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Kenna Collums

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THE MATRIX METHOD OF LINEAR DICHROISM

by
Kenna Collums

A thesis submitted to the faculty of The University of Mississippi in partial fulfillment
of the requirements of the Sally McDonnell Barksdale Honors College.

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Approved by

Advisor: Dr. Sandra Spiroff

Reader: Dr. Nagamani Vunnam

Reader: Dr. William Staton

THE MATRIX METHOD OF LINEAR DICHROISM

KENNA COLLUMS

ABSTRACT. This thesis discusses linear dichroism, and in particular the matrix method behind the spectroscopic technique. Linear dichroism uses the difference in the absorption of light that is parallel to the orientation axis and the absorption of light that is perpendicular to the orientation axis. From this process, the structure and function of molecules can be studied. The matrix method diagonalizes a Hamiltonian matrix with a unitary matrix. This Hamiltonian matrix is constructed from the transition energies, which are the diagonal elements, and coupling energies, which are off-diagonal elements.

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CONTENTS

1. INTRODUCTION

Linear dichroism is a spectroscopic method used by scientists to determine the structure, orientation, and properties of biological and chemical samples. It utilizes optical activity to produce information regarding the sample. After interpreting that information, certain properties of the molecule can be studied.

We use the matrix method of linear dichroism as a tool to interpret data from spectroscopy. The first step is to run a sample through the linear dichroism spectroscopy and receive data from it. From this information, transition energies of the molecule can be calculated; those energy values are then used to create a matrix. In general, we follow these three steps for the matrix method of linear dichroism:

- (1) First, we build a hamiltonian matrix E , like the one shown in Figure 1.1, which is constructed from the different energy transitions.
- (2) Next, we find U , the unitary matrix that diagonalizes E .
- (3) Then, we use U to diagonalize E with the equation $U^{-1}EU = E_{\text{diag}}$.

The diagonal matrix, E_{diag} , which contains eigenvalues for the diagonal elements, provides information about the chemical sample.

As mentioned above, the matrix in Figure 1.1 is hamiltonian. It is a motivating example in our study, and we will discuss it again in Section 4 in greater detail.

$$E = \begin{pmatrix} E_{n1} & \langle n1|V|\pi1\rangle & \langle n1|V|n2\rangle & \langle n1|V|\pi2\rangle \\ \langle \pi1|V|n1\rangle & E_{\pi1} & \langle \pi1|V|n2\rangle & \langle \pi1|V|\pi2\rangle \\ \langle n2|V|n1\rangle & \langle n2|V|\pi1\rangle & E_{n2} & \langle n2|V|\pi2\rangle \\ \langle \pi2|V|n1\rangle & \langle \pi2|V|\pi1\rangle & \langle \pi2|V|n2\rangle & E_{\pi2} \end{pmatrix}$$

Figure 1.1

(Bayley, Nielsen, and Schellman)

Figure 1.1 is the hamiltonian matrix corresponding to the two peptide, two energy transition system. There is an equation for each element of the matrix, and we input the value for different energy transitions for each element to give us every combination of energy transitions for the two peptides. The diagonalization of E gives us valuable details of a chemical sample.

The matrix method is most used for determining the structure, function, and properties of many biomolecules. Biomolecules are found in the human body and include proteins, lipids, nucleic acids, carbohydrates, and many others. The process of linear dichroism allows for the analysis of particular properties of a sample that can not be analyzed from other spectroscopic devices.

2. MATHEMATICAL BACKGROUND

2.1. Mathematical Definitions. In order to analyze the data from linear dichroism, we use matrices. A matrix is a rectangular array of information. The size of a matrix is given by the number of rows and columns it contains in that order. A matrix with two rows and three columns is said to be a 2×3 matrix. The following are all examples of matrices.

$$N = \begin{bmatrix} 1 & 2 \\ 0 & 7 \\ 4 & 5 \end{bmatrix} \quad H = \begin{bmatrix} 2 & 1-i \\ 1+i & 1 \end{bmatrix} \quad D = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 8 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad G = \begin{bmatrix} 0 & 0 & 3 \\ 0 & 1 & 0 \\ 2 & 0 & 0 \end{bmatrix}$$

3×2 2×2 3×3 3×3

We are specifically concerned with $2n \times 2n$ square matrices for the matrix method; e.g., 2×2 , 4×4 , 6×6 , etc. A **square matrix** is a matrix with an equal number of rows and columns. The matrices H , D , and G above are examples of a square matrix. This is because H has two rows and two columns and D and G both have three rows and three columns. A **diagonal matrix** is a square matrix where any non-zero entries, if they occur, must be on the main diagonal. An example of a diagonal matrix is the matrix D above because the only place there are non-zero elements is along the main diagonal. However, G is not a diagonal matrix because the non-zero elements are not along the main diagonal.

The identity matrix is also an example of a diagonal matrix. The **identity matrix** is a diagonal matrix with a 1 in every diagonal entry position. The matrices

$$I_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad I_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad I_4 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

are the 2×2 , 3×3 , and 4×4 identity matrices, respectively. When multiplying another matrix, say A , by I , the result is the original matrix; i.e., $AI = IA = A$, for some matrix A that is equal in size to I . Also, if A is invertible, then it has an

inverse matrix, A^{-1} , which when multiplied by the original matrix A produces the identity matrix; i.e., $AA^{-1} = A^{-1}A = I$.

The data received from linear dichroism spectroscopy is organized into the rows and columns of a matrix to create a hamiltonian matrix. To understand a hamiltonian matrix, we must first define a hermitian matrix. A square matrix H is a **hermitian matrix** if it has entries from \mathbb{C} and is equal to its own conjugate transpose; i.e., $H = H^*$. A hermitian matrix is also referred to as a **self-adjoint matrix**. For example, we see that H is a hermitian matrix because taking the conjugate transpose of H gives us the original matrix:

$$H = \begin{bmatrix} 2 & 1-i \\ 1+i & 1 \end{bmatrix} \quad \overline{H} = \begin{bmatrix} 2 & 1+i \\ 1-i & 1 \end{bmatrix} \quad \overline{H}^T = H^* = \begin{bmatrix} 2 & 1-i \\ 1+i & 1 \end{bmatrix}.$$

A hamiltonian matrix is obtained from a hermitian matrix. A $2n \times 2n$ matrix A is **hamiltonian** if and only if $(KA)^* = KA$, where $K = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$ and I_n is the $n \times n$ identity matrix. Note that KA is a hermitian matrix. For example, the matrix

$$A = \begin{bmatrix} -1-i & -1 \\ 2 & 1-i \end{bmatrix}$$

is a hamiltonian matrix since

$$KA = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} -1-i & -1 \\ 2 & 1-i \end{bmatrix} = \begin{bmatrix} 2 & 1-i \\ 1+i & 1 \end{bmatrix} = H$$

is a hermitian matrix.

