Finite Vector Space Representations

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What is a linear vector space?

The linear vector space representation of fields and operators is a powerful component in the toolbox of the mathematician, physicist, engineer and statistician. It enters in the analysis of a huge range of problems. Coming under alternative headings of "generalised fourier methods", "matrix methods", or "linear algebra", they are especially useful in the modern day as they allow problems to be formulated in a manner that is directly suitable for numerical solution by computer.

Vectors and matrices are structures that allow information to be represented in a systematic way. For our purposes a vector is a quantity that is a collection of numerical information. Along with the vector is its *representation* (the meanings attached to each element), which defines a *linear vector space*. Examples arise in basic physics, some quantities being fundamentally vector in nature, such as velocity or force that exist in two- or three-dimensional space. The representation in these examples is often of three cartesian directions of space (the *bases*), and the vector can be plotted, having a direction and a length. In such an example, the particular representation is not rigid. The representation can be changed by choosing different cartesian directions, by a rotation of the original axes. In the new representation, the components of the vector will have changed, not because the vector itself has changed, but because the representation has, and replotting the vector will yield the same absolute direction and length and it did before.

Vectors can have wider, but abstract, applications too. Commonly a field is represented as a vector. An example might be a two-dimensional field of some quantity constructed of a number of values on a finite grid covering the domain of the field. A possible representation of a vector might then be a sequence of kronecker delta functions at each position on the grid (these are a simple choice of bases). By associating each delta function with an element of the vector, the elements become the values of the field at each grid point. As in the case of the velocity or force, the vector will have a direction and length, but not in two- or three- dimensional space, but in an abstract N-dimensional space, where N is the number of grid points in the representation. This has a powerful conceptual value as all of the algebra that deals with vectors can now be applied to fields.

In this abstract application, there is the analogue of rotation of the basis. A new 'rotated' set of axes could be constructed by projecting the field onto an alternative basis set. A familiar example is the fourier decomposition of the field, which would yield a set of fourier coefficients that correspond to a representation of plane waves, each with a different wavenumber, instead of delta functions (the large dimensionality of the vector space makes it difficult to actually imagine the fourier transformation as a rotation!). Thus, by performing a fourier transform, we have represented the same field (i.e. vector) as an alternative set of coefficients. We can have either the vector in its real-space delta function representation, or the vector in its fourier-space representation.

Just as vectors can be used to represent fields, matrices are (linear) operators that act on these fields. For the purposes of this document, operators may be thought to come in two flavours. First there are the *transformation* or *rotation* operators - these are the kinds of operators that rotate the basis, transforming the representation. Acting with such a matrix does not fundamentally yield a new vector, but yields the same vector in a new representation, specified by the matrix. The fourier transform is an example of such an operator. The second kinds of operators might be referred to as *physical* or *statistical* operators, which perform specific physical or statistical roles. Many linear mathematical operations on the field have a matrix analogue, e.g. the laplacian operator, or the convolution operator, to name but two.

About this document

These notes are a description of three types of representation of vectors and physical operators. The simplest (section 1) is applicable to systems that are represented exclusively in terms of orthogonal basis vectors, and where both the input and output vectors of physical operators share the same vector space. A generalization of this (section 2) is for systems whose vector representations involve skew (non-orthogonal) basis vectors, which require a different treatment. Finally (section 3), considers the treatment of operators whose inputs and outputs do not share the same vector space. Here the technique of *singular value decomposition* is introduced.

To be clear and unambiguous, derivations are made using expanded (non-matrix) notation, but alongside the key equations, highlighted in boxes and using a separate equation numbering system, results are expressed in matrix notation, which is more compact. In so doing, many matrices - particularly transformation matrices - can be interpreted as an assembly of vectors. This introduces potential ambiguities as there are alternative conventions for doing this. Here, when assembling vectors into a matrix, the convention is used that each of the <u>columns</u> of the matrix holds each of the vectors (a lesser used convention, which is not used here, is to use the rows).

To be as general as possible, a dagger symbol (†) is used to represent the adjoint of a vector, matrix or operator. For vectors and matrices, this is the combined action of a transpose (^{T}) and complex conjugate (*). If all vectors and matrices contain purely real elements then the adjoint operation is equivalent to the transpose. Applying the adjoint operation to a scalar, means just take the complex conjugate.

Familiarity with certain matrix operations and concepts is assumed, e.g. taking the adjoint of a product of matrixes is equivalent to taking the adjoint of each individually, and reversing their order. Familiarity with the idea of an inverse matrix is also assumed.

1. Representation of vectors and operators in orthogonal bases

In this section we consider the representation of state vectors and operators in bases that have mutually orthogonal components. The eigenvectors of hermitian operators are mutually orthogonal and so this section has direct relevance to application around such operators.

1.1 Representation of a vector

In a basis comprised of $\hat{\phi}_i$ vectors, a vector $\hat{v}$ may be expressed,

$$\vec{v} = \sum_i v_i^\phi \hat{\phi}_i, \tag{1.1}$$

$$\hat{\phi}_i^\dagger \hat{\phi}_j = \delta_{ij}, \tag{1.2}$$

$$v_i^\phi = \hat{\phi}_i^\dagger \vec{v}, \tag{1.3}$$

while in an alternative basis of $\hat{\psi}_j$ the analogues are,

$$\vec{v} = \sum_j v_j^\psi \hat{\psi}_j, \tag{1.4}$$

$$\hat{\psi}_j^\dagger \hat{\psi}_i = \delta_{ij}, \tag{1.5}$$

$$v_j^\psi = \hat{\psi}_j^\dagger \vec{v}. \tag{1.6}$$

Define a relationship and an inverse relationship between the above two sets of bases,

$$\hat{\psi}_j = \sum_i T_{ij} \hat{\phi}_i, \tag{1.7}$$

$$\hat{\phi}_i = \sum_j U_{ji} \hat{\psi}_j, \tag{1.8}$$

where, for the matrix equivalents, $\mathbf{T} = \mathbf{U}^{-1}$. Use Eq. (1.2) to find matrix elements of $\mathbf{T}$ in Eq. (1.7),

$$T_{ij} = \hat{\phi}_i^\dagger \hat{\psi}_j, \tag{1.9}$$

and similarly use Eq. (1.5) in Eq. (1.8) to find the matrix elements of $\mathbf{U}$,

$$U_{ji} = \hat{\psi}_j^\dagger \hat{\phi}_i. \tag{1.10}$$

The right-hand-sides of Eqs. (1.9) and (1.10) are the adjoints of each other, implying,

$$U_{ji} = T_{ij}^* = T_{ji}^\dagger, \tag{1.11}$$

$$= (U^{-1})_{ji}^\dagger, \tag{1.12}$$

i.e. that the inverse transform operator between the two orthonormal bases is the same as the adjoint operator.

$$\boxed{(1.A) \qquad \mathbf{T} = \mathbf{U}^{-1} = \mathbf{U}^\dagger.}$$

1.2 Change in the representation of a vector

The **U** and **T** operators have been used to transform the basis elements, but they also can be made to transform the vectors themselves. Equation (1.1) is $\vec{v}$ in the ϕ-representation. In order to transform it to the ψ-representation, substitute Eq. (1.8) into Eq. (1.1),

$$\vec{v} \;=\; \sum_i v_i^{\phi} \sum_j U_{ji}\hat{\psi}_j \;=\; \sum_j \left(\sum_i U_{ji} v_i^{\phi}\right)\hat{\psi}_j. \tag{1.13}$$

By comparing Eq. (1.13) with Eq. (1.4), the bracketed term is seen to be the representation of $\vec{v}$ in the ψ-representation, i.e. that,

$$\begin{aligned} v_j^{\psi} &= \sum_i U_{ji} v_i^{\phi}, \\ &= \sum_i T^{\dagger}_{ji} v_i^{\phi}. \end{aligned} \tag{1.14}$$

$$\boxed{(1.B) \qquad \vec{v}^{\psi} \;=\; \mathbf{T}^{\dagger}\vec{v}^{\phi}.}$$

In Eq. (1.14), the property of the transforms, Eq. (1.11), has been used. In the same way, by substituting Eq. (1.7) into Eq. (1.4) and comparing to Eq. (1.1), one finds that,

$$\begin{aligned} v_i^{\phi} &= \sum_j T_{ij} v_j^{\psi}, \\ &= \sum_j U^{\dagger}_{ij} v_j^{\psi}. \end{aligned} \tag{1.15}$$

$$\boxed{(1.C) \qquad \vec{v}^{\phi} \;=\; \mathbf{U}^{\dagger}\vec{v}^{\psi}.}$$

In Eq. (1.15), the property, Eq. (1.11), has again been used.

