What *Can* the Answer be?

2. Reciprocal Basis and Dual Vectors

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We usually express vectors as a sum of *basis vectors* which are mutually perpendicular and of unit length. In some situations, such as the description of crystals, it is necessary to use basis vectors which have any length and any angle between them. Solving for the coefficients in such an expansion introduces the concept of *reciprocal vectors* or *dual vectors*. They are the natural language to use in describing phenomena periodic in space, such as waves and crystal lattices. Generalisation of this concept to infinite dimensions leads to Dirac's notation for quantum states.

At the end of Part I of this series I stated that concepts such as reciprocal basis vectors, dual spaces and co-vectors could be motivated from simple considerations starting from well-known identities in elementary vector analysis.

Let us begin with the resolution of an ordinary vector $\mathbf{v}$ in three-dimensional (Euclidean) space according to

$$\mathbf{v} = \mathbf{i}\, v_x + \mathbf{j}\, v_y + \mathbf{k}\, v_z \ . \qquad (1)$$

What are v_x, v_y and v_z in terms of $\mathbf{v}$? Clearly, $v_x = \mathbf{i} \cdot \mathbf{v}, v_y = \mathbf{j} \cdot \mathbf{v}$, $v_z = \mathbf{k} \cdot \mathbf{v}$. Therefore, if we introduce the *projection operator* $P_x = \mathbf{ii}$ (no dot or cross in between the two vectors!), and 'operate' with it on the arbitrary vector $\mathbf{v}$ by taking the dot product, the result $\mathbf{ii} \cdot \mathbf{v}$ is defined to be precisely $\mathbf{i}(\mathbf{i} \cdot \mathbf{v}) = \mathbf{i}\, v_x$, the component or part of $\mathbf{v}$ that lies along the unit vector $\mathbf{i}$. Similarly, we have projection operators $P_y = \mathbf{jj}$ and $P_z = \mathbf{kk}$. The *unit operator* (the operator that leaves any vector $\mathbf{v}$ unchanged) is evidently just the sum of *all* the projection operators, namely,

$$\mathbf{I} = P_x + P_y + P_z = \mathbf{ii} + \mathbf{jj} + \mathbf{kk}. \quad (2)$$

Thus Eq. (1) expresses the fact that

$$\mathbf{v} = \mathbf{I} \cdot \mathbf{v} = \mathbf{i}(\mathbf{i} \cdot \mathbf{v}) + \mathbf{j}(\mathbf{j} \cdot \mathbf{v}) + \mathbf{k}(\mathbf{k} \cdot \mathbf{v}). \quad (3)$$

We now ask the question: what is the counterpart of Eq. (3) in the case of *oblique axes* defined by three arbitrary, non-coplanar vectors **a**, **b** and **c** (*Figure 1*), instead of the rectangular axes defined by **i**, **j** and **k**?

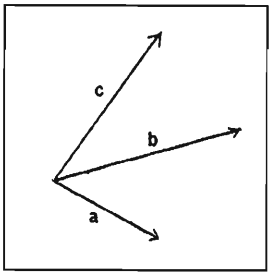

Figure 1 Oblique axes defined by a set of three arbitrary non-coplanar vectors a, b and c.

Once again, we can arrive at a solution by asking what the answer *can possibly be*. Writing

$$\mathbf{v} = \alpha\,\mathbf{a} + \beta\mathbf{b} + \gamma\mathbf{c}, \quad (4)$$

we observe that the coefficient α cannot involve any overlap[1] of **v** with either **b** or **c**; β cannot involve any overlap of **v** with either **c** or **a**; and γ cannot involve any overlap of **v** with either **a** or **b**. Therefore α *must* be proportional to that part of **v** which lies along $(\mathbf{b} \times \mathbf{c})$, i.e., to $[(\mathbf{b} \times \mathbf{c}) \cdot \mathbf{v}]$. Similar conclusions hold good for β and γ. Hence