A hamiltonian matrix must be of size $2n \times 2n$ because the matrix is organized into four submatrices, each of size $n \times n$. For the general case, a hamiltonian matrix appears as

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}$$

where $A, B, C,$ and D are $n \times n$ matrices. For example,

$$R = \begin{bmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \end{bmatrix}$$

Example of a 4×4 Hamiltonian Matrix with Real Entries [?]

is a very simple real hamiltonian matrix that is constructed of four 2×2 submatrices. Notice that $n = 2$ for the characteristic size of a hamiltonian matrix, which is $2n \times 2n$, making this a 4×4 matrix. This matrix has all real entries, but it is still considered to be in the vector space $\mathbb{C}^{2n \times 2n}$ since the imaginary parts can be equal to zero; i.e., $a + bi$, where $b = 0$. For clarification, a more complicated 4×4 hamiltonian matrix C with complex entries is included below.

$$C = \begin{bmatrix} -2 - i & 3 - i & 7 & i \\ 0 & -1 + i & -i & 5 \\ 2 & 1 + i & 2 - i & 0 \\ 1 - i & 4 & -3 - i & 1 + i \end{bmatrix}$$

Example of a 4×4 Hamiltonian Matrix with Complex Entries

Once we find the hamiltonian matrix A that corresponds to the molecule of interest, we must diagonalize it. A square matrix A is **diagonalizable** if there exists an invertible matrix P such that $P^{-1}AP$ is equal to a diagonal matrix. Then, we say that P diagonalizes A . In order to diagonalize a matrix, we must first identify the eigenvalues and eigenvectors. The **eigenvector** or **characteristic vector** of a square matrix A is a non-zero vector x such that for some scalar λ , $Ax = \lambda x$. The scalar λ is called an **eigenvalue** or **characteristic value** of A . [?]

The hamiltonian matrix is diagonalized with a unitary matrix. A **unitary matrix** (see Example ??) is a nonsingular complex matrix U such that the conjugate transpose of U is equal to the inverse of U ; i.e., $U^* = U^{-1}$. If the elements of U are real, then it is an **orthogonal matrix**, or a matrix where its transpose is equal to its inverse; i.e., $U^T = U^{-1}$. Examples of a unitary matrix U and an orthogonal matrix O are included below.

$$U = \frac{1}{2} \begin{bmatrix} 1+i & 1-i \\ 1-i & 1+i \end{bmatrix} \quad \text{and} \quad O = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$$

Many of the calculations that take place for the matrix method are done so within an inner product space, which is within a vector space. A vector space must satisfy the following ten axioms.

Definition:[?] Let V be an arbitrary nonempty set of objects on which the operations of addition and scalar multiplication are defined. By addition we mean a rule \oplus for associating with each pair of objects α and β in V an element $\alpha \oplus \beta$, called the **sum** of α and β ; by scalar multiplication we mean a rule \odot for associating with each scalar c and each object α in V an element $c \odot \alpha$, called the **scalar multiple** of α by c . If the following axioms are satisfied by all objects α, β, γ in V and all scalars c and d in a field F , then we call V a **vector space** and we call the objects in V **vectors**:

- (1) If α and β are objects in V , then $\alpha \oplus \beta$ is in V .
- (2) $\alpha \oplus \beta = \beta \oplus \alpha$
- (3) $\alpha \oplus (\beta \oplus \gamma) = (\alpha \oplus \beta) \oplus \gamma$
- (4) There is an object $\mathbf{0}$ in V such that $\mathbf{0} \oplus \alpha = \alpha \oplus \mathbf{0} = \alpha$
- (5) For each α in V , there is an object $-\alpha$ in V called the **negative** of α such that $\alpha \oplus (-\alpha) = (-\alpha) \oplus \alpha = \mathbf{0}$

(6) If c is any scalar and α is any object in V , then $c \odot \alpha$ is in V .

$$(7) c \odot (\alpha \oplus \beta) = c \odot \alpha \oplus c \odot \beta$$

$$(8) (c + d) \odot \alpha = c \odot \alpha \oplus d \odot \alpha$$

$$(9) c \odot (d \odot \alpha) = (cd) \odot \alpha$$

$$(10) 1 \odot \alpha = \alpha$$

Example 2.1. We will now prove that the set of $2n \times 2n$ matrices with entries from \mathbb{C} form a vector space by showing that it follows the ten axioms above. We will denote this space as $\mathbb{C}^{2n \times 2n}$. We will let α , β , and γ be objects in $\mathbb{C}^{2n \times 2n}$, and let c and d be scalars.

$$(1) \alpha + \beta \in \mathbb{C}^{2n \times 2n}$$

This is true because the addition of two matrices produces a matrix of the same size and \mathbb{C} is closed under addition.

$$(2) \alpha + \beta = \beta + \alpha \quad \text{and} \quad (3) \alpha + (\beta + \gamma) = (\alpha + \beta) + \gamma$$

Matrix addition is commutative and associative.

$$(4) \mathbf{0} + \alpha = \alpha + \mathbf{0} = \alpha$$

The zero object in the $\mathbb{C}^{2n \times 2n}$ vector space is the zero matrix, which is a matrix with a 0 for all entries.

$$(5) \alpha + (-\alpha) = -\alpha + \alpha = \mathbf{0}$$

The negative of α simply negates each entry in α , making all the entries 0 when added together.

$$(6) c \cdot \alpha \in \mathbb{C}^{2n \times 2n}$$

This statement is true since matrix scalar multiplication multiplies each matrix element by that scalar and \mathbb{C} is closed under multiplication.

$$(7) c \cdot (\alpha + \beta) = (c \cdot \alpha) + (c \cdot \beta) \quad \text{and} \quad (8) (c + d) \cdot \alpha = (c \cdot \alpha) + (d \cdot \alpha)$$

Scalar multiplication distributes over addition.

$$(9) \quad c \cdot (d \cdot \alpha) = cd \cdot \alpha$$

This equality is true since the same action takes place on the matrix in both the left and right side of the equation. On the left side of the equation, every entry of α is multiplied by d and then multiplied by c . On the right side, every entry is multiplied by cd , yielding the same result.

$$(10) \quad 1 \cdot \alpha = \alpha$$

The above statement is true since we are multiplying the matrix α by the scalar 1.

Definition:[?] Let F be the field of real numbers or the field of complex numbers, and V a vector space over F . An **inner product** on V is a function which assigns to each ordered pair of vectors α, β in V a scalar $(\alpha|\beta)$ in F in such a way that for all α, β, γ in V and all scalars c

$$(1) \quad (\alpha + \beta|\gamma) = (\alpha|\gamma) + (\beta|\gamma);$$

$$(2) \quad (c\alpha|\beta) = c(\alpha|\beta);$$

$$(3) \quad (\beta|\alpha) = \overline{(\alpha|\beta)};$$

$$(4) \quad (\alpha|\alpha) > 0 \text{ if } \alpha \neq 0.$$

Also, note that because of (2) and (3), $(\alpha|c\beta) = \bar{c}(\alpha|\beta)$.

An **inner product space** is a vector space with an inner product. We have included two examples to demonstrate an inner product space.

Example 2.2. Two examples of inner product spaces are listed below.

$$(1) \text{ Let } V \text{ be } \mathbb{C}^{2n \times 2n} \text{ and } (A|B) = \sum_{j,k} A_{jk} \bar{B}_{jk}. \text{ Then } V \text{ is an inner product space.}$$

$$(2) \text{ Let } V \text{ be } \mathbb{C}^2 \text{ and let } \alpha, \beta \in \mathbb{C}^2, \text{ say } \alpha = (\alpha_1, \alpha_2) \text{ and } \beta = (\beta_1, \beta_2). \text{ Then}$$

$$(\alpha|\beta) = \sum_j \alpha_j \cdot \bar{\beta}_j \text{ makes } V \text{ into an inner product space.}$$

We will illustrate the above terms in the following simple example of the hermitian matrix H .

Example 2.3. Recall that $H = \begin{bmatrix} 2 & 1-i \\ 1+i & 1 \end{bmatrix}$, and note that it is an element in the vector space $\mathbb{C}^{2 \times 2}$.