1.3 Representation of an operator

The operators **U** and **T** that transform between representations are shown in section 1.2 to be natural matrix quantities. We now consider the conversion of physical or statistical operators to matrix form. Here, we consider only those operators that act within the same representation, and are described exclusively by orthogonal basis members.

Let operator **O** act on $\vec{v}^2$ to give $\vec{v}^1$. It need not be a matrix operator at this stage - all we need know is how to operate with **O** on any basis member.

$$\vec{v}^2 \;=\; \mathbf{O}\vec{v}^1, \tag{1.16}$$

$$\sum_i v_i^{2,\phi}\hat{\phi}_i \;=\; \sum_i v_i^{1,\phi}\mathbf{O}\hat{\phi}_i. \tag{1.17}$$

In Eq. (1.17), the vectors have been expanded in the ϕ-representation. Now use Eq. (1.2) for the orthonormality of the $\hat{\phi}$ vectors,

$$(1.18) \qquad v_j^{2,\phi} \;=\; \sum_i \left(\hat{\phi}_j^\dagger \mathbf{O} \hat{\phi}_i\right) v_i^{1,\phi}.$$

This result allows us to derive the operator **O** in matrix form under the ϕ-representation. Equation (1.18) is the expanded form of a matrix equation, where the matrix elements are found in the bracketed term,

$$(1.19) \qquad O_{ji}^{\phi} \;=\; \hat{\phi}_j^\dagger \mathbf{O} \hat{\phi}_i.$$

$$\boxed{(1.D) \qquad \vec{v}^{2,\phi} \;=\; \mathbf{O}^{\phi} \vec{v}^{1,\phi}.}$$

Thus, acting on a field with the operator **O**, is equivalent to acting on the field expressed in the ϕ-representation with the matrix of the above elements.

Similarly, a matrix representation exists for the ψ-representation,

$$(1.20) \qquad O_{nm}^{\psi} \;=\; \hat{\psi}_n^\dagger \mathbf{O} \hat{\psi}_m.$$

$$\boxed{(1.E) \qquad \vec{v}^{2,\psi} \;=\; \mathbf{O}^{\psi} \vec{v}^{1,\psi}.}$$

The matrix elements of Eq. (1.20) would be applied to fields expressed in the ψ-representation. In a similar way to different possible representations of a vector, Eqs. (1.19) and (1.20) represent the same operator, but in two different representations.

1.4 Change in the representation of an operator

There exists a simple relationship between the two representations of the operator **O**, given as Eqs. (1.19) and (1.20) in section 1.3. Given the matrix in one representation, and a basis transformation to another (as used in section 1.1), one can find the matrix in the other representation.

Suppose that the matrix elements of **O** in the ϕ-representation - Eq. (1.19) - are known, what are the matrix elements in the ψ-representation - Eq. (1.20) - without calculating them from scratch? Substitute Eq. (1.7) into Eq. (1.20),

$$\begin{aligned}
O_{nm}^{\psi} \;&=\; \sum_i T_{in}^{*} \hat{\phi}_i^\dagger \mathbf{O} \sum_j T_{jm} \hat{\phi}_j, \\
&=\; \sum_i \sum_j T_{in}^{*} \left(\hat{\phi}_i^\dagger \mathbf{O} \hat{\phi}_j\right) T_{jm}, \\
(1.21) \qquad &=\; \sum_i \sum_j T_{ni}^{\dagger} \mathbf{O}_{ij}^{\phi} T_{jm}.
\end{aligned}$$

$$\boxed{(1.F) \qquad \mathbf{O}^{\psi} \;=\; \mathbf{T}^\dagger \mathbf{O}^{\phi} \mathbf{T}.}$$

The boxed expression is the matrix equation equivalent to Eq. (1.21) where the columns of the matrix **T** specify the ψ-basis vectors in terms of the ϕ-basis vectors - see Eq. (1.7). Similarly, the operator in the ϕ-representation can be found from it in the ψ-representation (substitute Eq. (1.8) into Eq. (1.19)),

$$O^{\phi}_{ji} = \sum_n \sum_m U^{\dagger}_{jn}\mathbf{O}^{\psi}_{nm}U_{mi}. \tag{1.22}$$

$$\boxed{(1.G) \qquad \mathbf{O}^{\phi} = \mathbf{U}^{\dagger}\mathbf{O}^{\psi}\mathbf{U}.}$$

The columns of the matrix $\mathbf{U}$ specify the ϕ-basis vectors in terms of the ψ-basis vectors - see Eq. (1.8).

1.5 The eigenrepresentation

If the $\hat{\psi}$ vectors are eigenvectors of the operator $\mathbf{O}$ then the ψ-representation of $\mathbf{O}$ has the special property of being diagonal, as shown here. If $\hat{\psi}_m$ is an eigenvector of $\mathbf{O}$ with eigenvalue λ_m then,

$$\mathbf{O}\hat{\psi}_m = \lambda_m\hat{\psi}_m. \tag{1.23}$$

The matrix elements O^{ψ}_{mn} of Eq. (1.20) are then,

$$\begin{aligned} O^{\psi}_{nm} &= \hat{\psi}^{\dagger}_n\mathbf{O}\hat{\psi}_m, \\ &= \lambda_m\hat{\psi}^{\dagger}_n\hat{\psi}_m, \\ &= \lambda_m\delta_{nm}, \qquad (1.24) \end{aligned}$$

meaning that $\mathbf{O}^{\psi}$ is diagonal. Thus the matrix form of an operator in its eigenvector representation is diagonal, and the diagonal elements are its eigenvalues. Let $\mathbf{O}^{\phi}$ (the operator in the ϕ-representation as in Eq. (1.19)) be the operator in a non-eigenrepresentation (the matrix $\mathbf{O}^{\phi}$ is non-diagonal). It can be *diagonalized* by transforming it - using Eq. (1.21) - into the basis of the eigenvectors. Thus, by choosing the columns of the matrix $\mathbf{T}$ to be the eigenvectors of $\mathbf{O}^{\phi}$, Eq. (1.21) would yield the matrix elements in the eigenrepresentation. Only the diagonal elements ($m = n$) need be computed, which are the eigenvalues, and all other elements are zero.

If the columns of the matrix $\mathbf{T}$ are the representation of the ψ-vectors (in the ϕ-representation) then the following is the eigenvalue equation, in matrix form, for all eigenvectors,

$$\boxed{(1.H) \qquad \mathbf{O}^{\phi}\mathbf{T} = \mathbf{T}\mathbf{O}^{\psi},}$$

and can be found from a simple rearrangement of the matrix Eq. (1.F) using the matrix relations of Eq. (1.A). In the above matrix equation, the diagonal elements of $\mathbf{O}^{\psi}$ are the eigenvalues.