$$\mathbf{v} = \lambda\,\mathbf{a}\,[(\mathbf{b} \times \mathbf{c}) \cdot \mathbf{v}] + \mu\mathbf{b}\,[(\mathbf{c} \times \mathbf{a}) \cdot \mathbf{v}] + \nu\mathbf{c}\,[(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{v}], \quad (5)$$

where the scalar factors λ, μ and ν are yet to be determined. The equivalence of all directions in space (the *isotropy of space*) suggests that λ, μ and ν must be equal to each other. This is easily borne out by setting $\mathbf{v} = \mathbf{a}, \mathbf{b}$ and **c** in turn. We find immediately that $\lambda = \mu = \nu = 1/[(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c}]$. [Here we have used the cyclic symmetry of the scalar triple product, namely, $(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c} = (\mathbf{b} \times \mathbf{c}) \cdot \mathbf{a} = (\mathbf{c} \times \mathbf{a}) \cdot \mathbf{b}$.] Therefore

$$\mathbf{v} = \frac{\mathbf{a}[(\mathbf{b} \times \mathbf{c}) \cdot \mathbf{v}] + \mathbf{b}\,[(\mathbf{c} \times \mathbf{a}) \cdot \mathbf{v}] + \mathbf{c}\,[(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{v}]}{[(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c}]}. \quad (6)$$

[1] Overlap here means 'dot product' (also called 'scalar product' or 'inner product'). This step in the argument can be understood in more detail as follows. Let us keep α fixed and vary β and γ. The vector **v** then varies over a plane parallel to the b-c. plane. All vectors in this plane have the same value of α, but their projections on the b-c plane vary, so α cannot depend on those. It can only depend on the projection onto a vector normal to the b-c plane, that is, $\mathbf{b} \times \mathbf{c}$.

In three dimensional space, no more than three vectors of a given set of vectors can be linearly independent.

There is another, equally instructive, way to arrive at Eq. (6). We begin with the well-known vector identity

$$\mathbf{u} \times (\mathbf{b} \times \mathbf{c}) = \mathbf{b}(\mathbf{u} \cdot \mathbf{c}) - \mathbf{c}\,(\mathbf{u} \cdot \mathbf{b}). \qquad (7)$$

(A proof of Eq. (7) based on general arguments was given in Part I.) Now suppose $\mathbf{u}$ is itself of the form $\mathbf{u} = \mathbf{v} \times \mathbf{a}$. Substitution in Eq. (7) gives

$$(\mathbf{v} \times \mathbf{a}) \times (\mathbf{b} \times \mathbf{c}) = \mathbf{b}\,[(\mathbf{v} \times \mathbf{a}) \cdot \mathbf{c}] - \mathbf{c}[(\mathbf{v} \times \mathbf{a}) \cdot \mathbf{b}]. \qquad (8)$$

The vector representing the quadruple cross product on the left-hand side is thus a linear combination of the vectors $\mathbf{b}$ and $\mathbf{c}$. It therefore lies in the plane formed by these two vectors. However, we could as well have written $\mathbf{b} \times \mathbf{c} = \mathbf{d}$, in which case

$$\begin{aligned}(\mathbf{v} \times \mathbf{a}) \times (\mathbf{b} \times \mathbf{c}) &= (\mathbf{v} \times \mathbf{a}) \times \mathbf{d} \\ &= \mathbf{a}\,(\mathbf{v} \cdot \mathbf{d}) - \mathbf{v}\,(\mathbf{a} \cdot \mathbf{d}) \\ &= \mathbf{a}\,[\mathbf{v} \cdot (\mathbf{b} \times \mathbf{c})] - \mathbf{v}\,[\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})]. \qquad (9)\end{aligned}$$

