Crystal Structure

In general, by *solid* we mean an equilibrium state with broken translation symmetry (in any spatial direction). That is, the solid is a state for which there exist observables—say, densities of particles—with spatially dependent expectation values, $A(\mathbf{r}) \neq A(\mathbf{r}')$. A *crystal* is a solid that features translation symmetry:

$$A(\mathbf{r} + \mathbf{T}) = A(\mathbf{r}) , \tag{1}$$

where $\mathbf{T}$ is one of the *translation vectors*. For a crystal, there exist an infinite number of translation vectors, but in d dimensions the number of linear independent translation vectors cannot be larger than d. For a genuine crystal, the number of linear independent translation vectors is exactly equal to d. There exist so-called *quasi*-crystals for which the number of linear independent translation vectors is smaller than d. Solids that do not possess translation symmetry at all are called *amorphous solids*, or *structural glasses*. In this course, we will be mostly dealing with genuine crystals.

The group of translations

All the translations with respect to which a given crystal is symmetric in the sense of Eq. (1) form a *group*. A group $\mathcal{G}$ is a set of objects obeying the following four axioms.

A1. For any two elements A and B of the group $\mathcal{G}$ there exists a *group operation* $\cdot$ (sometimes called a composition, a product, etc.) such that $A \cdot B \in \mathcal{G}$.

A2. Associativity: $(A \cdot B) \cdot C = A \cdot (B \cdot C)$.

A3. There exists an identity element $E \in \mathcal{G}$ such that for each $A \in \mathcal{G}$, $E \cdot A = A \cdot E = A$.

A4. For each $A \in \mathcal{G}$ there exists an inverse element $X \in \mathcal{G}$ such that $X \cdot A = A \cdot X = E$.

From these axioms, there are two elementary uniqueness theorems: (i) The identity element is unique, and (ii) For each $A \in \mathcal{G}$, its inverse element is unique. It is also trivially seen that if X is inverse to A, then A is inverse to X; and E is inverse to itself.

In the *Abelian* group, the group operation is commutative: $A \cdot B = B \cdot A$.

To make sure that all the translations that carry a crystal into itself form a group, $\mathcal{G}_T$, we observe that the elements of $\mathcal{G}_T$ can be associated with the translation vectors. Then the composition of two translations with the vectors $\mathbf{T}_1$ and $\mathbf{T}_2$ is yet another translation carrying a crystal into itself, with the translation vector $\mathbf{T}_3 = \mathbf{T}_1 + \mathbf{T}_2$. Since the addition of vectors is

associative, the axiom A2 is satisfied. The identity element is the translation by zero vector. And for the translation by the vector $\mathbf{T}$ the inverse element (trivially belonging to $\mathcal{G}_T$) is the translation by the vector $-\mathbf{T}$. Since the vector addition is commutative, the translation group is Abelian.

Primitive sets of translation vectors. Bravais lattice

Each translation vector $\mathbf{T}$ of the group $\mathcal{G}_T$ can be parameterized as a linear combination, with *integer* coefficients, of specially chosen three (for definiteness we work in three dimensions) translation vectors $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$:

$$\mathbf{T} \equiv \mathbf{T}_\mathbf{n} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \,. \tag{2}$$

Here we use a convenient integer-vector notation for the three integer coefficients: $\mathbf{n} = (n_1, n_2, n_3)$. Corresponding set of the three vectors is called *primitive*. The requirement that each of the numbers (n_1, n_2, n_3) be integer significantly constrains the choice of primitive sets. For example if we take the primitive set $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$ and replace $\mathbf{a}_1 \to \tilde{\mathbf{a}}_1 = 2\mathbf{a}_1$, the new set $(\tilde{\mathbf{a}}_1, \mathbf{a}_2, \mathbf{a}_3)$ will not be primitive, because $\mathbf{a}_1 = 0.5\tilde{\mathbf{a}}_1$. Still, there is an infinite number of choices of a primitive sets. An elementary step that allows one to go from one primitive set to yet another one is by replacing one of the vectors in the set by a sum of itself and the other vector of the same set, like $\mathbf{a}_1 \to \mathbf{a}_1 + \mathbf{a}_2$, etc. Note that iteratively repeating this procedure we can arrive at a primitive set having vectors of arbitrarily large lengths (but at the expense of having arbitrarily small angles between them)!