The content of this section on orthonormal systems is applicable if the operator, $\mathbf{O}$, is hermitian. This is due to an important property of hermitian operators - that their eigenfunctions are orthogonal, making them into a suitable basis set. In the remainder of section 1.5, we prove this property.

We now define a hermitian operator. A general property of operators (in fact the definition of the adjoint operator) is the following,

$$\hat{\psi}^{\dagger}_i\mathbf{O}\hat{\psi}_j = (\mathbf{O}^{\dagger}\hat{\psi}_i)^{\dagger}\,\hat{\psi}_j, \tag{1.25}$$

$$= (\hat{\psi}_j^\dagger \mathbf{O}^\dagger \hat{\psi}_i)^* . \tag{1.26}$$

A hermitian operator has the property that,

$$\mathbf{O} = \mathbf{O}^\dagger, \tag{1.27}$$

meaning that for such operators (from Eq. (1.26)),

$$\hat{\psi}_i^\dagger \mathbf{O} \hat{\psi}_j = (\hat{\psi}_j^\dagger \mathbf{O} \hat{\psi}_i)^* . \tag{1.28}$$

There are two important properties that can be deduced from Eq. (1.28) - that the eigenvalues of hermitian operators are real, and that their eigenvectors are mutually orthogonal. To show this, consider two eigenvectors of **O**,

$$\mathbf{O}\hat{\psi}_m = \lambda_m \hat{\psi}_m, \tag{1.29}$$

$$\mathbf{O}\hat{\psi}_n = \lambda_n \hat{\psi}_n. \tag{1.30}$$

For each of Eqs. (1.29) and (1.30), perform an inner product with the 'other' eigenvector and do not assume yet that the eigenvectors are orthogonal,

$$\hat{\psi}_n^\dagger \mathbf{O}\hat{\psi}_m = \lambda_m \hat{\psi}_n^\dagger \hat{\psi}_m, \tag{1.31}$$

$$\hat{\psi}_m^\dagger \mathbf{O}\hat{\psi}_n = \lambda_n \hat{\psi}_m^\dagger \hat{\psi}_n. \tag{1.32}$$

Take the adjoint of Eq. (1.31) and make use of the Hermitian property of Eq. (1.27),

$$\hat{\psi}_m^\dagger \mathbf{O}\hat{\psi}_n = \lambda_m^* \hat{\psi}_m^\dagger \hat{\psi}_n. \tag{1.33}$$

The left-hand-sides of Eqs. (1.32) and (1.33) are identical. The difference between these equations yields,

$$0 = (\lambda_m^* - \lambda_n)\, \hat{\psi}_m^\dagger \hat{\psi}_n. \tag{1.34}$$

The simultaneous properties of real eigenvalues ($\lambda_m^* = \lambda_m$) and orthogonal eigenvectors ($\hat{\psi}_m^\dagger \hat{\psi}_n = \delta_{mn}$) are consistent with Eq. (1.34). To satisfy this equation, either the difference of eigenvalues is zero, or the inner product is zero. The difference of eigenvalues is zero when $m = n$, allowing the inner product to be non-zero. When $m \neq n$, the difference between eigenvalues is non-zero, which means that the inner product must be zero.

Another final point regards the matrix elements of hermitian operators. Combining the hermitian property of **O**, Eq. (1.27) with Eq. (1.26) yields,

$$\hat{\psi}_i^\dagger \mathbf{O} \hat{\psi}_j = (\hat{\psi}_j^\dagger \mathbf{O} \hat{\psi}_i)^* ,$$

$$O_{ij}^{\psi} = O_{ji}^{\psi^*} . \tag{1.35}$$

This means that opposite matrix elements of hermitian operators are complex conjugates of each other. If the matrix elements are real, the the matrix is symmetric.

2. Representation of vectors and operators in skew bases

The matrix representation of hermitian operators (Eq. (1.27)) has special symmetry properties. More general matrices require a more general treatment and often require basis vectors that are skew to each other which do not satisfy the orthogonality property of Eqs. (1.2) or (1.5). In this section we discuss the vector spaces that are suitable as a representation of non-hermitian matrices, but still act within the same vector space.

2.1 Representation of a vector

Just as in section 1, a vector can be represented in a chosen basis,

$$\vec{v} = \sum_i v_i^{\phi} \hat{\phi}_i, \tag{2.1a}$$

but, unlike in section 1, the basis are now not assumed to be mutually orthogonal. Because of this, it is useful to define another set of basis, $\hat{\mathbf{\Phi}}_i$ (a *dual basis*) which goes alongside the $\hat{\phi}_i$. The dual representation of $\vec{v}$ is then,

$$\vec{v} = \sum_i v_i^{\mathbf{\Phi}} \hat{\mathbf{\Phi}}_i, \tag{2.1b}$$

the $\hat{\mathbf{\Phi}}_i$ (represented in upper case) being the *conjugate* or *adjoint* of $\hat{\phi}_i$ (represented in lower case). The basis set and its dual are intimately related having the following bi-orthogonality relations to make up for the fact that the bases are skew,

$$\hat{\mathbf{\Phi}}_i^{\dagger} \hat{\phi}_j = \delta_{ij}, \tag{2.2a}$$

$$\hat{\phi}_i^{\dagger} \hat{\mathbf{\Phi}}_j = \delta_{ij}, \tag{2.2b}$$

(in tensor calculus, the terms *covariant* and *contravariant* are used to distinguish between the bases). In section 1, in effect, these two sets also exist, but they are the same set. The bi-orthogonality property allows extraction of the expansion coefficients in Eqs. (2.1a) and (2.1b),

$$v_i^{\phi} = \hat{\mathbf{\Phi}}_i^{\dagger} \vec{v}, \tag{2.3a}$$

$$v_i^{\mathbf{\Phi}} = \hat{\phi}_i^{\dagger} \vec{v}. \tag{2.3b}$$

Analogous equations exist for another basis set, $\hat{\psi}_i$ and its dual $\hat{\mathbf{\Psi}}_i$,

$$\vec{v} = \sum_j v_j^{\psi} \hat{\psi}_j, \tag{2.4a}$$

$$\vec{v} = \sum_j v_j^{\mathbf{\Psi}} \hat{\mathbf{\Psi}}_j, \tag{2.4b}$$

$$\hat{\mathbf{\Psi}}_j^{\dagger} \hat{\psi}_i = \delta_{ji}, \tag{2.5a}$$

$$\hat{\psi}_j^{\dagger} \hat{\mathbf{\Psi}}_i = \delta_{ji}, \tag{2.5b}$$

$$v_j^{\psi} = \hat{\mathbf{\Psi}}_j^{\dagger} \vec{v}, \tag{2.6a}$$

$$v_j^{\mathbf{\Psi}} = \hat{\psi}_j^{\dagger} \vec{v}. \tag{2.6b}$$

Define relationships and inverse relationships between the above two sets of bases and their duals,

$$(2.7a)\qquad \hat{\psi}_j = \sum_i T_{ij}\hat{\phi}_i,$$

$$(2.7b)\qquad \hat{\mathbf{\Psi}}_j = \sum_i T'_{ij}\hat{\mathbf{\Phi}}_i,$$

$$(2.8a)\qquad \hat{\phi}_i = \sum_j U_{ji}\hat{\psi}_j,$$

$$(2.8b)\qquad \hat{\mathbf{\Phi}}_i = \sum_j U'_{ji}\hat{\mathbf{\Psi}}_j,$$

where, for the matrix equivalents, $\mathbf{T} = \mathbf{U}^{-1}$ and $\mathbf{T}' = \mathbf{U}'^{-1}$. Use Eqs. (2.2a), (2.2b), (2.5a) and (2.5b) to find matrix elements of $\mathbf{T}$, $\mathbf{T}'$, $\mathbf{U}$ and $\mathbf{U}'$,