The *same* vector is therefore a linear combination of the two vectors $\mathbf{a}$ and $\mathbf{v}$, and thus lies in the plane formed by them. As the four vectors $\mathbf{v}$, $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ may be chosen quite arbitrarily, this appears to be paradoxical. However, we must now recall that these are vectors in three-dimensional space, *in which no more than three vectors of a given set of vectors can be linearly independent*, i.e., non-coplanar. In other words, if the vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ are a linearly independent set, the fourth vector $\mathbf{v}$ *must* be expressible as a linear combination of these, precisely by equating the expressions found in Eqs. (8) and (9) and solving for $\mathbf{v}$. The result, after once again using the cyclic symmetry of the scalar triple product and some rearrangement, is precisely Eq. (6). This is the counterpart of the resolution in Eq. (3) of an arbitrary vector $\mathbf{v}$ along orthogonal axes. The answer to our problem of resolving a vector $\mathbf{v}$ in an arbitrary basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is thus

$$\mathbf{v} = \mathbf{a}\,(\mathbf{A}\cdot\mathbf{v}) + \mathbf{b}\,(\mathbf{B}\cdot\mathbf{v}) + \mathbf{c}\,(\mathbf{C}\cdot\mathbf{v}), \qquad (10)$$

where

$$\mathbf{A} = \frac{\mathbf{b}\times\mathbf{c}}{V},\ \mathbf{B} = \frac{\mathbf{c}\times\mathbf{a}}{V},\ \mathbf{C} = \frac{\mathbf{a}\times\mathbf{b}}{V}\quad , \qquad (11)$$

with $V = (\mathbf{a}\times\mathbf{b})\cdot\mathbf{c}$. The notation V arises from the fact that the modulus of $(\mathbf{a}\times\mathbf{b})\cdot\mathbf{c}$ is the volume of the parallelopiped formed by the vectors **a**, **b** and **c**. The vectors **A**, **B** and **C** form the so-called *reciprocal basis*. The terminology is most familiar in crystallography: if **a**, **b**, **c** are the primitive basis vectors of a lattice, **A**, **B**, **C** are the basis vectors of the 'reciprocal' lattice. It is immediately verified that

$$\mathbf{A}\cdot\mathbf{a} = \mathbf{B}\cdot\mathbf{b} = \mathbf{C}\cdot\mathbf{c} = 1, \qquad (12)$$

which helps explain why the term 'reciprocal basis' is used; also,

$$\mathbf{A}\cdot\mathbf{b} = \mathbf{A}\cdot\mathbf{c} = \mathbf{B}\cdot\mathbf{a} = \mathbf{B}\cdot\mathbf{c} = \mathbf{C}\cdot\mathbf{a} = \mathbf{C}\cdot\mathbf{b} = 0. \qquad (13)$$

In fact, the reciprocal basis is *defined* in books on crystallography by Eqs. (12) and (13); the solutions are just the vectors in (11). It is easy to check that the general formula of Eq. (10) reduces to Eq. (3) in the special case of an orthogonal basis.

In what space do the reciprocal basis vectors (**A**, **B**, **C**) 'live'? If the original basis vectors (**a**, **b**, **c**) have the physical dimensions of length, Eqs. (11) show that (**A**, **B**, **C**) have the physical dimensions of $(\text{length})^{-1}$. In crystallography and solid state physics this fact is used to define a 'reciprocal lattice' in wavenumber space, in which (**A**, **B**, **C**) are the primitive lattice vectors. Why does one do this? It is not my intention to go into crystal physics here, but two good reasons (among several others) may be cited. In crystal physics, we have to deal very frequently with periodic functions, i.e., functions that satisfy $f(\mathbf{r}) = f(\mathbf{r}+\mathbf{R})$ where **R** is any lattice vector $m\mathbf{a} + n\mathbf{b} + p\mathbf{c}$, and where m, n and p take on

integer values. Such a function can be expanded in a Fourier series of the form

$$f(\mathbf{r}) = \sum_{\mathbf{G}} f_{\mathbf{G}} \exp(i\mathbf{G} \cdot \mathbf{r}). \tag{14}$$

