A guide to matrix representations

We start by considering, for definiteness, a three-dimensional vector space. We meet many of these in the course; the most obvious one is the space of ordinary 3-d position vectors, but it could be the set of second-order polynomials, or the space of functions $f(\theta, \phi)$ for which

$$-\hbar^2 \left(\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial f(\theta,\phi)}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2 f(\theta,\phi)}{\partial\phi^2} \right) = 2\hbar^2 f(\theta,\phi), \tag{1}$$

or the energy eigenstates of the 2-d harmonic oscillator with $E = 3\hbar\omega$, or of the 3-d harmonic oscillator with $E = \frac{5}{2}\hbar\omega$, or the symmetric states of two spin-$\frac{1}{2}$ particles, or the spin states of a Z^0 boson.... The first of these is a real vector space, the second could be real or complex but the rest are all complex. To avoid confusion with ordinary position vectors, and also with column vectors, we will call the members of the space "states", and denote them $|\psi\rangle$, where ψ is some convenient label which may take many forms.

The space we are discussing has an inner product between pairs of states. For position vectors it is the scalar product, for the two functions $f(\theta, \phi)$ and $g(\theta, \phi)$ it is $\int_0^{2\pi} \int_0^{\pi} f^*(\theta,\phi) g(\theta,\phi) \sin\theta \mathrm{d}\theta \mathrm{d}\phi$, for the energy eigenstates it is $\int \phi^*(\mathbf{r})\psi(\mathbf{r})\mathrm{d}^d\mathbf{r}$ (with $d = 2$ or 3), and so on. The inner product is denoted $\langle\phi|\psi\rangle$, where f, ψ, ϕ are all labels. $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$.

In our space, we choose three normalised basis state $\{|1\rangle, |2\rangle, |3\rangle\}$ which are orthogonal to one another: $\langle 1|1\rangle = \langle 2|2\rangle = \langle 3|3\rangle = 1$ and $\langle 1|2\rangle = \langle 2|3\rangle = \langle 1|3\rangle = 0$. (Again, 1, 2 and 3 are just labels; in position space they would be written as unit vectors $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$). Any state in the space can be written as a sum over these three basis states:

$$|\psi\rangle = v_1|1\rangle + v_2|2\rangle + v_3|3\rangle$$

and the list of numbers—**coefficients**— (v_1, v_2, v_3) defines the state. It isn't actually the state, but it fully specifies the state (given that we know the basis). We say that the number triplet is a **representation** of the state. Clearly $|1\rangle$ is represented by $(1, 0, 0)$, $|2\rangle$ by $(0, 1, 0)$ and $|3\rangle$ by $(0, 0, 1)$. Because of orthogonality, $v_1 = \langle 1|\psi\rangle$ etc.

Operators change states into other states. An operator is fully defined by what it does to the states of the basis, since then we can find what it does to any other state. And the state produced by the operator from, say, $|1\rangle$ can like any other state be written in terms of $\{|1\rangle, |2\rangle, |3\rangle\}$. So we might have

$$\hat{Q}|1\rangle = a|1\rangle + b|2\rangle + c|3\rangle, \qquad \hat{Q}|2\rangle = d|1\rangle + e|2\rangle + f|3\rangle, \qquad \hat{Q}|3\rangle = g|1\rangle + h|2\rangle + k|3\rangle$$

and hence

$$|\xi\rangle \equiv \hat{Q}|\psi\rangle = (av_1 + dv_2 + gv_3)|1\rangle + (bv_1 + ev_2 + hv_3)|2\rangle + (cv_1 + fv_2 + kv_3)|3\rangle$$

or equivalently, denoting these coeffients (w_1, w_2, w_3),

$$\begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} = \begin{pmatrix} a & d & g \\ b & e & h \\ c & f & k \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$$

The action of $\hat{Q}$ on any state $|\alpha\rangle$ can be found from the action of this matrix on the number triplet which represents $|\alpha\rangle$. So, in this basis, the matrix represents $\hat{Q}$.

If we want to pick out a particular element of the matrix, say the 2nd row, 3rd column, here denoted h, we see that it is the coefficient of $|2\rangle$ in $\hat{Q}|3\rangle$, or $\langle 2|\hat{Q}|3\rangle$. We usually write that element of a matrix $\mathbf{Q}$ as Q_{23}, so $Q_{ij} = \langle i|\hat{Q}|j\rangle$.