$$(2.9a)\qquad T_{ij} = \hat{\mathbf{\Phi}}_i^\dagger\hat{\psi}_j,$$

$$(2.9b)\qquad T'_{ij} = \hat{\phi}_i^\dagger\hat{\mathbf{\Psi}}_j,$$

$$(2.10a)\qquad U_{ji} = \hat{\mathbf{\Psi}}_j^\dagger\hat{\phi}_i,$$

$$(2.10b)\qquad U'_{ji} = \hat{\psi}_j^\dagger\hat{\mathbf{\Phi}}_i.$$

Some of the right hand sides of the above four equations are the adjoints of others. Namely, Eq. (2.9a) is the conjugate of Eq. (2.10b) and Eq. (2.9b) of Eq. (2.10a). This means that the following relationships hold,

$$(2.11a)\qquad U'_{ji} = T^*_{ij} = T^\dagger_{ji},$$

$$(2.12a)\qquad = (U^{-1})^\dagger_{ji},$$

$$(2.11b)\qquad U_{ji} = T'^*_{ij} = T'^\dagger_{ji},$$

$$(2.12b)\qquad = (U'^{-1})^\dagger_{ji}.$$

$$\boxed{(2.Aa)\qquad \mathbf{T} = \mathbf{U}^{-1} = \mathbf{U}'^\dagger,}$$

$$\boxed{(2.Ab)\qquad \mathbf{T}' = \mathbf{U}'^{-1} = \mathbf{U}^\dagger.}$$

These results mean that the inverse operator transforming between the bases is the same as the adjoint of the operator acting between its dual bases.

2.2 Change in the representation of a vector

The $\mathbf{U}$, $\mathbf{T}$, $\mathbf{U}'$ and $\mathbf{T}'$ operators have been used to transform the basis elements, but they also can be made to transform the vectors themselves. Equation (2.1a) is $\vec{v}$ in the ϕ-representation. In order to transform it to the ψ-representation, substitute Eq. (2.8a) into Eq. (2.1a),

$$(2.13)\qquad \vec{v} = \sum_i v_i^\phi \sum_j U_{ji}\hat{\psi}_j = \sum_j\left(\sum_i U_{ji}v_i^\phi\right)\hat{\psi}_j.$$

By comparing Eq. (2.13) with Eq. (2.4a), the bracketed term is seen to be the representation of $\vec{v}$ in the ψ-representation, i.e. that,

$$v_j^{\psi} = \sum_i U_{ji} v_i^{\phi},$$

$$= \sum_i T_{ji}'^{\dagger} v_i^{\phi}. \tag{2.14}$$

$$\boxed{(2.B) \qquad \vec{v}^{\psi} = \mathbf{T}'^{\dagger} \vec{v}^{\phi}.}$$

In Eq. (2.14), the property of the transforms, Eq. (2.11b), has been used. Although we are transforming a vector from the ϕ- to the ψ-representation, the $\mathbf{T}'$ - Eq. (2.7b) - (rather than the $\mathbf{T}$) operator has been used, which transforms between the dual of these representations. This is due to the fact that the bases are skew. In the same way, by substituting Eq. (2.7a) into Eq. (2.4a) and comparing to Eq. (2.1a), one finds that,

$$v_i^{\phi} = \sum_j T_{ij} v_j^{\psi},$$

$$= \sum_j U_{ij}'^{\dagger} v_j^{\psi}. \tag{2.15}$$

$$\boxed{(2.C) \qquad \vec{v}^{\phi} = \mathbf{U}'^{\dagger} \vec{v}^{\psi}.}$$

In Eq. (2.15), the property of the transforms, Eq. (2.11a), has been used. These are very similar results to those proven in section 1 for transformations between vectors represented with orthogonal basis sets.

2.3 Representation of an operator

The operators $\mathbf{U}$, $\mathbf{U}'$, $\mathbf{T}$ and $\mathbf{T}'$ that transform between representations are shown, in section 2.2, to be natural matrix quantities. We now consider the conversion of physical operators to matrix form. Here we consider those operators that act within the same representation but, unlike in section 1, the basis members do not have to be orthogonal.

Let operator $\mathbf{O}$ act on $\vec{v}^2$ to give $\vec{v}^1$. It need not be a matrix operator at this stage - all we need to know is how to operate with $\mathbf{O}$ on any basis member.

$$\vec{v}^2 = \mathbf{O}\vec{v}^1, \tag{2.16}$$

$$\sum_i v_i^{2,\phi} \hat{\phi}_i = \sum_i v_i^{1,\phi} \mathbf{O} \hat{\phi}_i. \tag{2.17}$$

In Eq. (2.17), the vectors have been expanded in the ϕ-representation. This is the same treatment as for the orthogonal systems. Now use Eq. (2.2a) for the bi-orthonormality between the $\hat{\phi}$ and $\hat{\mathbf{\Phi}}$ vectors,

$$v_j^{2,\phi} = \sum_i \left(\hat{\mathbf{\Phi}}_j^{\dagger} \mathbf{O} \hat{\phi}_i \right) v_i^{1,\phi}. \tag{2.18}$$

This result allows us to derive the operator **O** in matrix form under the ϕ-representation. Equation (2.18) is the expanded form of a matrix equation, where the matrix elements are found in the bracketed term,

$$O^{\phi}_{ji} = \hat{\mathbf{\Phi}}^{\dagger}_{j}\mathbf{O}\hat{\phi}_{i}. \tag{2.19a}$$

$$\boxed{\vec{v}^{2,\phi} = \mathbf{O}^{\phi}\vec{v}^{1,\phi}.} \tag{2.Da}$$

Thus, acting on a field with the operator **O**, is equivalent to acting on the field expressed in the ϕ-representation with the matrix of the above elements. There is a slight peculiarity with the results for skew systems: although the form of the right hand side of Eq. (2.19a), for the matrix elements, suggests a transference of the basis from ϕ to $\mathbf{\Phi}$, the vectors before ($\vec{v}^{1,\phi}$) and after ($\vec{v}^{2,\phi}$) the action of $\mathbf{O}^{\phi}$, remain in the ϕ-representation.

Similarly, a matrix representation exists for the $\mathbf{\Phi}$-representation,

$$O^{\mathbf{\Phi}}_{ij} = \hat{\phi}^{\dagger}_{i}\mathbf{O}\hat{\mathbf{\Phi}}_{j}. \tag{2.19b}$$

$$\boxed{\vec{v}^{2,\mathbf{\Phi}} = \mathbf{O}^{\mathbf{\Phi}}\vec{v}^{1,\mathbf{\Phi}}.} \tag{2.Db}$$

Similarly for the ψ and $\mathbf{\Psi}$-representations,

$$O^{\psi}_{nm} = \hat{\mathbf{\Psi}}^{\dagger}_{n}\mathbf{O}\hat{\psi}_{m}. \tag{2.20a}$$

$$\boxed{\vec{v}^{2,\psi} = \mathbf{O}^{\psi}\vec{v}^{1,\psi}.} \tag{2.Ea}$$

$$O^{\mathbf{\Psi}}_{mn} = \hat{\psi}^{\dagger}_{m}\mathbf{O}\hat{\mathbf{\Psi}}_{n}. \tag{2.20b}$$

$$\boxed{\vec{v}^{2,\mathbf{\Psi}} = \mathbf{O}^{\mathbf{\Psi}}\vec{v}^{1,\mathbf{\Psi}}.} \tag{2.Eb}$$

2.4 Change in the representation of an operator

There exists simple relationships between the representations of the operator **O**. We will examine the relationships between **O** in the ϕ- and ψ-basis sets, as specified in section 2.3 (Eqs. (2.19a) and (2.20a) respectively). Given the matrix in one representation, and a basis transformation to another (as used in section 2.1), one can find the matrix in the other representation.