The summation over $\mathbf{G}$ runs over *precisely the vectors of the reciprocal lattice*, i.e., $\mathbf{G} = h\mathbf{A} + k\mathbf{B} + l\mathbf{C}$, where (h, k, l) are integers. The second noteworthy point is that the Bragg condition for diffraction (of X-rays, electrons, neutrons, etc.) from a crystal is expressible in a very simple form in terms of $\mathbf{G}$, namely, $2\mathbf{k} \cdot \mathbf{G} = \mathbf{G}^2$ (where $\mathbf{k}$ is the wave vector of the incident beam). Likewise, the Laue conditions for diffraction maxima reduce to just $\mathbf{G} \cdot \mathbf{a} = h$, $\mathbf{G} \cdot \mathbf{b} = k$, $\mathbf{G} \cdot \mathbf{c} = l$ (which follow directly from Eqs. (12) and (13) and the definition of $\mathbf{G}$).

We are now at a point where the concepts of *ket* and *bra vectors* can be introduced naturally. Going back to Eq. (1), we note the following. Any vector $\mathbf{v}$ can be represented in the form of a *column matrix* according to

$$\mathbf{v} = \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} v_x + \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} v_y + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} v_z \tag{15}$$

(Here and in what follows, we shall freely use the '=' symbol between an abstract quantity and its *representation* in any form.) To save space, let us write $(1\ 0\ 0)^T$ for the column matrix $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$. T stands for 'transpose'. In this way of representing vectors, therefore,

$$\mathbf{i} = (1\ 0\ 0)^T,\ \mathbf{j} = (0\ 1\ 0)^T,\ \mathbf{k} = (0\ 0\ 1)^T. \tag{16}$$

We could also identify these with unit ket vectors denoted by $|e_1\rangle$, $|e_2\rangle$ and $|e_3\rangle$ respectively. Operating on a general vector $\mathbf{v} = (v_x, v_y, v_z)^T$, the projection operator P_x = **ii** introduced below Eq. (1) must yield the component $\mathbf{i}\, v_x = (v_x\ 0\ 0)^T$. This is achieved if we identify P_x with the 3×3 *matrix* $(1\ 0\ 0)^T$ $(1\ 0\ 0)$. In other words, the **i** on the left in **ii** really stands for the column vector $(1\ 0\ 0)^T$ or the ket vector $|e_1\rangle$, while the **i** on the right stands for the row vector $(1\ 0\ 0)$ – it is now natural to identify it with the bra vector $\langle e_1|$. The operator P_x is therefore $|e_1\rangle\langle e_1|$; similarly, $P_y = |e_2\rangle\langle e_2|$ and $P_z = |e_3\rangle\langle e_3|$. The 'resolution of the identity', Eq. (2), reads

$$|e_1\rangle\langle e_1| + |e_2\rangle\langle e_2| + |e_3\rangle\langle e_3| = \mathbf{I}. \qquad (17)$$

The component v_x, which we saw was simply the scalar or dot product $\mathbf{i}\cdot\mathbf{v}$, is now written as the 'inner product' $\langle e_1|\,\langle \mathrm{v}\rangle$ where we have used the ket vector $|\mathrm{v}\rangle$ to denote the vector $\mathbf{v} = (v_x, v_y, v_z)^T$. We can then go on to generalize this idea of ket vectors and their "adjoint bra vectors" to n-dimensional Euclidean spaces, and then to infinite-dimensional Hilbert spaces. The whole treatment provides an admittedly heuristic, but easily digested, method of introducing the machinery of linear vector spaces (e.g., for quantum mechanics) to students of physics whose background in this regard comprises little more than some familiarity with elementary matrix analysis — the situation most commonly encountered.