First we find the eigenvalues of H .

$$\begin{vmatrix} 2-c & 1-i \\ 1+i & 1-c \end{vmatrix} = (2-c)(1-c) - (1-i)(1+i) = c(c-3) = 0$$

Solving for c , we obtain the eigenvalues $c_1 = 3$ and $c_2 = 0$.

Next, we substitute each eigenvalue into the matrix and find a basis for the null space; i.e., we find $X = \begin{bmatrix} x \\ y \end{bmatrix}$ that satisfies $HX = c_i X$, which will give us the eigenvectors. For $c_1 = 3$, we calculate

$$\left[\begin{array}{cc|c} 2-3 & 1-i & 0 \\ 1+i & 1-3 & 0 \end{array} \right] = \left[\begin{array}{cc|c} -1 & 1-i & 0 \\ 1+i & -2 & 0 \end{array} \right] = \left[\begin{array}{cc|c} 1 & -1+i & 0 \\ 1+i & -2 & 0 \end{array} \right] = \left[\begin{array}{cc|c} 1 & -1+i & 0 \\ 0 & 0 & 0 \end{array} \right]$$

Thus

$$x + (-1+i)y = 0, \text{ and}$$

$$x = (1-i)y.$$

Hence, the eigenvector corresponding to the eigenvalue $c_1 = 3$ is

$$x_1 = \begin{bmatrix} 1-i \\ 1 \end{bmatrix}.$$

If we evaluate the eigenvector corresponding to the eigenvalue $c_2 = 0$ in the same manner, we find that

$$x_2 = \begin{bmatrix} -\frac{1}{2} + \frac{1}{2}i \\ 1 \end{bmatrix}.$$

Now that we have found the eigenvalues and eigenvectors, we use those to diagonalize the matrix. Set $P = \begin{bmatrix} 1-i & -\frac{1}{2} + \frac{1}{2}i \\ 1 & 1 \end{bmatrix}$. Then $P^{-1} = \begin{bmatrix} \frac{2}{3(1-i)} & \frac{1}{3} \\ -\frac{2}{3(1-i)} & \frac{2}{3} \end{bmatrix}$.

The next step is to calculate $P^{-1}HP = D$ to find the diagonal matrix D corresponding to H .

$$P^{-1}HP = \begin{bmatrix} \frac{2}{3(1-i)} & \frac{1}{3} \\ -\frac{2}{3(1-i)} & \frac{2}{3} \end{bmatrix} \begin{bmatrix} 2 & 1-i \\ 1+i & 1 \end{bmatrix} \begin{bmatrix} 1-i & -\frac{1}{2} + \frac{1}{2}i \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 3 & 0 \\ 0 & 0 \end{bmatrix} = D$$

Although the matrix P diagonalizes H , P is not a unitary matrix. The eigenvectors form an orthogonal basis, which we can see by calculating the inner product of x_1 and x_2 . Using the standard inner product on \mathbb{C}^2 , we have

$$(x_1|x_2) = (1-i, 1) \cdot \overline{\left(-\frac{1}{2} + \frac{1}{2}i, \bar{1}\right)} = 0.$$

Then, we take the norm of x_1 and x_2 to obtain an orthonormal basis. For x_1 , we have $\sqrt{(1-i)(1+i) + 1^2} = \sqrt{3}$. To be specific:

$$\left(\frac{1}{\sqrt{3}}x_1 \mid \frac{1}{\sqrt{3}}x_1 \right) = 1.$$

Similarly, for x_2 , we have $\sqrt{\left(-\frac{1}{2} + \frac{1}{2}i\right)\left(-\frac{1}{2} - \frac{1}{2}i\right) + 1^2} = \sqrt{\frac{3}{2}}$. So we obtain

$$\alpha_1 = \frac{1}{\sqrt{3}} \begin{bmatrix} 1-i \\ 1 \end{bmatrix} = \begin{bmatrix} \frac{1-i}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{bmatrix} \quad \text{and} \quad \alpha_2 = \frac{1}{\sqrt{\frac{3}{2}}} \begin{bmatrix} -\frac{1}{2} + \frac{1}{2}i \\ 1 \end{bmatrix} = \begin{bmatrix} \frac{-\frac{1}{2} + \frac{1}{2}i}{\sqrt{\frac{3}{2}}} \\ \frac{1}{\sqrt{\frac{3}{2}}} \end{bmatrix}$$

for the orthonormal basis. Then the unitary invertible matrix is

$$U = \begin{bmatrix} \frac{\sqrt{3}}{3} - \frac{\sqrt{3}}{3}i & -\frac{\sqrt{6}}{6} + \frac{\sqrt{6}}{6}i \\ \frac{\sqrt{3}}{3} & \frac{\sqrt{6}}{3} \end{bmatrix}.$$

Taking the inverse of U , we obtain

$$U^{-1} = \frac{\sqrt{2} + \sqrt{2}i}{2} \begin{bmatrix} \frac{\sqrt{6}}{3} & \frac{\sqrt{6}}{6} - \frac{\sqrt{6}}{6}i \\ -\frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} - \frac{\sqrt{3}}{3}i \end{bmatrix}.$$

Then, we can calculate the transition matrix

$$D = U^{-1}HU = \begin{bmatrix} 3 & 0 \\ 0 & 0 \end{bmatrix}.$$

In calculations involving imaginary numbers, sometimes roots of imaginary numbers appear. For example, one might have $\sqrt{1+2i}$. We explain what we mean by this expression. Note that $1+2i = \sqrt{5} \exp(i\theta) = \sqrt{5}(\cos \theta + i \sin \theta)$. Also, $\tan \theta = \frac{2}{1}$, hence $\theta = \arctan 2$. It is a solution to the complex equation $z^2 = z_0$. These solutions take the form $c_k = \sqrt{r_0} \exp[i(\frac{\theta}{2} + \frac{2k\pi}{1})]$ for $z_0 = r_0 \exp(i\theta)$ for $k = 0, 1$. Therefore, $z^2 = 1+2i$ has solutions $c_1 = \sqrt[4]{5} \exp[i(\frac{\theta}{2})]$ and $c_2 = \sqrt[4]{5} \exp[i(\frac{\theta}{2} + \pi)]$.

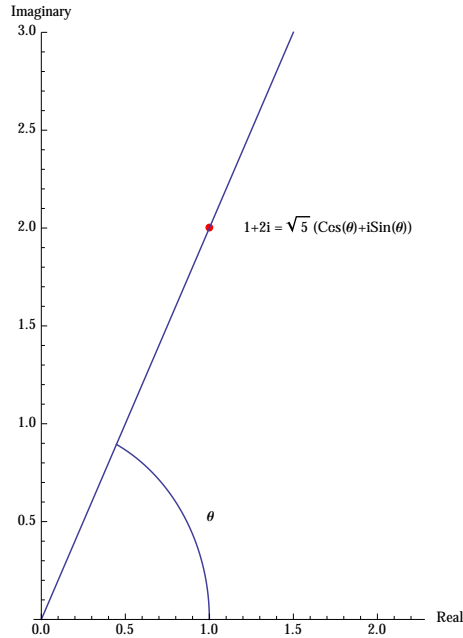


Figure 2.1

2.2. Mathematical Theorems. A fundamental step in the matrix method of linear dichroism is the diagonalization of hamiltonian matrices. Recall that hamiltonian matrices are closely related to hermitian matrices. One of the most important mathematical results is that hermitian matrices are always diagonalizable. Our ultimate goal is to prove this result, which is Corollary ?? below. In this subsection, we establish the mathematics necessary to understand the proof of Corollary ?. Another interesting result is that the eigenvalues of hermitian matrices are always real numbers.