Suppose that the matrix elements of **O** in the ϕ-representation - Eq. (2.19a) - are known, what are the matrix elements of **O** in the ψ-representation - Eq. (2.20a) - without calculating them from scratch? Substitute Eqs. (2.7a) and (2.7b) into Eq. (2.20a),

$$\begin{aligned} O^{\psi}_{mn} &= \sum_i T'^{*}_{im}\hat{\mathbf{\Phi}}^{\dagger}_{i}\mathbf{O} \sum_j T_{jn}\hat{\phi}_{j}, \\ &= \sum_i \sum_j T'^{*}_{im}\left(\hat{\mathbf{\Phi}}^{\dagger}_{i}\mathbf{O}\hat{\phi}_{j}\right)T_{jn}, \end{aligned}$$

$$\text{(2.21)} \qquad = \sum_i \sum_j T'^{\dagger}_{mi} O^{\phi}_{ij} T_{jn}.$$

$$\boxed{\text{(2.}F\text{)} \qquad \mathbf{O}^{\psi} = \mathbf{T}'^{\dagger}\mathbf{O}^{\phi}\mathbf{T}.}$$

The boxed expression is the matrix equation equivalent to Eq. (2.21) where the columns of the matrix **T** specify the ψ-basis vectors in terms of the ϕ-basis vectors - see Eq. (2.7a), and the columns of the matrix $\mathbf{T}'$ specify the $\mathbf{\Psi}$-basis vectors in terms of the $\mathbf{\Phi}$-basis vectors - see Eq. (2.7b). Similarly, the operator in the ϕ-representation can be found from it in the ψ-representation (substitute Eqs. (2.8a) and (2.8b) into Eq. (2.19a)),

$$\text{(2.22)} \qquad O^{\phi}_{ji} = \sum_n \sum_m U'^{\dagger}_{jm} O^{\psi}_{mn} U_{ni}.$$

$$\boxed{\text{(2.}G\text{)} \qquad \mathbf{O}^{\phi} = \mathbf{U}'^{\dagger}\mathbf{O}^{\psi}\mathbf{U}.}$$

2.5 The eigenrepresentation

If the $\hat{\psi}$ vectors are eigenvectors of the operator **O** (and the $\hat{\mathbf{\Psi}}$ are bi-orthogonal to these) then the ψ-representation of **O** has the special property of being diagonal, as shown here. If $\hat{\psi}_m$ is an eigenvector of **O** with eigenvalue λ_m then,

$$\text{(2.23)} \qquad \mathbf{O}\hat{\psi}_m = \lambda_m \hat{\psi}_m.$$

The matrix elements O^{ψ}_{mn} of Eq. (2.20a) are then,

$$\begin{aligned} O^{\psi}_{nm} &= \hat{\mathbf{\Psi}}^{\dagger}_n \mathbf{O} \hat{\psi}_m, \\ &= \lambda_m \hat{\mathbf{\Psi}}^{\dagger}_n \hat{\psi}_m, \\ \text{(2.24)} \qquad &= \lambda_m \delta_{nm}, \end{aligned}$$

meaning that $\mathbf{O}^{\psi}$ is diagonal. Thus the matrix form of an operator in its eigenvector representation is diagonal, and the diagonal elements are its eigenvalues. Let $\mathbf{O}^{\phi}$ (the operator in the ϕ-representation as in Eq. (2.19a)) be the operator in a non-eigenrepresentation (the matrix $\mathbf{O}^{\phi}$ is non-diagonal). It can be *diagonalized* by transforming it - using Eq. (2.21) - into the basis of the eigenvectors. Thus, by choosing the columns of the matrix **T** to be the eigenvectors of $\mathbf{O}^{\phi}$, and the columns of the matrix $\mathbf{T}'$ to be bi-orthogonal to these, Eq. (2.21) would yield the matrix elements in the eigenrepresentation. Only the diagonal elements ($m = n$) need be computed, which are the eigenvalues, and all other elements are zero.

If the columns of the matrix **T** are the representation of the ψ-vectors (in the ϕ-representation) then the following is the eigenvalue equation, in matrix form, for all eigenvectors,

$$\boxed{\text{(2.}H\text{)} \qquad \mathbf{O}^{\phi}\mathbf{T} = \mathbf{T}\mathbf{O}^{\psi},}$$

and can be found from a simple rearrangement of the matrix Eq. (2.F) using the matrix relations of Eqs. (2.Aa) and (2.Ab). In the above matrix equation, the diagonal elements of $\mathbf{O}^{\psi}$ are the eigenvalues.

Until now, nothing has been said about the dual space basis vectors, $\hat{\mathbf{\Psi}}$, apart from being bi-orthogonal to the $\hat{\psi}$ basis vectors. If the $\hat{\psi}$ vectors are eigenvectors of $\mathbf{O}$, then the set of bi-orthogonal vectors, $\hat{\mathbf{\Psi}}$, are found to be eigenvectors of the adjoint operator, $\mathbf{O}^\dagger$.

Take the eigenvalue equation for $\hat{\psi}_m$ (Eq. (2.23)) and perform an inner product with $\hat{\mathbf{\Psi}}_n$, but unlike in Eq. (2.24), do not assume for now that $\hat{\mathbf{\Psi}}_n$ is bi-orthogonal to $\hat{\psi}_m$,

$$\hat{\mathbf{\Psi}}_n^\dagger \mathbf{O} \hat{\psi}_m = \lambda_m \hat{\mathbf{\Psi}}_n^\dagger \hat{\psi}_m. \tag{2.25}$$

The adjoint of this equation is,

$$\hat{\psi}_m^\dagger \mathbf{O}^\dagger \hat{\mathbf{\Psi}}_n = \lambda_m^* \hat{\psi}_m^\dagger \hat{\mathbf{\Psi}}_n. \tag{2.26}$$

Next, allow $\hat{\mathbf{\Psi}}_n$ to be an eigenvector of $\mathbf{O}^\dagger$, with eigenvalue μ_n, then perform an inner product with $\hat{\psi}_m$,

$$\mathbf{O}^\dagger \hat{\mathbf{\Psi}}_n = \mu_n \hat{\mathbf{\Psi}}_n,$$

$$\hat{\psi}_m^\dagger \mathbf{O}^\dagger \hat{\mathbf{\Psi}}_n = \mu_n \hat{\psi}_m^\dagger \hat{\mathbf{\Psi}}_n. \tag{2.27}$$

The left-hand-sides of Eqs. (2.26) and (2.27) are identical. The difference between these two equations yields,

$$0 = (\lambda_m^* - \mu_n)\, \hat{\psi}_m^\dagger \hat{\mathbf{\Psi}}_n. \tag{2.28}$$

The simultaneous properties of the two sets of eigenvalues being related by $\lambda_m^* = \mu_m$ (the eigenvalues are complex conjugates of each other), and bi-orthogonal eigenvectors ($\hat{\psi}_m^\dagger \hat{\mathbf{\Psi}}_n = \delta_{mn}$) are consistent with Eq. (2.28). To satisfy this equation, either the difference of eigenvalues is zero, or the inner product is zero. The difference of eigenvalues is zero when $m = n$, allowing the inner product to be non-zero. When $m \neq n$, the difference between eigenvalues is non-zero, which means that the inner product must be zero.

