Representations Using Matrices *

When we begin discussing operators and integrals of operators operating on functions, the idea of representing these integrals in a matrix form emerges. If we have a set of basis functions, $\{\phi_1, \phi_2, \phi_3, \cdots\}$ and we attempt to expand a function in terms of these basis functions, in the form

$$\sum_n c_n \phi_n$$

where n runs over the size of the basis set, and c_n are constants (numbers), then it is convenient to treat these constants as vectors themselves, i.e., to form a row vector

$$\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ \vdots \end{pmatrix} \tag{1}$$

To express one of these basis vectors, one would write

$$\phi_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \tag{2}$$

while

$$\phi_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \tag{3}$$

etc..

A_{op} would have the form:

$$A_{op} = \begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} & a_{1,4} & a_{1,5} & \cdots \\ a_{2,1} & a_{2,2} & a_{2,3} & a_{2,4} & a_{2,5} & \cdots \\ a_{3,1} & a_{3,2} & a_{3,3} & a_{3,4} & a_{3,5} & \cdots \\ a_{4,1} & a_{4,2} & a_{4,3} & a_{4,4} & a_{4,5} & \cdots \\ a_{5,1} & a_{5,2} & a_{5,3} & a_{5,4} & a_{5,5} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \ddots \end{pmatrix}$$

where

$$a_{i,j} =< i|A_{op}|j >= \int \phi_i^* A_{op} \phi_j d\tau$$

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Then,

$$A_{op}| >= \begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} & a_{1,4} & a_{1,5} & \cdots \\ a_{2,1} & a_{2,2} & a_{2,3} & a_{2,4} & a_{2,5} & \cdots \\ a_{3,1} & a_{3,2} & a_{3,3} & a_{3,4} & a_{3,5} & \cdots \\ a_{4,1} & a_{4,2} & a_{4,3} & a_{4,4} & a_{4,5} & \cdots \\ a_{5,1} & a_{5,2} & a_{5,3} & a_{5,4} & a_{5,5} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \ddots \end{pmatrix} \otimes \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ \vdots \end{pmatrix} \tag{4}$$

which is often written as

$$A_{op}| >= \sum_{\ell=1}^{\ell=dim} a_{m,\ell} c_\ell \phi_\ell$$

(and we should point out that often, the summation sign (and limits) are discarded, under the rule that repeated indices are automatically to be summed. Also, the upper dimension could be "infinite"). This results in a column vector of the form

$$A_{op}| >= \begin{pmatrix} a_{1,1}c_1\phi_1 + a_{1,2}c_2\phi_2 + a_{1,3}c_3\phi_3 + \cdots \\ a_{2,1}c_1\phi_1 + a_{2,2}c_2\phi_2 + a_{2,3}c_3\phi_3 + \cdots \\ a_{3,1}c_1\phi_1 + a_{3,2}c_2\phi_2 + a_{3,3}c_3\phi_3 + \cdots \\ a_{4,1}c_1\phi_1 + a_{4,2}c_2\phi_2 + a_{4,3}c_3\phi_3 + a_{4,4}c_4\phi_4 \\ a_{5,1}c_1\phi_1 + a_{5,2}c_2\phi_2 + a_{5,3}c_3\phi_3 + a_{5,4}c_4\phi_4 \\ \vdots \end{pmatrix} \tag{5}$$

The convention is to associate a row vector with the complex conjugate transpose, i.e.,

$$\left(\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ \vdots \end{pmatrix}^T \right)^* \rightarrow (c_1^*, c_2^*, c_3^*, c_4^*, c_5^*, \cdots)$$

so that

$$\begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} & a_{1,4} & a_{1,5} & \cdots \\ a_{2,1} & a_{2,2} & a_{2,3} & a_{2,4} & a_{2,5} & \cdots \\ a_{3,1} & a_{3,2} & a_{3,3} & a_{3,4} & a_{3,5} & \cdots \\ a_{4,1} & a_{4,2} & a_{4,3} & a_{4,4} & a_{4,5} & \cdots \\ a_{5,1} & a_{5,2} & a_{5,3} & a_{5,4} & a_{5,5} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \ddots \end{pmatrix} = \int \left\{ (c_1^*, c_2^*, c_3^*, c_4^*, c_5^*, \cdots) \otimes A_{op} \otimes \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ \cdots \end{pmatrix} d\tau \right\}$$

where $< j|A_{op}|i >= a_{i,j}$. Notice that the functions ϕ_i are hidden from view, although they are still there, since integration (normally) would require us to know what these functions are, as well as the operator (A_{op} in an equivalent coördinate system.

We note that if the set $\{\phi_i\}$ have as members eigenfunctions of A_{op}, then this matrix becomes diagonal, since each element becomes

$$< j|A_{op}|i > \rightarrow < j|\alpha_i|i > \rightarrow \alpha_i \delta_{i,j}$$

where α_i is the i^{th} eigenvalue of A_{op} with eigenfunction $|i >$.