{1} - \mathbf{A})\mathbf{x} = \mathbf{c}$$

for $\mathbf{x}$ The most straightforward way to proceed is to invert $\omega\mathbf{1} - \mathbf{A}$, i.e.,

$$\mathbf{x} = (\omega\mathbf{1} - \mathbf{A})^{-1}\mathbf{c} = \mathbf{G}(\omega)\mathbf{c}$$

If we want $\mathbf{x}$ as a function of ω we need to invert the matrix for *each* value of ω. However, if we diagonalize A, we can write

$$x_i = \sum_j (\mathbf{G}(\omega))_{ij} c_j = \sum_{j\alpha} \frac{U_{i\alpha}U_{j\alpha}^* c_j}{\omega - a_\alpha}$$

It is now computationally simple to evaluate $\mathbf{x}$ as a function of ω.

Exercise 1.13 If

$$\mathbf{A} = \begin{pmatrix} a & b \\ b & a \end{pmatrix}$$

show that

$$f(\mathbf{A}) = \begin{pmatrix} \frac{1}{2}[f(a+b) + f(a-b)] & \frac{1}{2}[f(a+b) - f(a-b)] \\ \frac{1}{2}[f(a+b) - f(a-b)] & \frac{1}{2}[f(a+b) + f(a-b)] \end{pmatrix}$$

1.2 ORTHOGONAL FUNCTIONS, EIGENFUNCTIONS, AND OPERATORS

We know from the theory of Fourier series that it is possible to represent a sufficiently well-behaved function $f(x)$ on some interval as an infinite linear combination of sines and cosines with coefficients that depend on the function. Thus any such function can be represented by specifying these coefficients. This seems very similar to the idea of expanding a vector in terms of a set of basis vectors. The purpose of this section is to explore this similarity. We consider an infinite set of functions $\{\psi_i(x), i = 1, 2, \ldots\}$ that