To recap, if we use the symbol $\underset{\{1,2,3\}}{\longrightarrow}$ to mean "is represented in the $\{|1\rangle,\ |2\rangle,\ |3\rangle\}$ basis by", we have

$$|\psi\rangle \underset{\{1,2,3\}}{\longrightarrow} \mathbf{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} \equiv \begin{pmatrix} \langle 1|\psi\rangle \\ \langle 2|\psi\rangle \\ \langle 3|\psi\rangle \end{pmatrix}; \qquad \hat{Q} \underset{\{1,2,3\}}{\longrightarrow} \mathbf{Q} = \begin{pmatrix} \langle 1|\hat{Q}|1\rangle & \langle 1|\hat{Q}|2\rangle & \langle 1|\hat{Q}|3\rangle \\ \langle 2|\hat{Q}|1\rangle & \langle 2|\hat{Q}|2\rangle & \langle 2|\hat{Q}|3\rangle \\ \langle 3|\hat{Q}|1\rangle & \langle 3|\hat{Q}|2\rangle & \langle 3|\hat{Q}|3\rangle \end{pmatrix}$$

and

$$|\xi\rangle = \hat{Q}|\psi\rangle \underset{\{1,2,3\}}{\longrightarrow} \mathbf{w} = \mathbf{Q}\mathbf{v}.$$

Often the basis has been chosen to be a set of eigenstates of some operator $\hat{R}$, in which case we use a shorter notation $\underset{R}{\longrightarrow}$ (but note that the order of the state matters for the actual form of the representation).

Now the states

$$|1'\rangle = \tfrac{1}{2}|1\rangle + \tfrac{i}{\sqrt{2}}|2\rangle - \tfrac{1}{2}|3\rangle, \quad |2'\rangle = \sqrt{\tfrac{1}{2}}(|1\rangle + |3\rangle), \quad |3'\rangle = \tfrac{1}{2}|1\rangle - \tfrac{i}{\sqrt{2}}|2\rangle - \tfrac{1}{2}|3\rangle$$

satisfy $\langle 1'|1'\rangle = \langle 2'|2'\rangle = \langle 3'|3'\rangle = 1$ and $\langle 1'|2'\rangle = \langle 1'|3'\rangle = \langle 2'|3'\rangle = 0$, so they are an equally good choice for a basis (in a complex space). But in this new basis, the column vectors and matrices which represent states and operators will be different. For instance $|\psi\rangle = v'_1|1'\rangle + v'_2|2'\rangle + v'_3|3'\rangle$ where

$$v_1 = \tfrac{1}{2}v'_1 + \sqrt{\tfrac{1}{2}}v'_2 + \tfrac{1}{2}v'_3, \quad v_2 = \tfrac{i}{\sqrt{2}}(v'_1 - v'_3), \quad v_3 = -\tfrac{1}{2}v'_1 + \sqrt{\tfrac{1}{2}}v'_2 - \tfrac{1}{2}v'_3$$

or

$$\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \sqrt{\frac{1}{2}} & \frac{1}{2} \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ -\frac{1}{2} & \sqrt{\frac{1}{2}} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} v'_1 \\ v'_2 \\ v'_3 \end{pmatrix}.$$

If we call the matrix $\mathbf{S}$, then we see that its columns are just the representations of the new states $\{|1'\rangle, |2'\rangle, |3'\rangle\}$ in the old basis $\{|1\rangle, |2\rangle, |3\rangle\}$: $\mathbf{S}_{23} = \langle 2|3'\rangle$ etc.

