

FINITE VECTOR SPACES: MATRIX ELEMENTS

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education, sec 3.6.

An operator, such as the hamiltonian, can be expressed as matrix elements relative to a particular basis. We've looked at the case where the basis has an infinite number of dimensions. There are some quantum mechanical systems (for example, spin) where the dimension of the basis is finite. In such cases, we can find a finite set of eigenvectors (or eigenfunctions) and their corresponding eigenvalues.

Suppose for example that we have a system containing only two states. We can use any two linearly independent vectors as a basis for this system. For example, we might choose

$$|1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad (1)$$

$$|2\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad (2)$$

We could equally well have chosen:

$$|1'\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad (3)$$

$$|2'\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad (4)$$

where the $\frac{1}{\sqrt{2}}$ in front normalizes the vectors. There are, of course, an infinite number of other choices.

Now suppose we have a hamiltonian in this two-state system, and that its matrix elements relative to the first basis are

$$H = \begin{bmatrix} a & b \\ b & c \end{bmatrix} \quad (5)$$

for some constants a, b, c . Since H is hermitian, the only constraints on it are that the diagonal elements must be real, and $H_{mn} = H_{nm}^*$. In our example, we'll assume that all its elements are real, so the matrix as given must

be hermitian. (In the most general hamiltonian, the off-diagonal elements could be complex, with one the conjugate of the other.)

Relative to the first basis we have

$$\langle 1|H|1\rangle = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} a & b \\ b & c \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = a \quad (6)$$

and similarly for the other elements.

We could work out the components of H relative to the other basis by doing the multiplication:

$$\langle 1'|H|1'\rangle = \frac{1}{2} \begin{bmatrix} 1 & -1 \end{bmatrix} \begin{bmatrix} a & b \\ b & c \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1}{2}(a - 2b + c) \quad (7)$$

and so on.

In this system, the standard time-independent Schrödinger equation is

$$H|v\rangle = E|v\rangle \quad (8)$$

where $|v\rangle$ is a stationary state, which is just another vector. This is just an eigenvalue/eigenvector problem from elementary linear algebra.

However, in the general case, neither of the bases above consists of eigenvectors of H , so we can do the standard eigenvalue/eigenvector calculation to find them. To get the eigenvalues we calculate

$$\det \begin{bmatrix} a - E & b \\ b & c - E \end{bmatrix} = 0 \quad (9)$$

which has solutions

$$E = \frac{1}{2} \left[a + c \pm \sqrt{a^2 + 4b^2 + c^2 - 2ac} \right] \quad (10)$$

The corresponding eigenvectors are found by solving the linear equation

$$\begin{bmatrix} a & b \\ b & c \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = E \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \quad (11)$$

We get

$$\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \frac{2b}{c - a \pm \sqrt{a^2 + 4b^2 + c^2 - 2ac}} \\ 1 \end{bmatrix} \quad (12)$$

These vectors can be normalized, but it gets a bit messy.

For the special case of $a = c$, the situation simplifies a fair bit. We get

$$E = a \pm b \quad (13)$$

$$\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \pm 1 \\ 1 \end{bmatrix} \quad (14)$$

In this case, the eigenvectors, when normalized and with the sign reversed, *are* those of the second basis given above:

$$\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \pm 1 \end{bmatrix} \quad (15)$$

Now that we have the eigenvectors, we can analyze a system that starts out in any initial state we like. Suppose its initial state is

$$S(0) = \begin{bmatrix} g \\ h \end{bmatrix} \quad (16)$$

We need to express this in terms of the eigenvectors, so we get

$$S(0) = \frac{(g+h)}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \frac{(g-h)}{2} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad (17)$$

The general time dependent solution is then

$$S(t) = \frac{(g+h)}{2} e^{-i(a+b)t/\hbar} \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \frac{(g-h)}{2} e^{-i(a-b)t/\hbar} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad (18)$$

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