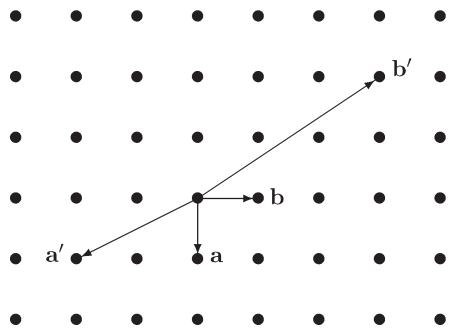


1.3. GENERAL INTRODUCTION TO SPACE GROUPS



**Figure 1.3.2.1**  
Conventional basis  $\mathbf{a}$ ,  $\mathbf{b}$  and a non-conventional basis  $\mathbf{a}'$ ,  $\mathbf{b}'$  for the square lattice.

*Example*

The square lattice

$$\mathbf{L} = \mathbb{Z}^2 = \left\{ \begin{pmatrix} m \\ n \end{pmatrix} \mid m, n \in \mathbb{Z} \right\}$$

in  $\mathbb{V}^2$  has the vectors

$$\mathbf{a} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

as its standard lattice basis. But

$$\mathbf{a}' = \begin{pmatrix} 1 \\ -2 \end{pmatrix}, \quad \mathbf{b}' = \begin{pmatrix} -2 \\ 3 \end{pmatrix}$$

is also a lattice basis of  $\mathbf{L}$ : on the one hand  $\mathbf{a}'$  and  $\mathbf{b}'$  are integral linear combinations of  $\mathbf{a}$ ,  $\mathbf{b}$  and are thus contained in  $\mathbf{L}$ . On the other hand

$$-3\mathbf{a}' - 2\mathbf{b}' = \begin{pmatrix} -3 \\ 6 \end{pmatrix} + \begin{pmatrix} 4 \\ -6 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \mathbf{a}$$

and

$$-2\mathbf{a}' - \mathbf{b}' = \begin{pmatrix} -2 \\ 4 \end{pmatrix} + \begin{pmatrix} 2 \\ -3 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \mathbf{b},$$

hence  $\mathbf{a}$  and  $\mathbf{b}$  are also integral linear combinations of  $\mathbf{a}'$ ,  $\mathbf{b}'$  and thus the two bases  $\mathbf{a}$ ,  $\mathbf{b}$  and  $\mathbf{a}'$ ,  $\mathbf{b}'$  both span the same lattice (see Fig. 1.3.2.1).

The example indicates how the different lattice bases of a lattice  $\mathbf{L}$  can be described. Recall that for a vector  $\mathbf{v} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$  the coefficients  $x$ ,  $y$ ,  $z$  are called the *coordinates* and

the vector  $\begin{pmatrix} x \\ y \\ z \end{pmatrix}$  is called the *coordinate column* of  $\mathbf{v}$  with respect

to the basis  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$ . The coordinate columns of the vectors in  $\mathbf{L}$  with respect to a lattice basis are therefore simply columns with three integral components. In particular, if we take a second lattice basis  $\mathbf{a}'$ ,  $\mathbf{b}'$ ,  $\mathbf{c}'$  of  $\mathbf{L}$ , then the coordinate columns of  $\mathbf{a}'$ ,  $\mathbf{b}'$ ,  $\mathbf{c}'$  with respect to the first basis are columns of integers and thus the basis transformation  $\mathbf{P}$  such that  $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\mathbf{P}$  is an integral  $3 \times 3$  matrix. But if we interchange the roles of the two bases, they are related by the inverse transformation  $\mathbf{P}^{-1}$ , i.e.  $(\mathbf{a}, \mathbf{b}, \mathbf{c}) = (\mathbf{a}', \mathbf{b}', \mathbf{c}')\mathbf{P}^{-1}$ , and the argument given above asserts that  $\mathbf{P}^{-1}$  is also an integral matrix. Now, on the one hand  $\det \mathbf{P}$  and  $\det \mathbf{P}^{-1}$  are both integers (being determinants of integral matrices), on the other hand  $\det \mathbf{P}^{-1} = 1/\det \mathbf{P}$ . This is only possible if  $\det \mathbf{P} = \pm 1$ .

Summarizing, the different lattice bases of a lattice  $\mathbf{L}$  are obtained by transforming a single lattice basis  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$  with integral transformation matrices  $\mathbf{P}$  such that  $\det \mathbf{P} = \pm 1$ .

**1.3.2.2. Metric properties**

In the three-dimensional vector space  $\mathbb{V}^3$ , the *norm* or *length* of

a vector  $\mathbf{v} = \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix}$  is (due to Pythagoras' theorem) given by

$$|\mathbf{v}| = \sqrt{v_x^2 + v_y^2 + v_z^2}.$$

From this, the *scalar product*

$$\mathbf{v} \cdot \mathbf{w} = v_x w_x + v_y w_y + v_z w_z \text{ for } \mathbf{v} = \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix}, \mathbf{w} = \begin{pmatrix} w_x \\ w_y \\ w_z \end{pmatrix}$$

is derived, which allows one to express angles by

$$\cos \angle(\mathbf{v}, \mathbf{w}) = \frac{\mathbf{v} \cdot \mathbf{w}}{|\mathbf{v}| |\mathbf{w}|}.$$

The definition of a norm function for the vectors turns  $\mathbb{V}^3$  into a *Euclidean space*. A lattice  $\mathbf{L}$  that is contained in  $\mathbb{V}^3$  inherits the metric properties of this space. But for the lattice, these properties are most conveniently expressed with respect to a lattice basis. It is customary to choose basis vectors  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$  which define a right-handed coordinate system, i.e. such that the matrix with columns  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$  has a positive determinant.

*Definition*

For a lattice  $\mathbf{L} \subseteq \mathbb{V}^3$  with lattice basis  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$  the *metric tensor* of  $\mathbf{L}$  is the  $3 \times 3$  matrix

$$\mathbf{G} = \begin{pmatrix} \mathbf{a} \cdot \mathbf{a} & \mathbf{a} \cdot \mathbf{b} & \mathbf{a} \cdot \mathbf{c} \\ \mathbf{b} \cdot \mathbf{a} & \mathbf{b} \cdot \mathbf{b} & \mathbf{b} \cdot \mathbf{c} \\ \mathbf{c} \cdot \mathbf{a} & \mathbf{c} \cdot \mathbf{b} & \mathbf{c} \cdot \mathbf{c} \end{pmatrix}.$$

If  $\mathbf{A}$  is the  $3 \times 3$  matrix with the vectors  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$  as its columns, then the metric tensor is obtained as the matrix product  $\mathbf{G} = \mathbf{A}^T \cdot \mathbf{A}$ . It follows immediately that the metric tensor is a symmetric matrix, i.e.  $\mathbf{G}^T = \mathbf{G}$ .

*Example*

Let

$$\mathbf{a} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{c} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

be the basis of a lattice  $\mathbf{L}$ . Then the metric tensor of  $\mathbf{L}$  (with respect to the given basis) is

$$\mathbf{G} = \begin{pmatrix} 3 & 2 & 0 \\ 2 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

With the help of the metric tensor the scalar products of arbitrary vectors, given as linear combinations of the lattice basis, can be computed from their coordinate columns as follows: If  $\mathbf{v} = x_1\mathbf{a} + y_1\mathbf{b} + z_1\mathbf{c}$  and  $\mathbf{w} = x_2\mathbf{a} + y_2\mathbf{b} + z_2\mathbf{c}$ , then