3. Representation of vectors and operators in multiple bases (with application to singular vectors)

In sections 1 and 2, the 'input' and 'output' vector spaces of the operator **O** are identical (the difference between the two sections being the orthogonality or bi-orthogonality of the basis members). In this section we consider the representations of state vectors and operators necessary to describe the action of operators that span two different spaces. That is for those operators that act on a vector in one vector space (called the *right space* since it falls on the right hand side of the operator), and yield a vector in another (called the *left space*). The left and right spaces are each taken to be orthogonal spaces (see below).

The separate left and right vector spaces are necessary to describe the action of physical operators considered in this section. The sizes of each space can be different, and so we must define from the start the number of bases in each space. Let the left space have α basis members and the right space have β. We did not specify the number of members in previous sections since it was constant. Another important number is the rank of the operator, γ which is discussed in section 3.5.

3.1 Representation of left and right vectors

A vector belonging to the left vector space can be represented in a chosen left basis,

$$\vec{v}^L = \sum_{m=1}^{\alpha} v_m^{\phi,L} \hat{\phi}_m^L, \tag{3.1a}$$

and a vector belonging to the right vector space can be represented in a right basis,

$$\vec{v}^R = \sum_{i=1}^{\beta} v_i^{\phi,R} \hat{\phi}_i^R, \tag{3.1b}$$

where the two bases are separate. Note the different upper limits on the summations. The left and right members are each orthogonal sets, which allows the coefficients $v_m^{\phi,L}$ and $v_i^{\phi,R}$ to be found,

$$\hat{\phi}_m^{L\dagger} \hat{\phi}_n^L = \delta_{mn}, \tag{3.2a}$$

$$\hat{\phi}_i^{R\dagger} \hat{\phi}_j^R = \delta_{ij}, \tag{3.2b}$$

$$v_m^{\phi,L} = \hat{\phi}_m^{L\dagger} \vec{v}^L, \tag{3.3a}$$

$$v_i^{\phi,R} = \hat{\phi}_i^{R\dagger} \vec{v}^R. \tag{3.3b}$$

In an alternative left basis and an alternative right basis, the analogues of the above are,

$$\vec{v}^L = \sum_{m=1}^{\alpha} v_m^{\psi,L} \hat{\psi}_m^L, \tag{3.4a}$$

$$\vec{v}^R = \sum_{i=1}^{\beta} v_i^{\psi,R} \hat{\psi}_i^R, \tag{3.4b}$$

$$(3.5a)\qquad \hat{\psi}_m^{L\,\dagger}\hat{\psi}_n^L = \delta_{mn},$$

$$(3.5b)\qquad \hat{\psi}_i^{R\dagger}\hat{\psi}_j^R = \delta_{ij},$$

$$(3.6a)\qquad v_m^{\psi,L} = \hat{\psi}_m^{L\,\dagger}\vec{v}^L,$$

$$(3.6b)\qquad v_i^{\psi,R} = \hat{\psi}_i^{R\dagger}\vec{v}^R.$$

Define relationships and inverse relationships between the $\hat{\phi}_m^L$ and $\hat{\psi}_n^L$ bases and the $\hat{\phi}_i^R$ and $\hat{\psi}_j^R$ bases,

$$(3.7a)\qquad \hat{\psi}_n^L = \sum_{m=1}^{\alpha} T_{mn}^L\hat{\phi}_m^L,$$

$$(3.7b)\qquad \hat{\psi}_j^R = \sum_{i=1}^{\beta} T_{ij}^R\hat{\phi}_i^R,$$

$$(3.8a)\qquad \hat{\phi}_m^L = \sum_{n=1}^{\alpha} U_{nm}^L\hat{\psi}_n^L,$$

$$(3.8b)\qquad \hat{\phi}_i^R = \sum_{j=1}^{\beta} U_{ji}^R\hat{\psi}_j^R,$$

where, for the matrix equivalents, $\mathbf{T}^L = \mathbf{U}^{L-1}$ and $\mathbf{T}^R = \mathbf{U}^{R-1}$. Use Eqs. (3.2a), (3.2b), (3.5a) and (3.5b) to find matrix elements of $\mathbf{T}^L$, $\mathbf{T}^R$, $\mathbf{U}^L$ and $\mathbf{U}^R$,

$$(3.9a)\qquad T_{mn}^L = \hat{\phi}_m^{L\,\dagger}\hat{\psi}_n^L,$$

$$(3.9b)\qquad T_{ij}^R = \hat{\phi}_i^{R\dagger}\hat{\psi}_j^R,$$

$$(3.10a)\qquad U_{nm}^L = \hat{\psi}_n^{L\dagger}\hat{\phi}_m^L,$$

$$(3.10b)\qquad U_{ji}^R = \hat{\psi}_j^{R\dagger}\hat{\phi}_i^R.$$

Some of the right hand sides of the above four equations are the adjoints of others. Namely, Eq. (3.9a) is the conjugate of Eq. (3.10a) and Eq. (3.9b) of Eq. (3.10b). This means that the following relationships hold,

$$(3.11a)\qquad U_{nm}^L = T_{mn}^{L\;*} = T_{nm}^{L\;\dagger},$$

$$(3.12a)\qquad = (U^{L^{-1}})_{nm,}^{\dagger}$$

$$(3.11b)\qquad U_{ji}^R = T_{ij}^{R*} = T_{ji}^{R\dagger},$$

$$(3.12b)\qquad = (U^{R^{-1}})_{ji}^{\dagger}.$$

$$\boxed{(3.Aa)\qquad \mathbf{T}^L = \mathbf{U}^{L^{-1}} = \mathbf{U}^{L^\dagger},}$$

$$\boxed{(3.Ab)\qquad \mathbf{T}^R = \mathbf{U}^{R^{-1}} = \mathbf{U}^{R^\dagger}.}$$

3.2 Change in the representation of vectors

The $\mathbf{U}^L$, $\mathbf{T}^L$, $\mathbf{U}^R$ and $\mathbf{T}^R$ operators have been used to transform the basis elements, but they also can be made to transform the vectors themselves. Equation (3.1) is $\vec{v}^L$ in the ϕ^L-representation. In order to transform it into the ψ^L-representation, substitute Eq. (3.8a) into Eq. (3.1a),

$$\vec{v}^L = \sum_{m=1}^{\alpha} v_m^{\phi,L} \sum_{n=1}^{\alpha} U_{nm}^L \hat{\psi}_n^L = \sum_{n=1}^{\alpha} \left(\sum_{m=1}^{\alpha} U_{nm}^L v_m^{\phi,L} \right) \hat{\psi}_n^L. \tag{3.13}$$

By comparing Eq. (3.13) with Eq. (3.4a), the bracketed term is seen to be the representation of $\vec{v}^L$ in the ψ^L-representation, i.e. that,

$$\begin{aligned} v_n^{\psi,L} &= \sum_{m=1}^{\alpha} U_{nm}^L v_m^{\phi,L}, \\ &= \sum_{m=1}^{\alpha} {T_{nm}^L}^{\dagger} v_m^{\phi,L}. \end{aligned} \tag{3.14a}$$

$$\boxed{(3.Ba) \qquad \vec{v}^{\psi,L} = \mathbf{T}^{L^{\dagger}} \vec{v}^{\phi,L}.}$$

In Eq. (3.14a), the property of the transforms, Eq. (3.11a), has been used. In the same way, by substituting Eq. (3.7a) into Eq. (3.4a) and comparing to Eq. (3.1a), one finds the inverse relationship,

$$\begin{aligned} v_n^{\phi,L} &= \sum_{m=1}^{\alpha} T_{nm}^L v_m^{\psi,L}, \\ &= \sum_{m=1}^{\alpha} {U_{nm}^L}^{\dagger} v_m^{\psi,L}. \end{aligned} \tag{3.15a}$$

$$\boxed{(3.Ca) \qquad \vec{v}^{\phi,L} = \mathbf{U}^{L^{\dagger}} \vec{v}^{\psi,L}.}$$

In Eq. (3.15a), the property of the transforms, Eq. (3.11a), has been used.