Let us now translate our findings for oblique axes to this language of ket and bra vectors. Writing **a**, **b** and **c** as the ket vectors $|a\rangle$, $|b\rangle$ and $|c\rangle$ respectively, Eq. (12) suggests at once that the reciprocal basis vectors **A**, **B** and **C** are in fact to be identified with bra vectors $\langle A|$, $\langle B|$ and $\langle C|$. Equation (12) is the statement that the corresponding inner products are normalized to unity, i.e.,

$$\langle A|a\rangle = \langle B|b\rangle = \langle C|c\rangle = 1. \qquad (18)$$

In crystallography, however, the structure of the lattice may force us to stick to the non-orthogonal basis as the natural and more useful one, supplemented by the reciprocal basis.

The expansion of an arbitrary vector **v** in Eq. (10) reads, in this language,

$$|v\rangle = (\langle A|v\rangle)|a\rangle + (\langle B|v\rangle)|b\rangle + (\langle C|v\rangle)|c\rangle. \qquad (19)$$

In other words, the resolution of the identity given by Eq. (17) for orthogonal coordinates is now replaced by

$$|a\rangle\langle A| + |b\rangle\langle B| + |c\rangle\langle C| = \mathbf{I}. \qquad (20)$$

The space spanned by the reciprocal basis vectors **A**, **B** and **C** (more generally, by bra vectors) may be regarded as a kind of *dual* of the original space spanned by the vectors **a**, **b** and **c**. [This statement is a bit loose and glosses over certain technical details, but is quite acceptable at the present level of rigour.] It turns out that we can prove that the dual space is actually *isomorphic* to the original space, provided the latter is finite-dimensional (in our case, it is three dimensional). 'Isomorphic to' does not mean 'identical with', of course, but it does mean that the properties of the two spaces are essentially the same. This isomorphism between a linear vector space and its dual space *may* sometimes be valid even for infinite-dimensional spaces. A common but nontrivial example in physics occurs in elementary quantum mechanics: the position space wavefunction of a particle moving in one spatial dimension is a member of the linear vector space of square-integrable functions (of one real variable $x \in \mathbf{R}$). Its Fourier transform has a physical interpretation as the corresponding wavefunction in momentum space. This is also square-integrable, and is a member of an *isomorphic* vector space of square-integrable functions (of one real variable, $p \in \mathbf{R}$).

We have seen how 'reciprocal' vectors (in a 'dual' vector space) arise naturally if we work with an oblique set of axes. The distinction between the original space and the dual space exists in any case, but it may be blurred in the case of an orthogonal basis set like (**i**, **j**, **k**) in a real vector space because the reciprocal

basis appears to coincide with the original basis. When faced with a non-orthogonal basis set, the usual practice in quantum mechanics is to construct an orthogonal basis by, say, the Gram-Schmidt procedure. In crystallography, however, the structure of the lattice may force us to stick to the non-orthogonal basis as the natural and more useful one, supplemented, as we have seen, by the reciprocal basis. It must be remembered that we have been working in three-dimensional Euclidean space for the greater part. What if the number of dimensions we have to deal with is not equal to three? (For one thing, the 'cross product' of two vectors is a vector only in three dimensions!) What if the space itself is curved? Do vectors and reciprocal vectors (or *bra* vectors), living in the dual vector space, have anything to do with the distinction between *contravariant* and *covariant* vectors, (or 'upstairs' and 'downstairs' indices), *tangent* and *cotangent* spaces, and maybe even the Lagrangian and Hamiltonian formalisms in classical mechanics? The answer is 'yes', implying that some profound aspects of the physical world are lurking behind the simple geometrical questions we have been discussing. We shall touch upon these matters in the next part of this series.

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65	64	63	62	61	60	59	58	57	90
66	37	36	35	34	33	32	31	56	89
67	38	17	16	15	14	13	30	55	88
68	39	18	5	4	3	12	29	54	87
69	40	19	6	1	2	11	28	53	86
70	41	20	7	8	9	10	27	52	85
71	42	21	22	23	24	25	26	51	84
72	43	44	45	46	47	48	49	50	83
73	74	75	76	77	78	79	80	81	82

Prime numbers occur along the diagonals in a square spiral arrangement of consecutive integers — Discovered by Stanislaw Ulam in 1963.