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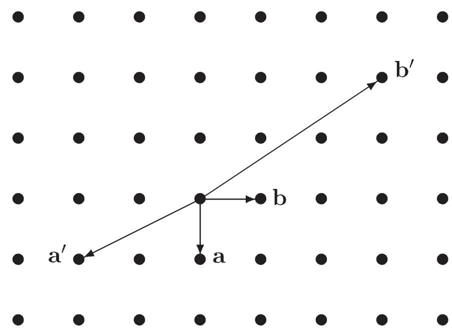


Figure 1.3.2.1
Conventional basis **a**, **b** and a non-conventional basis **a**′, **b**′ for the square lattice.

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 **L**: on the one hand **a**′ and **b**′ are integral linear combinations of **a**, **b** and are thus contained in **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 **a** and **b** are also integral linear combinations of **a**′, **b**′ and thus the two bases **a**, **b** and **a**′, **b**′ both span the same lattice (see Fig. 1.3.2.1).

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

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

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 **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 **a**, **b**, **c** which define a right-handed coordinate system, *i.e.* such that the matrix with columns **a**, **b**, **c** has a positive determinant.

Definition

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

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

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

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 **L**. Then the metric tensor of **L** (with respect to the given basis) is

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

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

$$\mathbf{v} \cdot \mathbf{w} = (x_1\, y_1\, z_1) \cdot \boldsymbol{G} \cdot \begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix}.$$

From this it follows how the metric tensor transforms under a basis transformation $\boldsymbol{P}$. If $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}$, then the metric tensor $\boldsymbol{G}'$ of $\mathbf{L}$ with respect to the new basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ is given by

$$\boldsymbol{G}' = \boldsymbol{P}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{P}.$$

An alternative way to specify the geometry of a lattice in $\mathbb{V}^3$ is using the *cell parameters*, which are the lengths of the lattice basis vectors and the angles between them.

Definition

For a lattice $\mathbf{L}$ in $\mathbb{V}^3$ with lattice basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ the *cell parameters* (also called *lattice parameters*, *lattice constants* or *metric parameters*) are given by the lengths

$$a = |\mathbf{a}| = \sqrt{\mathbf{a} \cdot \mathbf{a}}, \quad b = |\mathbf{b}| = \sqrt{\mathbf{b} \cdot \mathbf{b}}, \quad c = |\mathbf{c}| = \sqrt{\mathbf{c} \cdot \mathbf{c}}$$

of the basis vectors and by the interaxial angles

$$\alpha = \angle(\mathbf{b}, \mathbf{c}), \quad \beta = \angle(\mathbf{c}, \mathbf{a}), \quad \gamma = \angle(\mathbf{a}, \mathbf{b}).$$

Owing to the relation $\mathbf{v} \cdot \mathbf{w} = |\mathbf{v}|\,|\mathbf{w}| \cos \angle(\mathbf{v}, \mathbf{w})$ for the scalar product of two vectors, one can immediately write down the metric tensor in terms of the cell parameters:

$$\boldsymbol{G} = \begin{pmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ac\cos\beta & bc\cos\alpha & c^2 \end{pmatrix}.$$

1.3.2.3. Unit cells

A lattice $\mathbf{L}$ can be used to subdivide $\mathbb{V}^3$ into cells of finite volume which all have the same shape. The idea is to define a suitable subset $\mathbf{C}$ of $\mathbb{V}^3$ such that the translates of $\mathbf{C}$ by the vectors in $\mathbf{L}$ cover $\mathbb{V}^3$ without overlapping. Such a subset $\mathbf{C}$ is called a *unit cell* of $\mathbf{L}$, or, in the more mathematically inclined literature, a *fundamental domain* of $\mathbb{V}^3$ with respect to $\mathbf{L}$. Two standard constructions for such unit cells are the *primitive unit cell* and the *Voronoï domain* (which is also known by many other names).

Definition

Let $\mathbf{L}$ be a lattice in $\mathbb{V}^3$ with lattice basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$.