Corollary 2.4. [?, Theorem 18 Corollary] *Let A be an $n \times n$ Hermitian (self-adjoint) matrix. Then there is a unitary matrix U such that $U^{-1}AU$ is diagonal (A is unitarily equivalent to a diagonal matrix). If A is a real symmetric matrix, there is a real orthogonal matrix U such that $U^{-1}AU$ is diagonal.*

The first step toward our goal is the following theorem. Theorem ?? shows that, given an inner product space and a linear functional, there exists a unique vector β that determines the linear functional; i.e., $f(\alpha) = (\alpha|\beta)$. This is important because the existence of the vector and its uniqueness are utilized in the proof of Theorem ??.

Theorem 2.5. [?, Theorem 8.6] *Let V be a finite-dimensional inner product space, and f a linear functional on V . Then there exists a unique vector β in V such that $f(\alpha) = (\alpha|\beta)$ for all α in V .*

Proof. Let $\{\alpha_1, \alpha_2, \dots, \alpha_n\}$ be an orthonormal basis for V . Put

$$\beta = \sum_{j=1}^n \overline{f(\alpha_j)} \alpha_j$$

and let f_β be the linear functional defined by

$$f_\beta(\alpha) = (\alpha|\beta).$$

Then

$$\begin{aligned}
 f_\beta(\alpha_k) &= (\alpha_k|\beta) = (\alpha_k|\sum_j \overline{f(\alpha_j)}\alpha_j) = \overline{(\sum_{j=1}^n \overline{f(\alpha_j)}\alpha_j|\alpha_k)} = \sum_{j=1}^n \overline{(\overline{f(\alpha_j)}\alpha_j|\alpha_k)} = \\
 &= \sum_{j=1}^n \overline{f(\alpha_j)(\alpha_j|\alpha_k)} = \sum_{j=1}^n \overline{f(\alpha_j)(\alpha_j|\alpha_k)} = \sum_{j=1}^n f(\alpha_j)\overline{(\alpha_j|\alpha_k)} = \sum_{j=1}^n f(\alpha_j)(\alpha_k|\alpha_j) = \\
 &= f(\alpha_1)(\alpha_k|\alpha_1) + \dots + f(\alpha_n)(\alpha_k|\alpha_n) = f(\alpha_1) \times 0 + \dots + f(\alpha_k)(\alpha_k|\alpha_k) + \dots + f(\alpha_n) \times 0 = \\
 &= f(\alpha_1) \times 0 + \dots + f(\alpha_k) \times 1 + \dots + f(\alpha_n) \cdot 0 = f(\alpha_k)
 \end{aligned}$$

since $(\alpha_k|\alpha_j)$ is orthonormal. Since this is true for each α_k , it follows that $f = f_\beta$. Now suppose γ is a vector in V such that $(\alpha|\beta) = (\alpha|\gamma)$ for all α . Then $(\beta-\gamma|\beta-\gamma) = (\beta|\beta) - (\gamma|\beta) - (\gamma|\beta) + (\gamma|\gamma) = 0$. Thus $\beta - \gamma = \mathbf{0}$ and $\beta = \gamma$. Thus there is exactly one vector β determining the linear functional f in the stated manner. \square

The equality within the inner product space proven in this theorem is important because it is used to prove other theorems, namely Theorem ??, as well.

Theorem 2.6. [?, Theorem 8.7] *For any linear operator T on a finite-dimensional inner product space V , there exists a unique linear operator T^* on V such that*

$$(2-2) \quad (T\alpha|\beta) = (\alpha|T^*\beta)$$

for all α, β in V .

Proof. Let β be any vector in V . Then $\psi : \alpha \rightarrow (T\alpha|\beta)$ is a linear functional on V .

We can show that ψ is a linear functional by

$$(i) \psi(\alpha + \gamma) = (T(\alpha + \gamma)|\beta) = (T\alpha + T\gamma|\beta) = (T\alpha|\beta) + (T\gamma|\beta) = \psi(\alpha) + \psi(\gamma), \text{ and}$$

$$(ii) \psi(k\alpha) = (T(k\alpha)|\beta) = (kT\alpha|\beta) = k(T\alpha|\beta) = k\psi(\alpha).$$

By Theorem ?? there is a unique vector β' in V such that $(T\alpha|\beta) = (\alpha|\beta')$ for every α in V . Let T^* denote the mapping $\beta \rightarrow \beta'$:

$$\beta' = T^*\beta.$$

We have (2-2), but we must verify that T^* is a linear operator. Let β, γ be in V and

let c be a scalar. Then for any α ,

$$\begin{aligned}
 (\alpha|T^*(c\beta + \gamma)) &= (T\alpha|c\beta + \gamma) \\
 &= (T\alpha|c\beta) + (T\alpha|\gamma) \\
 &= \bar{c}(T\alpha|\beta) + (T\alpha|\gamma) \\
 &= \bar{c}(\alpha|T^*\beta) + (\alpha|T^*\gamma) \\
 &= (\alpha|cT^*\beta) + (\alpha|T^*\gamma) \\
 &= (\alpha|cT^*\beta) + (\alpha|T^*\gamma) \\
 &= (\alpha|cT^*\beta + T^*\gamma).
 \end{aligned}$$

Thus $T^*(c\beta + \gamma) = cT^*\beta + T^*\gamma$ by the uniqueness argument in Theorem ?? and T^* is linear.

The uniqueness of T^* is clear. For any β in V , the vector $T^*\beta$ is uniquely determined as the vector β' such that $(T\alpha|\beta) = (\alpha|\beta')$ for every α . \square

Theorem ?? proves a result on the matrix associated to a linear operator.

Theorem 2.7. [?, Theorem 8.8] *Let V be a finite-dimensional inner product space and let $\mathcal{B} = \{\alpha_1, \dots, \alpha_n\}$ be an (ordered) orthonormal basis for V . Let T be a linear operator on V and let A be the matrix of T in the ordered basis \mathcal{B} . Then $A_{kj} = (T\alpha_j|\alpha_k)$.*

Proof. Since \mathcal{B} is an orthonormal basis, we have

$$\alpha = \sum_{k=1}^n (\alpha|\alpha_k)\alpha_k.$$

The matrix A is defined by

$$T\alpha_j = \sum_{k=1}^n A_{kj}\alpha_k$$

and since

$$T\alpha_j = \sum_{k=1}^n (T\alpha_j|\alpha_k)\alpha_k$$

we have $A_{kj} = (T\alpha_j|\alpha_k)$. \square

The next result shows that the matrix of the conjugate transpose of a linear operator is simply the conjugate transpose of the matrix associated to said linear operator.

Corollary 2.8. [?, Theorem 8 Corollary] *Let V be a finite-dimensional inner product space, and let T be a linear operator on V . In any orthonormal basis for V , the matrix of T^* is the conjugate transpose of the matrix of T .*

Proof. Let $\beta = \{\alpha_1, \dots, \alpha_n\}$ be an orthonormal basis for V , let $A = [T]_\beta$ and $B = [T^*]_\beta$. According to Theorem ??,

$$\begin{aligned} A_{kj} &= (T\alpha_j | \alpha_k) \\ B_{kj} &= (T^*\alpha_j | \alpha_k). \end{aligned}$$

By the definition of T^* we then have

$$\begin{aligned} B_{kj} &= (T^*\alpha_j | \alpha_k) \\ &= \overline{(\alpha_k | T^*\alpha_j)} \\ &= \overline{(T\alpha_k | \alpha_j)} \\ &= \overline{A_{jk}} \end{aligned}$$

So $B_{kj} = \overline{A_{jk}} = A_{kj}^*$. □

The next theorem is interesting since we notice that even though the hermitian matrix, which is associated to the hamiltonian matrix that we build, may have complex entries, we still obtain real eigenvalues. Also, it is used in the proof of Theorem ??.