Similar results exist for transformations between the two bases of the right space. By substituting Eq. (3.8b) into Eq. (3.1b) and comparing to Eq. (3.4b), one finds that,

$$\begin{aligned} v_j^{\psi,R} &= \sum_{i=1}^{\beta} U_{ji}^R v_i^{\phi,R}, \\ &= \sum_{i=1}^{\beta} T_{ji}^{R^{\dagger}} v_i^{\phi,R}. \end{aligned} \tag{3.14b}$$

$$\boxed{(3.Bb) \qquad \vec{v}^{\psi,R} = \mathbf{T}^{R^{\dagger}} \vec{v}^{\phi,R}.}$$

In Eq. (3.14b), the property of the transforms, Eq. (3.11b), has been used. In the same way, by substituting Eq. (3.7b) into Eq. (3.4b) and comparing to Eq. (3.1b), one finds the inverse relationship,

$$v_j^{\phi,R} = \sum_{i=1}^{\beta} T_{ji}^R v_i^{\psi,R},$$

(3.15b) $$= \sum_{i=1}^{\beta} U_{ji}^{R^\dagger} v_i^{\psi,R}.$$

(3.Cb) $$\boxed{\vec{v}^{\phi,R} = \mathbf{U}^{R^\dagger} \vec{v}^{\psi,R}.}$$

In Eq. (3.15b), the property of the transforms, Eq. (3.11b), has been used. These are very similar results to those proven in section 1, for the left and right bases separately.

3.3 Representation of an operator

The operators $\mathbf{U}^L$, $\mathbf{U}^R$, $\mathbf{T}^L$ and $\mathbf{T}^R$ that transform between representations are shown, in section 3.2, to be natural matrix quantities. We now consider the conversion of physical operators to matrix form. Here we consider those matrices that straddle two different vector spaces (the operators considered in section 1.3 are a subset of the operators used here, which are special in that the two spaces happen to be the same).

Let the operator $\mathbf{O}$ act on $\vec{v}^R$ to give $\vec{v}^L$. It need not be a matrix operator at this stage - all we need to know is how to operate with $\mathbf{O}$ on any right basis member to give a combination of left basis members.

(3.16) $$\vec{v}^L = \mathbf{O}\vec{v}^R,$$

(3.17) $$\sum_{m=1}^{\alpha} v_m^{\phi,L} \hat{\phi}_m^L = \sum_{m=1}^{\beta} v_m^{\phi,R} \mathbf{O} \hat{\phi}_m^R.$$

In Eq. (3.17), the vectors have been expanded in the ϕ-representation in the left and right spaces. This is the same treatment as for the orthogonal systems. Now use Eq. (3.2a) for the orthonormality of the left basis vectors,

(3.18) $$v_n^{\phi,L} = \sum_{m=1}^{\beta} \left(\hat{\phi}_n^{L^\dagger} \mathbf{O} \hat{\phi}_m^R\right) v_m^{\phi,R},$$

for $1 \leqslant n \leqslant \alpha$. This result allows us to derive the operator $\mathbf{O}$ in matrix form under the ϕ-representation. Equation (3.18) is the expanded form of a matrix equation, where the matrix elements are found in the bracketed term,

(3.19a) $$O_{nm}^{\phi\phi} = \hat{\phi}_n^{L^\dagger} \mathbf{O} \hat{\phi}_m^R.$$

(3.Da) $$\boxed{\vec{v}^{\phi,L} = \mathbf{O}^{\phi\phi} \vec{v}^{\phi,R}.}$$

Thus, acting on a field with the operator $\mathbf{O}$, is equivalent to acting on the field expressed in the ϕ^R-representation with the matrix, $\mathbf{O}^{\phi\phi}$, of the above elements to yield a vector in the ϕ^L-representation.

Similarly, a matrix representation exists for the ψ-representation in each of the left and right bases, (3.19*b*) $$O^{\psi\psi}_{nm} = \hat{\psi}^{L^\dagger}_n \mathbf{O} \hat{\psi}^R_m.$$

$$\boxed{(3.Db) \qquad \vec{v}^{\psi,L} = \mathbf{O}^{\psi\psi} \vec{v}^{\psi,R}.}$$

Expressions for the matrix elements when one vector space is in the ϕ-representation and the other in the ψ-representation are,

(3.20*a*) $$O^{\psi\phi}_{nm} = \hat{\psi}^{L^\dagger}_n \mathbf{O} \hat{\phi}^R_m.$$

$$\boxed{(3.Ea) \qquad \vec{v}^{\psi,L} = \mathbf{O}^{\psi\phi} \vec{v}^{\phi,R}.}$$

(3.20*b*) $$O^{\phi\psi}_{nm} = \hat{\phi}^{L^\dagger}_n \mathbf{O} \hat{\psi}^R_m.$$

$$\boxed{(3.Eb) \qquad \vec{v}^{\phi,L} = \mathbf{O}^{\phi\psi} \vec{v}^{\psi,R}.}$$

3.4 Change in the representation of an operator

There exists simple relationships between the above representations of the operator **O**. We will examine the relationships between **O** in the ϕ- and ψ-basis sets (in the left and right cases), as specified in section 3.3. Given the matrix in one representation, and a basis transformation to another (as used in section 3.1), one can find the matrix in the other representation.

Suppose that the matrix elements of **O** in the ϕ-representation - Eq. (3.19a) - are known, what are the matrix elements of **O** in the ψ-representation - Eq. (3.19b) - without calculating them from scratch? Substitute Eqs. (3.7a) and (3.7b) into Eq. (3.19b),

$$O^{\psi\psi}_{nm} = \sum_{i=1}^{\alpha} T^{L^*}_{in} \hat{\phi}^{L^\dagger}_i \mathbf{O} \sum_{j=1}^{\beta} T^R_{jm} \hat{\phi}^R_j,$$

$$= \sum_{i=1}^{\alpha} \sum_{j=1}^{\beta} T^{L^*}_{in} \left(\hat{\phi}^{L^\dagger}_i \mathbf{O} \hat{\phi}^R_j \right) T^R_{jm},$$

(3.21) $$= \sum_{i=1}^{\alpha} \sum_{j=1}^{\beta} T^{L^\dagger}_{ni} O^{\phi\phi}_{ij} T^R_{jm}.$$

$$\boxed{(3.F) \qquad \mathbf{O}^{\psi\psi} = \mathbf{T}^{L^\dagger} \mathbf{O}^{\phi\phi} \mathbf{T}^R.}$$

The boxed expression is the matrix equation equivalent to Eq. (3.21) where the columns of the matrix $\mathbf{T}^L$ specify the ψ^L-basis vectors in terms of the ϕ^L-basis vectors - see Eq. (3.7a) and the columns of the matrix $\mathbf{T}^R$ specify the ψ^R-basis vectors in terms of the ϕ^R-basis vectors - see Eq. (3.7b). Similarly, the operator in the ϕ-representation can be found from it in the ψ-representation (substitute Eqs. (3.8a) and (3.8b) into Eq. (3.19a)),

(3.22) $$O^{\phi\phi}_{nm} = \sum_{i=1}^{\alpha} \sum_{j=1}^{\beta} U^{L^\dagger}_{ni} O^{\psi\psi}_{ij} U^R_{jm}.$$

$$(3.G) \qquad \mathbf{O}^{\phi\phi} = \mathbf{U}^{L^\dagger}\mathbf{O}^{\psi\psi}\mathbf{U}^R.$$

The columns of the matrix $\mathbf{U}^L$ specify the ϕ^L-basis vectors in terms of the ψ^L-basis vectors - see Eq. (3.8a) and the columns of the matrix $\mathbf{U}^R$ specify the ϕ^R-basis vectors in terms of the ψ^R-basis vectors - see Eq. (3.8b).