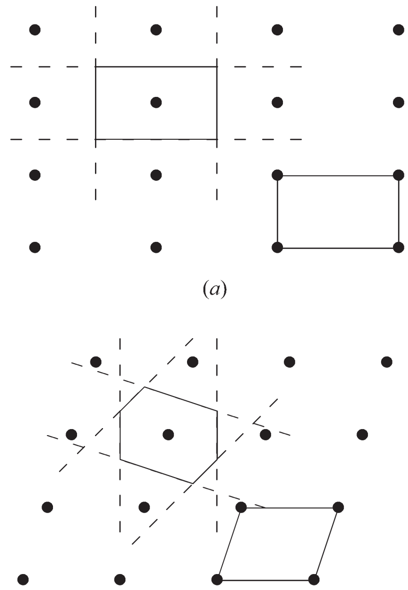
(i) The set $\mathbf{C} := \{x\mathbf{a} + y\mathbf{b} + z\mathbf{c} \mid 0 \le x, y, z < 1\}$ is called the *primitive unit cell* of $\mathbf{L}$ with respect to the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$. The primitive unit cell is the parallelepiped spanned by the vectors of the given basis.

(ii) The set $\mathbf{C} := \{\mathbf{w} \in \mathbb{V}^3 \mid |\mathbf{w}| \le |\mathbf{w} - \mathbf{v}| \text{ for all } \mathbf{v} \in \mathbf{L}\}$ is called the *Voronoï domain* or *Dirichlet domain* or *Wigner–Seitz cell* or *Wirkungsbereich* or *first Brillouin zone* (for the case of reciprocal lattices in dual space, see Section 1.3.2.5) of $\mathbf{L}$ (around the origin).

The Voronoï domain consists of those points of $\mathbb{V}^3$ that are closer to the origin than to any other lattice point of $\mathbf{L}$.

See Fig. 1.3.2.2 for examples of these two types of unit cells in two-dimensional space.

It should be noted that the attribute ‘primitive’ for a unit cell is often omitted. The term ‘unit cell’ then either denotes a primitive unit cell in the sense of the definition above or a slight generalization of this, namely a cell spanned by vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ which are not necessarily a lattice basis. This will be discussed in detail in the next section. If a unit cell in the even more general sense of a cell whose translates cover the whole space without overlap (thus including *e.g.* Voronoï domains) is meant, this should be indicated by the context.



(*a*)

(*b*)

Figure 1.3.2.2
Voronoï domains and primitive unit cells for a rectangular lattice (*a*) and an oblique lattice (*b*).

The construction of the Voronoï domain is independent of the basis of $\mathbf{L}$, as the Voronoï domain is bounded by planes bisecting the line segment between the origin and a lattice point and perpendicular to this segment. In two-dimensional space, the Voronoï domain is simply bounded by lines, in three-dimensional space it is bounded by planes and more generally it is bounded by $(n-1)$-dimensional hyperplanes in n-dimensional space.

The boundaries of the Voronoï domain and its translates overlap, thus in order to get a proper fundamental domain, part of the boundary has to be excluded from the Voronoï domain.

The volume V of the unit cell can be expressed both *via* the metric tensor and *via* the cell parameters. One has

$$\begin{aligned} V^2 &= \det \boldsymbol{G} \\ &= a^2b^2c^2(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma) \end{aligned}$$

and thus

$$V = abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}.$$

Although the cell parameters depend on the chosen lattice basis, the volume of the unit cell is not affected by a transition to a different lattice basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$. As remarked in Section 1.3.2.1, two lattice bases are related by an integral basis transformation $\boldsymbol{P}$ of determinant ± 1 and therefore $\det \boldsymbol{G}' = \det(\boldsymbol{P}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{P}) = \det \boldsymbol{G}$, *i.e.* the determinant of the metric tensor is the same for all lattice bases.

Assuming that the vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ form a *right-handed* system, the volume can also be obtained *via*

$$V = \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \mathbf{b} \cdot (\mathbf{c} \times \mathbf{a}) = \mathbf{c} \cdot (\mathbf{a} \times \mathbf{b}).$$

1.3.2.4. Primitive and centred lattices

The definition of a lattice as given in Section 1.3.2.1 states that a lattice consists precisely of the integral linear combinations of the vectors in a lattice basis. However, in crystallographic