Theorem 2.9. [?, Theorem 8.15] *Let V be an inner product space and T a self-adjoint (Hermitian) linear operator on V . Then each characteristic value of T is real, and characteristic vectors of T associated with distinct characteristic values are orthogonal.*

Proof. Suppose c is a characteristic value of T , i.e., that $T\alpha = c\alpha$ for some non-zero vector α . Then

$$\begin{aligned} c(\alpha|\alpha) &= (c\alpha|\alpha) \\ &= (T\alpha|\alpha) \\ &= (\alpha|T\alpha) \\ &= (\alpha|c\alpha) \\ &= \bar{c}(\alpha|\alpha) \end{aligned}$$

by the properties of inner product spaces. In summary, $c(\alpha|\alpha) = \bar{c}(\alpha|\alpha)$. Therefore, $c(\alpha|\alpha) - \bar{c}(\alpha|\alpha) = 0$, which implies $(c - \bar{c})(\alpha|\alpha) = 0$. This is happening in \mathbb{C} , which has the Zero Product Property (if $ab = 0$, then either $a = 0$ or $b = 0$). Since $(\alpha|\alpha) \neq 0$, we must have $c = \bar{c}$. Suppose we also have $T\beta = d\beta$ with $\beta \neq 0$. Then

$$\begin{aligned} c(\alpha|\beta) &= (T\alpha|\beta) \\ &= (\alpha|T\beta) \\ &= (\alpha|d\beta) \\ &= \bar{d}(\alpha|\beta) \\ &= d(\alpha|\beta). \end{aligned}$$

If $c \neq d$, then $(\alpha|\beta) = 0$. □

The following theorem shows that every hermitian operator has at least one non-zero eigenvector. This fact is necessary for the proof of Theorem ??.

Theorem 2.10. [?, Theorem 8.16] *On a finite-dimensional inner product space of positive dimension, every self-adjoint operator has a (non-zero) characteristic vector.*

Proof. Let V be an inner product space of dimension n , where $n > 0$, and let T be a self-adjoint operator on V . Choose an orthonormal basis β for V and let $A = [T]_{\beta}$. Since $T = T^*$, we have $A = A^*$. Now let W be the space of $n \times 1$ matrices over \mathbb{C} , with inner product $(X|Y) = Y^*X$. Then $U(X) = AX$ defines a self-adjoint linear

operator U on W . The characteristic polynomial, $\det(xI - A)$, is a polynomial of degree n over the complex numbers; every polynomial over \mathbb{C} of positive degree has a root. Thus, there is a complex number c such that $\det(cI - A) = 0$. This means that $A - cI$ is singular, or that there exists a non-zero X such that $AX = cX$. Since the operator U (multiplication by A) is self-adjoint, it follows from Theorem ?? that c is real. If V is a real vector space, we may choose X to have real entries. For then A and $A - cI$ have real entries, and since $A - cI$ is singular, the system $(A - cI)X = 0$ has a non-zero real solution X . It follows that there is a non-zero vector α in V such that $T\alpha = c\alpha$. \square

Theorem ?? proves that if a subspace is invariant under a linear operator T , then the complement of that subspace is invariant under T^* . This fact is useful for the proof of Theorem ??.

Theorem 2.11. [?, Theorem 8.17] *Let V be a finite-dimensional inner product space, and let T be any linear operator on V . Suppose W is a subspace of V which is invariant under T . Then the orthogonal complement of W is invariant under T^* .*

Proof. We recall that the fact that W is invariant under T does not mean that each vector in W is left fixed by T ; it means that if α is in W then $T\alpha$ is in W . Let β be in W^\perp . We must show that $T^*\beta$ is in W^\perp , that is, that $(\alpha|T^*\beta) = 0$ for every α in W . If α is in W , then $T\alpha$ is in W , so $(T\alpha|\beta) = 0$ by the definition of W^\perp . But $(T\alpha|\beta) = (\alpha|T^*\beta)$ by Theorem ?? \square

Finally, we give the last theorem necessary to prove our corollary. It establishes the fact that the orthonormal basis of a hermitian matrix consists of its characteristic vectors.

Theorem 2.12. [?, Theorem 8.18] *Let V be a finite-dimensional inner product space, and let T be a self-adjoint linear operator on V . Then there is an orthonormal basis for V , each vector of which is a characteristic vector to T .*

Proof. We are assuming $\dim V > 0$. By Theorem ??, T has a characteristic vector α . Let $\alpha_1 = \frac{\alpha}{\|\alpha\|}$, the norm of α , so that α_1 is also a characteristic vector for T and $\|\alpha_1\| = 1$. We can show that α_1 is also a characteristic vector by $T\alpha_1 = T(\frac{1}{\|\alpha\|}\alpha) = \frac{1}{\|\alpha\|}T\alpha = \frac{1}{\|\alpha\|}c\alpha = c\frac{1}{\|\alpha\|}\alpha = c\alpha_1$. If $\dim V = 1$, then $\{\alpha_1\}$ is the orthonormal basis and we are done. Now we proceed by induction on the dimension of V . Let W be the one-dimensional subspace spanned by the vector α_1 . The statement that α_1 is a characteristic vector for T simply means that W is invariant under T . By Theorem ??, the orthogonal complement W^\perp is invariant under $T^* = T$. Now W^\perp , with the inner product from V , is an inner product space of dimension one less than the dimension of V since $\dim V = \dim W + \dim W^\perp$ and $\dim W = 1$. Let U be the linear operator induced on W^\perp by T , that is, the restriction of T to W^\perp . Then U is self-adjoint, and by the induction hypothesis, W^\perp has an orthonormal basis $\{\alpha_2, \dots, \alpha_n\}$ consisting of characteristic vectors for U . Now each of these vectors is also a characteristic vector for T , and since $V = W \oplus W^\perp$, we conclude that $\{\alpha_1\} \cup \{\alpha_2, \dots, \alpha_n\} = \{\alpha_1, \dots, \alpha_n\}$ is the desired basis for V . \square

Now we are in a position to prove Corollary ??, which was our goal of this section.

Proof of Corollary ??. Let V be $\mathbb{C}^{n \times 1}$, with the standard inner product, and let T be the linear operator on V which is represented by A in the standard ordered basis. Since $A = A^*$, we have $T = T^*$. Let $\mathcal{U} = \{\alpha_1, \dots, \alpha_n\}$ be an ordered orthonormal basis for V , such that $T\alpha_j = c_j\alpha_j$, for $j = 1, \dots, n$. If $D = [T]_{\mathcal{U}}$, then D is the diagonal matrix with diagonal entries c_1, \dots, c_n . Let U be the matrix with column

vectors $\alpha_1, \dots, \alpha_n$. Then $D = U^{-1}AU$. In case each entry of A is real, we can take V to be \mathbb{R}^n , with the standard inner product, and repeat the argument. In this case, U will be a unitary matrix with real entries, i.e., a real orthogonal matrix. \square

We recall Example ?? of a simple hermitian matrix to illustrate some of the theory established above. We note that the matrix is diagonalizable by a unitary matrix and that all of its eigenvalues are real.