We can show that $\mathbf{S}$ is unitary, so $\mathbf{S}^{-1} = \mathbf{S}^\dagger$, and mutiplying the equation above by $\mathbf{S}^\dagger$ gives

$$\begin{pmatrix} v'_1 \\ v'_2 \\ v'_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & -\frac{i}{\sqrt{2}} & -\frac{1}{2} \\ \sqrt{\frac{1}{2}} & 0 & \sqrt{\frac{1}{2}} \\ \frac{1}{2} & \frac{i}{\sqrt{2}} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}.$$

So

$$\mathbf{v}' = \mathbf{S}^\dagger\mathbf{v}, \qquad \text{and} \quad \mathbf{v} = \mathbf{S}\mathbf{v}'$$

If in the new basis, $\xi = w'_1|1'\rangle + w'_2|2'\rangle + w'_3|3'\rangle$,

$$\mathbf{w}' = \mathbf{S}^\dagger\mathbf{w} = \mathbf{S}^\dagger\mathbf{Q}\mathbf{v} = \mathbf{S}^\dagger\mathbf{Q}\mathbf{S}\mathbf{S}^\dagger\mathbf{v} = \mathbf{Q}'\mathbf{v}',$$

where in the last-but-one step we inserted the identity matrix $\mathbf{I} = \mathbf{S}\mathbf{S}^\dagger$. So in the new basis, the representation of $\hat{Q}$ is $\mathbf{Q}' = \mathbf{S}^\dagger\mathbf{Q}\mathbf{S}$.

We chose a particular set of new states here, but it should be clear that *any* unitary matrix $\mathbf{S}$ corresponds to a change to some new basis. (If the space is real, we are restricted to real unitary matrices, also called orthogonal matrices.) Since the eigenstates of a Hermitian operator $\hat{A}$ are always orthogonal, so are the eigenvectors of its representation $\mathbf{A}$ in some basis. We can construct a matrix $\mathbf{S}$ whose columns are these (normalised) eigenvectors, and this effects a change of basis to one in which $\mathbf{A}'$ is diagonal. The representation of states and operators in this basis would be denoted by $\xrightarrow[A]{}$. Here $\mathbf{S}$ is *not* the representation of an operator, but a way of obtaining representations of the *same* states and operators in *different* representations.

A concrete example is given by the space of solutions to Eq.(1), in which the differential operator is in fact $\hat{\mathbf{L}}^2$. The basis we use most often is the set of three states which are also eigenstates of $\hat{L}_z$, $-i\hbar\partial/\partial\phi$; these are the three $l = 1$ spherical harmonics with $m = \{1, 0, -1\}$. If we use these as our initial basis, the second basis we considered consists of the eigenstates of $\hat{L}_y$. Then we can explicitly construct representations of the operators in the L_y basis, given those in the initial ($\hat{L}_z$) basis:

$$\hat{L}_z \xrightarrow[L_z]{} \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad \hat{L}_x \xrightarrow[L_z]{} \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad \hat{L}_y \xrightarrow[L_z]{} \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

$$\hat{L}_z \xrightarrow[L_y]{} \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad \hat{L}_x \xrightarrow[L_y]{} \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad \hat{L}_y \xrightarrow[L_y]{} \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Clearly since the first set of matrices satisfy the required commutation relations, $[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$ and cyclic permutations thereof, so do the second set.

When we are discussing spaces of (restricted sets of) functions, such as solutions of Eq.(1), or degenerate states of the 2 or 3-dimensional harmonic oscillator, the distinction between the states and their representations is not too hard to keep in mind: any number triplet (v_1, v_2, v_3) represents a linear combination of basis functions and hence another function. In more abstract spaces like spin space, though, the distinction is perhaps harder to keep in mind, because we don't have a representation-independent mathematical description of the states, only words like "spin-up along the z axis". However at another level the functions themselves become just another representation (or "realisation") of the abstract vector space: the differential operators and spherical harmonics are a realisation of the abstract angular momentum algebra. So we can write

$$|l{=}1, m{=}1\rangle \xrightarrow[L_z]{} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad \xrightarrow[L_y]{} \begin{pmatrix} 1/2 \\ 1/\sqrt{2} \\ 1/2 \end{pmatrix}$$
$$\xrightarrow[x]{} \langle \mathbf{r}|l{=}1, m{=}1\rangle = Y_1^1(\theta, \phi)$$

where $\xrightarrow[x]{}$ or $\xrightarrow[\mathbf{r}]{}$ means "is represented in the position basis by".

Two symbols are typically used for the matrix which changes the representation, $\mathbf{S}$ and $\mathbf{U}$ (one stands for "similarity transform", which reflects the "similarity" of all relations between vectors and operators in the two bases, the other for "unitary". Unfortunately both $\hat{U}(t)$ and $\hat{\mathbf{S}}$ have special meanings, so we should have been more imaginative!