3.5 The 'eigenrepresentation' (singular vectors and singular values)

Unlike for operators that preserve the vector space, it is not possible here to write an eigenvalue equation (like Eq. (1.23)). We can, however, write the following,

$$(3.23) \qquad \mathbf{O}\hat{\psi}^R_m = \lambda_m \hat{\psi}^L_m.$$

The vectors $\hat{\psi}^R_m$ and $\hat{\psi}^L_m$ take the role of the eigenvectors considered before. In the above equation, they are called the right and left *singular vectors*. The scalar λ_m takes the role of the eigenvalue. It is called the *singular value* here. These singular vectors and the singular value satisfy other eigenvalue equations as discussed later.

If we choose to represent $\mathbf{O}$ in the basis vectors that satisfy Eq. (3.23), the matrix elements $O^{\psi\psi}_{nm}$ of Eq. (3.19b) are then,

$$\begin{aligned} O^{\psi\psi}_{nm} &= \hat{\psi}^{L^\dagger}_n \mathbf{O}\hat{\psi}^R_m, \\ &= \lambda_m \hat{\psi}^{L^\dagger}_n \hat{\psi}^L_m, \\ (3.24) \qquad &= \lambda_m \delta_{nm}, \end{aligned}$$

meaning that $\mathbf{O}^{\psi\psi}$ is 'diagonal'. The diagonality property is not strictly true, since only a square matrix can be diagonal and $\mathbf{O}^{\psi\psi}$ is a $\alpha \times \beta$ matrix. Equation (3.24) actually says that the square submatrix of dimension $\alpha \times \alpha$ or $\beta \times \beta$ (depending on whether α or β respectively is smaller) at the top left of the full matrix is diagonal. Thus the matrix form of an operator in its singular vector representation is 'diagonal', and the diagonal elements are its singular values. Let $\mathbf{O}^{\phi\phi}$ (the operator in the ϕ-representation as in Eq. (3.19a)) be the operator in a non-singular vector representation (the matrix $\mathbf{O}^{\phi\phi}$ is non-diagonal). It can be '*diagonalized'* by transforming it - using Eq. (3.21) - into the basis of the left and right singular vectors. Thus, by choosing the columns of the matrix $\mathbf{T}^L$ to be the left singular vectors of $\mathbf{O}^{\phi\phi}$ (to find these see Eq. (3.29b) below) and the columns of the matrix $\mathbf{T}^R$ to be the right singular vectors of $\mathbf{O}^{\phi\phi}$ (to find these see Eq. (3.29a) below), Eq. (3.21) would yield the matrix elements in the singular representation. Only the first α or β (depending on which is smaller) diagonal elements ($m = n$) need be computed, which are the singular values, and all other elements are zero.

If the columns of the matrix $\mathbf{T}^L$ are the representation of the ψ^L-vectors (in the ϕ^L-representation) and the columns of the matrix $\mathbf{T}^R$ are the representation of the ψ^R-vectors (in the ϕ^R-representation) then the following is the singular value equation, Eq. (3.23), in matrix form, for all singular vectors,

$$(3.Ha) \qquad \mathbf{O}^{\phi\phi}\mathbf{T}^R = \mathbf{T}^L\mathbf{O}^{\psi\psi},$$

and can be found from a simple rearrangement of the matrix Eq. (3.F) using the matrix relations of Eqs. (3.Aa) and (3.Ab). In the above matrix equation, the diagonal elements of $\mathbf{O}^{\psi\psi}$ are the singular values.

Another singular value equation that can be written is the following,

$$\mathbf{O}^{\dagger}\hat{\psi}_n^L = \mu_n\hat{\psi}_n^R, \tag{3.25}$$

which has singular value μ_n. We shall show that this is consistent with Eq. (3.23) if the left and right singular vectors form orthogonal sets, and that the two sets of singular values (λ_n in Eq. (3.23) and μ_n in Eq. (3.25)) are real and identical.

Perform the inner product of $\hat{\psi}_n^L$ with Eq. (3.23), and take the adjoint of the result and do not yet assume that the singular vectors are orthogonal,

$$\hat{\psi}_m^{R\dagger}\mathbf{O}^{\dagger}\hat{\psi}_n^L = \lambda_m^*\hat{\psi}_m^{L\dagger}\hat{\psi}_n^L. \tag{3.26}$$

Perform the inner product of $\hat{\psi}_m^R$ with Eq. (3.25),

$$\hat{\psi}_m^{R\dagger}\mathbf{O}^{\dagger}\hat{\psi}_n^L = \mu_n\hat{\psi}_m^{R\dagger}\hat{\psi}_n^R. \tag{3.27}$$

The left-hand-sides of Eqs. (3.26) and (3.27) are identical. This yields,

$$\lambda_m^*\hat{\psi}_m^{L\dagger}\hat{\psi}_n^L = \mu_n\hat{\psi}_m^{R\dagger}\hat{\psi}_n^R. \tag{3.28}$$

The simultaneous properties of real and identical singular values ($\lambda_m^* = \mu_m$) and orthogonal singular vectors ($\hat{\psi}_m^{L\dagger}\hat{\psi}_n^L = \delta_{mn}$ and $\hat{\psi}_m^{R\dagger}\hat{\psi}_n^R = \delta_{mn}$) are consistent with Eq. (3.28). Note though that orthogonality is guaranteed only when $m, n \leqslant \gamma$ where γ is the *rank* of the matrix operator $\mathbf{O}^{\phi\phi}$ (or indeed in any other representation). γ has the general property that $\gamma \leqslant \min(\alpha, \beta)$ and can be found by counting the non-zero singular values. If a singular value is zero then Eq. (3.28) is satisfied without the need for the singular vectors to be orthogonal.

Equation (3.25) then has the following matrix equivalent for all singular vectors, which can be found from the matrix Eq. (3.Ha) using the matrix relations of Eqs. (3.Aa) and (3.Ab),

$$\boxed{(3.Hb) \qquad \mathbf{O}^{\phi\phi\dagger}\mathbf{T}^L = \mathbf{T}^R\mathbf{O}^{\psi\psi\dagger}.}$$

The left and right singular vectors, and the square of the singular values can be found from solving a couple of eigenvalue equations which can be formed by considering Eqs. (3.23) and (3.25) simultaneously (with $\lambda_m = \mu_m$),

$$\mathbf{O}^{\dagger}\mathbf{O}\hat{\psi}_m^R = \lambda_m^2\hat{\psi}_m^R, \tag{3.29a}$$

$$\mathbf{O}\mathbf{O}^{\dagger}\hat{\psi}_m^L = \lambda_m^2\hat{\psi}_m^L. \tag{3.29b}$$

In matrix form, the above eigenvalue equations can be written as,

$$\boxed{(3.Ia) \qquad \mathbf{O}^{\phi\phi\dagger}\mathbf{O}^{\phi\phi}\mathbf{T}^R = \mathbf{T}^R\mathbf{O}^{\psi\psi\dagger}\mathbf{O}^{\psi\psi},}$$

$$\boxed{(3.Ib) \qquad \mathbf{O}^{\phi\phi}\mathbf{O}^{\phi\phi\dagger}\mathbf{T}^L = \mathbf{T}^L\mathbf{O}^{\psi\psi}\mathbf{O}^{\psi\psi\dagger},}$$

which can be derived directly from Eqs. (3.Ha) and (3.Hb).

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