3. CHEMISTRY BACKGROUND

Chemists spend a great deal of time studying molecules and how they behave under different conditions. **Molecules** are made of atoms that are bonded together, and **atoms** are the fundamental units of a chemical element. **Electrons** are the negatively charged particles that surround the center of the atom, and these are of particular interest in the study of molecules.

Within a molecule, electrons are found either in the ground state or an excited state. The **ground state** is simply the normal state of the electron, and it is the lowest energy level in which that electron can exist. When a molecule absorbs energy, an electron can be excited to a higher energy level, as shown in Figure 3.1. The energy required to move the electron to a different state depends on where the electron is originally and to which state it travels.

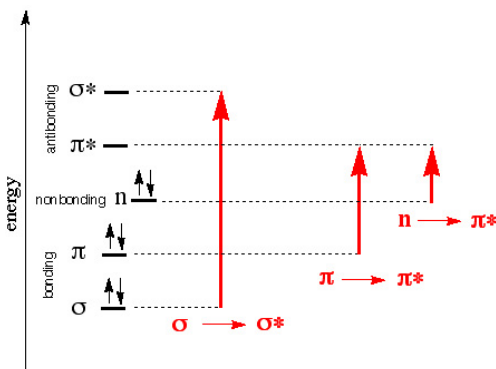


Figure 3.1

www.chem.ucla.edu/~bacher/UV-vis/uv_vis_tetracyclone.html.html

Fig. 3.1: When using the matrix method for a molecule containing two peptide groups, we are concerned with energy transitions from π to π^* and from n to π^* . When an electron is excited (when it absorbs energy), it will jump to a higher energy state.

In the electron cloud surrounding the **nucleus**, which is the center of the atom, there are different atomic orbitals and energy levels. Each atomic orbital has a unique shape. The s atomic orbital, seen in the first column in Fig. 3.2, has a spherical shape, and it is the simplest of the orbitals. The p orbital, shown in the second column of Fig. 3.2, is often described as a dumbbell shape. The shape of the d orbital is not as easy to visualize, but it is often seen as a clover or as a dumbbell on both the x -axis and y -axis, which is seen in the third column of Fig. 3.2.

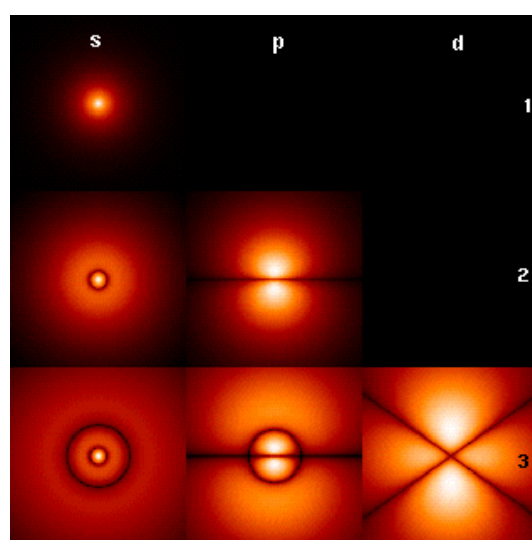


Figure 3.2 (Michael Diederich)

Fig. 3.2: The s , p , and d columns correspond to the different atomic orbitals, and the rows correspond to the different energy levels at each orbital. The brighter areas indicate a higher probability density for electrons in that location.

At each orbital there are different energy levels. As we get farther away from the nucleus, the energy levels get larger, with 1 being the lowest and the closest to the nucleus. We see the shape of each orbital and the likelihood of finding electrons in a specific place in Fig. 3.2, which shows probability density for electrons in a hydrogen atom. From the periodic table, we know that hydrogen has only one

electron since its atomic number is 1 and it is neutral in this case (refer to The Periodic Table in the Appendix).

Notice that the blocks for $1p$, $1d$, and $2d$ are completely black, meaning that there is a probability of 0 for finding an electron in that energy level and orbital. This is due to the fact that in the first energy level, only the s orbital exists, and in the second energy level, only the s and p orbitals exist.

Linear dichroism is one of the many spectroscopic methods used in chemistry to study molecules and their behavior. A **spectroscopic method** is one that is used to observe how a chemical sample will react with light. It utilizes the difference in the absorption of light that is parallel to the orientation axis and the absorption of light that is perpendicular to the orientation axis. This type of method allows us to see which wavelengths are absorbed by that sample and to what extent the energy is absorbed. Given that we know the wavelength, λ , from the spectroscopic data, we can calculate the energy, E , by combining the two equations

$$E = hf \quad \text{and} \quad \lambda f = c$$

into the single equation

$$E = \frac{hc}{\lambda},$$

where $h = 6.626 \times 10^{-34} \text{ m}^2\text{kg/s}$ is Planck's constant and $c = 3 \times 10^8 \text{ m/s}$ is the speed of light. Note that we now only have one variable, the wavelength, needed to calculate energy.

Linear dichroism is very useful for studying biomolecules, and in particular, peptides. **Peptides** are chains of amino acids linked together by peptide bonds. Amino acids all have the same basic molecular skeleton in common. There is an amino group, which is the NH_2 group in green (on the left), and there is a carboxyl group, which is the $COOH$ group shown in yellow (on the right), both bonded to the central carbon atom. Amino acids also have a hydrogen attached to the central

carbon. For the side chain, R represents an arbitrary group that is attached to the central carbon. This amino acid structure is shown in Figure 3.3.

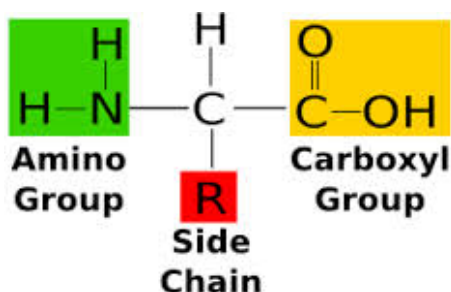


Figure 3.3

http://education-portal.com/cimages/multimages/16/amino_acid_structure.png

Fig. 3.3 This figure shows the molecular skeleton of all amino acids. The central carbon atom in an amino acid has two functional groups (an amino group and a carboxyl group) and a hydrogen atom attached to it. There is also a side chain that differs for every amino acid, which determines how the amino acids are classified.

There are twenty common amino acids in the human body, and any combination of those can be linked together by a peptide bond to form a peptide. Figure 3.4 shows two examples, one with two amino acids linked together and one with three amino acids linked together.

We consider dipeptides, like the one on the left of Figure 3.4, in the next section. Corresponding to dipeptides there is a specific hamiltonian matrix, which is $2n \times 2n$. It takes into account each peptide, each transition, and every combination of the transitions of the two peptides. We will specifically look at a dipeptide with two energy transitions, making the hamiltonian matrix a 4×4 matrix so that it represents every combination of energy transitions of the two peptides.

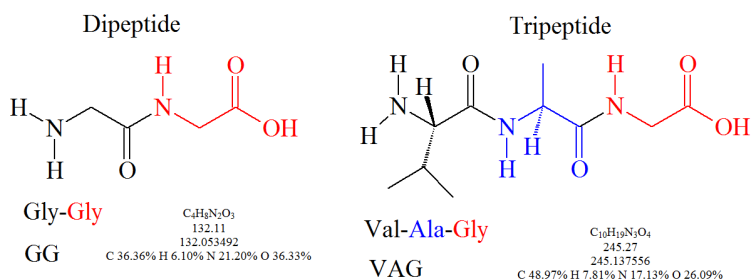


Figure 3.4

<http://blogbiosyn.files.wordpress.com/2013/09/peptides-1.png>

Fig. 3.4 This figure shows two examples of a peptide. The first example is called a dipeptide because it has two linked amino acids, which are both glycine in this case. The second example is a tripeptide since there are three amino acids linked together, which are valine, alanine, and glycine in this example.

When we receive the absorbance graph from the spectroscopic data, it shows the absorbance of the chromophores in the peptide. A **chromophore** is a part of the molecule that absorbs light. For proteins, the chromophores are the peptide bond, tryptophan, cysteine, and tyrosine, which is three of the twenty common amino acids. The range of wavelengths for the two chromophores for proteins is about 190 – 235nm, so we will consider that range for information in the spectroscopic graph.

4. DISCUSSION

We have taken the matrix for molecules containing two peptide groups given in [?] and rewrote it as

$$E = \begin{pmatrix} E_{n1} & \langle n1|V|\pi1\rangle & \langle n1|V|n2\rangle & \langle n1|V|\pi2\rangle \\ \langle \pi1|V|n1\rangle & E_{\pi1} & \langle \pi1|V|n2\rangle & \langle \pi1|V|\pi2\rangle \\ \langle n2|V|n1\rangle & \langle n2|V|\pi1\rangle & E_{n2} & \langle n2|V|\pi2\rangle \\ \langle \pi2|V|n1\rangle & \langle \pi2|V|\pi1\rangle & \langle \pi2|V|n2\rangle & E_{\pi2} \end{pmatrix}$$

Figure 4.1

(Bayley, Nielsen, and Schellman)

Figure 4.1 is the hamiltonian matrix representing the two peptide, two energy transition system.

where the two peptide groups are represented by 1 and 2, and the two energy transitions are represented by n (the $n - \pi^*$ transition) and π (the $\pi - \pi^*$ transition).

The diagonal elements represent the change in energy in one of the energy transitions of a single peptide group in the molecule. For example, E_{n1} is the change in energy from n to π^* of peptide 1.

The off-diagonal elements represent the change in energy in a coupling or mixing of the different states. It is considered a mixing of different states when the same peptide group undergoes multiple transitions. The coupling of the states refers to both peptide groups undergoing energy transitions. For example, $\langle n1|V|\pi1\rangle$ is a mixing of the $n - \pi^*$ transition and $\pi - \pi^*$ transition in peptide 1 while peptide 2 remains in the ground state, and $\langle n1|V|n2\rangle$ is a coupling of the n to π^* transitions in both peptide 1 and peptide 2.

For clarity, we give the hamiltonian matrix for two peptides and one energy transition, P , and the hamiltonian matrix for one peptide and two energy transitions, T . Again, the peptides are represented by 1 and 2, and the energy transitions are n

and π . Note that both P and T meet the $2n \times 2n$ size requirement for hamiltonian matrices since they are both 2×2 .

$$P = \begin{bmatrix} E_{n1} & \langle n1|V|n2\rangle \\ \langle n2|V|n1\rangle & E_{n2} \end{bmatrix} \quad \text{and} \quad T = \begin{bmatrix} E_{n1} & \langle n1|V|\pi1\rangle \\ \langle \pi1|V|n1\rangle & E_{\pi1} \end{bmatrix}$$

The elements of the original hamiltonian matrix, E , are calculated using different methods. There are four methods of calculation for fourteen of the sixteen elements, while two of the elements can be thought of as equal to zero since their value is negligible. We have replaced the elements in Figure 4.1 with their corresponding method of calculation in Figure 4.2.

$$\begin{pmatrix} E_{n1} & CAE & 0 & \mu_2 m_1 \\ CAE & E_{\pi1} & \mu_1 m_2 & K \\ 0 & \mu_1 m_2 & E_{n2} & CAE \\ \mu_2 m_1 & K & CAE & E_{\pi2} \end{pmatrix}$$

Figure 4.2

(Bayley, Nielsen, and Schellman)

This matrix is modified from the matrix in Figure 4.1 to show the methods by which each elements' value is calculated.

The CAE method is named for Condon, Altar, and Erying [?], whose paper the method was originally presented in. It is used to measure the transition energy of the mixing of states in the same peptide while the other peptide remains in the ground state.

The second method, shown as K in Fig. 4.2, is named for Kirkwood and Moffitt [?][?], who studied the calculations for these elements. We use this method to calculate the energy it takes to transition from π to π^* in peptide 1 and peptide 2.

The third way to calculate the transition energy is represented by μm . This method involves the coupling of the states, so it is used to measure the energy absorbed when peptide 1 and peptide 2 are both excited to a higher state.

Two of the matrix elements are now 0 because the energy for these calculations is negligible. The energy for these elements is the coupling of the $n - \pi^*$ transitions of both peptides, and it can be seen in Figure 3.1 that this energy transition is the smallest. It is comparatively so small that it can be thought of as equal to 0.

The graphs below show the linear dichroism spectroscopy (Figure 4.3) and the circular dichroism spectroscopy (Figure 4.4). The peptide bond and tryptophan are the chromophores in the Cadherin protein. The graph we receive from the linear dichroism spectroscopy provides information regarding the orientation of the chromophores within the peptides.

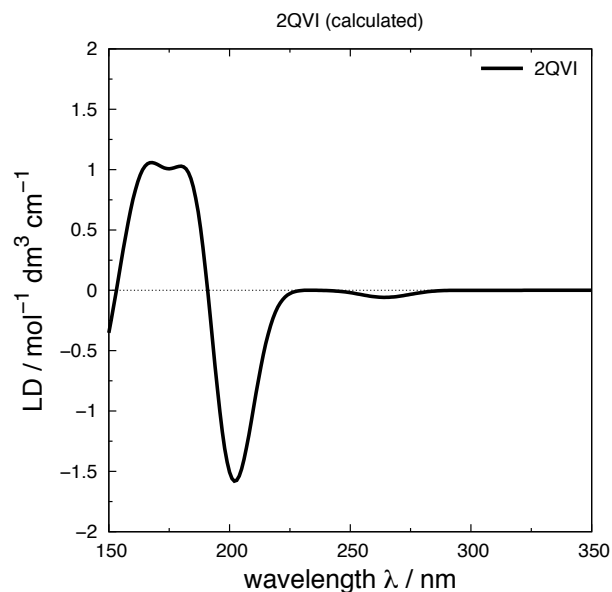


Figure 4.3 [?]

Fig. 4.3 shows the linear dichroism graph for the Cadherin protein.

Closely related to linear dichroism is circular dichroism. Whereas linear dichroism depends on linearly polarized light, circular dichroism depends on circularly polarized light. For the analysis of the the circular dichroism graph, we consider elements in the range of $190 - 235\text{nm}$ for wavelength. The first local minima in the graph can be disregarded because it is outside of the range we consider for useful information. The minimum is due to the peptide bond chromophore, and the maximum is due to the tryptophan chromophore. Because there is only one minima in the range $190 - 235$, that tells us that the Cadherin protein has a β -sheet secondary structure. If there were two minima in the range, then we could tell that the secondary structure of the protein was an α -helix.

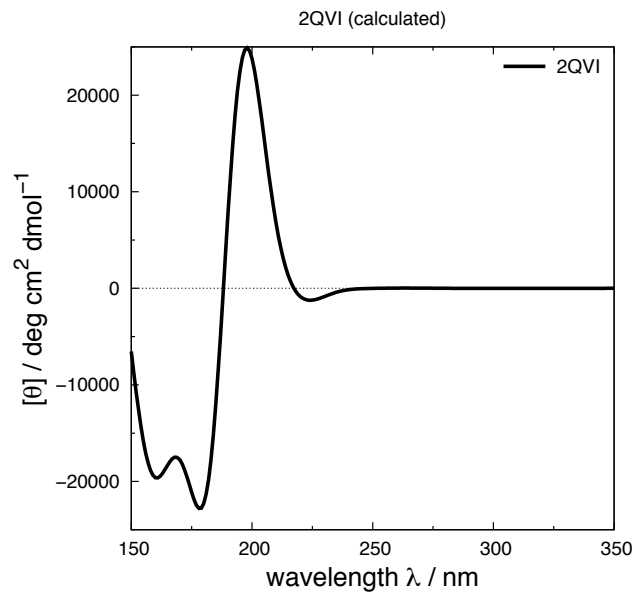


Figure 4.4 [?]

Fig. 4.4 shows the circular dichroism graph for the Cadherin protein.

After we analyze a sample by linear dichroism and use the matrix method, we obtain information about the conformation of the sample and the orientation of molecules within the sample. Circular dichroism spectroscopy is key in learning about the secondary structure of proteins. The possibilities for the secondary structure of a protein are either an α -helix, a β sheet, or a random coil. For example, DNA is structured in an α -helical shape, shown in Figure 4.5. It is possible to use linear dichroism to learn about the orientation of the backbone of DNA. Knowing about these characteristics of a biomolecule is helpful in identifying its biological function. It is possible to study many biomolecules and determine the structures using linear dichroism.



Figure 4.5

<http://www.veriware.org/images/dna/dna-helix.png>

Fig. 4.5 Deoxyribonucleic acid (DNA) has the secondary structure of an α -helix. The red and blue areas are the backbone of DNA, and the turns of those two strings is what gives DNA its shape.

Linear dichroism is also used to follow the kinetics of certain reactions [?]. For example, it is useful for determining the extent of the effects of an enzyme on

a biological system. We can determine ligand binding as well. When a ligand binds, the conformation of the peptide changes. This causes the absorbance of the wavelength corresponding to the peptide bond chromophore to change by either absorbing at a higher or lower wavelength. This important application is very useful in drug designing since it can show us whether or not a drug is binding, and therefore whether or not it is effective.

Linear dichroism is important for understanding the chemical structure of biomolecules in the human body. Many molecules found in the body are difficult to study because of the length or solubility, but linear dichroism enables us to study long and insoluble molecules. For example, it can be used study fibrous proteins, which are difficult to study with other techniques since fibers are usually insoluble and vary in length. Linear dichroism is crucial to furthering our understanding of the proteins in the human body.

APPENDIX-THE PERIODIC TABLE OF ELEMENTS

Periodic Table of Elements

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18																														
1 H Hydrogen 1.00794	<div style="display: flex; justify-content: space-between;"> <div> <p>Atomic # Symbol Name Atomic Mass</p> <p>C Solid Hg Liquid H Gas Rf Unknown</p> </div> <div> <p>Metals</p> <p>Alkali metals Alkaline earth metals Lanthanoids Actinoids Transition metals Poor metals Other nonmetals</p> </div> <div> <p>Nonmetals</p> <p>Noble gases</p> </div> </div>																2 He Helium 4.002602																														
3 Li Lithium 6.941	4 Be Beryllium 9.012182															5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.9984032	10 Ne Neon 20.1797																										
11 Na Sodium 22.98976928	12 Mg Magnesium 24.3050															13 Al Aluminum 26.9815386	14 Si Silicon 28.0855	15 P Phosphorus 30.973762	16 S Sulfur 32.065	17 Cl Chlorine 35.453	18 Ar Argon 39.948																										
19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.955912	22 Ti Titanium 47.887	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938045	26 Fe Iron 55.845	27 Co Cobalt 58.933195	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.64	33 As Arsenic 74.9216	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.798																														
37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90585	40 Zr Zirconium 91.224	41 Nb Niobium 92.90638	42 Mo Molybdenum 95.96	43 Tc Technetium (97.9072)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.90550	46 Pd Palladium 106.42	47 Ag Silver 107.8682	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.60	53 I Iodine 126.905447	54 Xe Xenon 131.293																														
55 Cs Cesium 132.9054519	56 Ba Barium 137.327	67-71														80 Hg Mercury 200.59	81 Tl Thallium 204.3833	82 Pb Lead 207.2	83 Bi Bismuth 208.98040	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222.0176)																									
87 Fr Francium (223)	88 Ra Radium (226)	89-103														104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (266)	107 Bh Bohrium (264)	108 Hs Hassium (277)	109 Mt Meitnerium (268)	110 Ds Darmstadtium (271)	111 Rg Roentgenium (272)	112 Uub Ununbium (285)	113 Uut Ununtrium (284)	114 Uuq Ununquadium (289)	115 Uup Ununpentium (288)	116 Uuh Ununhexium (282)	117 Uus Ununseptium	118 Uuo Ununoctium (284)																	
<p>For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.</p> <p>Design and Interface Copyright © 1997 Michael Dayah (michael@dayah.com). http://www.ptable.com/</p>																																															
<table border="1"> <tbody> <tr> <td>57 La Lanthanum 138.90547</td> <td>58 Ce Cerium 140.115</td> <td>59 Pr Praseodymium 140.90765</td> <td>60 Nd Neodymium 144.242</td> <td>61 Pm Promethium (145)</td> <td>62 Sm Samarium 150.36</td> <td>63 Eu Europium 151.964</td> <td>64 Gd Gadolinium 157.25</td> <td>65 Tb Terbium 158.92535</td> <td>66 Dy Dysprosium 162.50</td> <td>67 Ho Holmium 164.93032</td> <td>68 Er Erbium 167.259</td> <td>69 Tm Thulium 168.93421</td> <td>70 Yb Ytterbium 173.054</td> <td>71 Lu Lutetium 174.967</td> </tr> <tr> <td>89 Ac Actinium (227)</td> <td>90 Th Thorium 232.03806</td> <td>91 Pa Protactinium 231.03688</td> <td>92 U Uranium 238.02891</td> <td>93 Np Neptunium (237)</td> <td>94 Pu Plutonium (244)</td> <td>95 Am Americium (243)</td> <td>96 Cm Curium (247)</td> <td>97 Bk Berkelium (247)</td> <td>98 Cf Californium (251)</td> <td>99 Es Einsteinium (252)</td> <td>100 Fm Fermium (257)</td> <td>101 Md Mendelevium (258)</td> <td>102 No Nobelium (259)</td> <td>103 Lr Lawrencium (262)</td> </tr> </tbody> </table>																		57 La Lanthanum 138.90547	58 Ce Cerium 140.115	59 Pr Praseodymium 140.90765	60 Nd Neodymium 144.242	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.92535	66 Dy Dysprosium 162.50	67 Ho Holmium 164.93032	68 Er Erbium 167.259	69 Tm Thulium 168.93421	70 Yb Ytterbium 173.054	71 Lu Lutetium 174.967	89 Ac Actinium (227)	90 Th Thorium 232.03806	91 Pa Protactinium 231.03688	92 U Uranium 238.02891	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (262)
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<http://www.ptable.com/Images/periodic\%20table.png>

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KENNA COLLUMS

E-mail address: kmcollum@go.olemiss.edu