In accordance with the parameterization (2), all the translation vectors of the group $\mathcal{G}_T$ form a lattice, each site of which is conveniently labelled with the integer-vector subscript $\mathbf{n}$. This lattice is called *Bravais lattice* (after Auguste Bravais who introduced it in 1850). The geometric shape of the Bravais lattice does not depend on the choice of the primitive set. Indeed, an alternative way of introducing the Bravais lattice is to take some point in space—call it the origin—and consider the set of all points that can be obtained from the origin by applying all the translations of the group $\mathcal{G}_T$. Hence, the Bravais lattice is nothing but a geometric way of visualizing $\mathcal{G}_T$. What does depend on the choice of the primitive set, however, is the *labeling* of the sites of the Barvais lattice. The integer vector $\mathbf{n}$ ascribed to a given site of the Bravais lattice is unambiguously related to the choice of the primitive set, and, *vice versa*, if each site of the Bravais lattice is naturally labelled with an array of integers (n_1, n_2, n_3), then corresponding primitive set is given by the three translation vectors going from the origin to the sites $(1, 0, 0)$, $(0, 1, 0)$, and $(0, 0, 1)$.

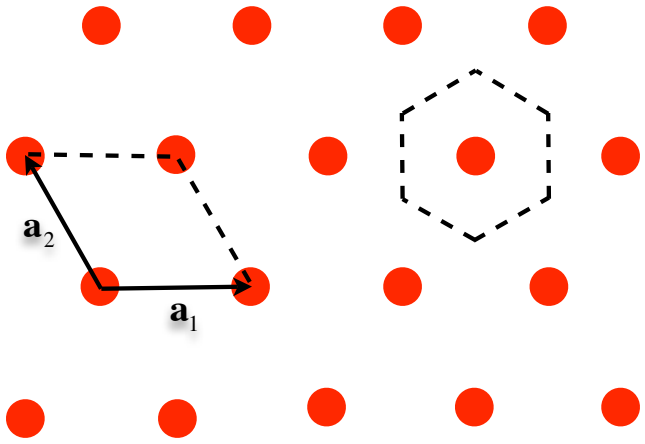

Figure 1: Hexagonal lattice: $|\mathbf{a}_1| = |\mathbf{a}_2|$, the angle between $\mathbf{a}_1$ and $\mathbf{a}_2$ is $2\pi/3$. The vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ are the primitive set forming the primitive parallelogram. The dashed hexagon is the Wigner-Seitz primitive cell.

With the notion of Bravais lattice, it is easy to exhaustively describe all possible choices of primitive sets. A translation vector $\mathbf{T}$ is *primitive* if it cannot be represented as an integer multiple of yet another translation vector $\mathbf{T}_0$ (that is it cannot be represented as $\mathbf{T} = m\mathbf{T}_0$, with some integer $m > 1$). By definition, each of the vectors in a primitive set is primitive. Does it work other way around: Can we construct a primitive set starting from *any* primitive vector? The answer is 'yes', and we are in a position to describe all possible ways of doing that. It is convenient to start with 2D, where a choice of a primitive translation vector $\mathbf{a}_1$ splits the Bravais lattice into a stack of one-dimensional lattices—lines of points—the vector $\mathbf{a}_1$ being the primitive translation vector for each of them. Consider the line that contains the origin of our 2D Bravais lattice, call it the base line. There are two lines that are the closest to the base line. The two are equivalent, so we pick up just one of them and call it the nearest line. It is rather obvious now that *any* vector $\mathbf{a}_2$ that connects the origin to any point on the nearest line can be chosen as a complimentary to $\mathbf{a}_1$ primitive vector to form a primitive set $(\mathbf{a}_1, \mathbf{a}_2)$; and it is also obvious that there are no other choices of $\mathbf{a}_2$ for given $\mathbf{a}_1$. Now we go from 2D to 3D. Here one can start with *any* plane of lattice points containing the origin and the fixed primitive vector $\mathbf{a}_1$. This plane (call it the base plane) is a 2D Bravais lattice for which we can choose—in accordance with the above-discussed 2D rules—a primitive vector $\mathbf{a}_2$ such that $(\mathbf{a}_1, \mathbf{a}_2)$ is a primitive set. The original 3D lattice then splits into a stack of 2D lattices obtained by translations of the base plane. Take one of the two planes closest to the base plane, call it the nearest plane. In a direct analogy with 2D case, all possible choices of $\mathbf{a}_3$ are then given by vectors connecting the origin to one of the points in the nearest plane.

A natural choice of a primitive set, minimizing the lengths of the vectors of the set, is as follows. Let $\mathbf{a}_1$ be the shortest (and thus obviously primitive) translation vector. The vector $\mathbf{a}_2$ is then chosen to be the shortest of all translation vectors carrying the origin to one of the Bravais lattice sites in the line closest to the line of sites formed by translating the origin by integer multiples of $\mathbf{a}_1$. In 3D, the vector $\mathbf{a}_3$ is then chosen to be the shortest of all translation vectors carrying the origin to one of the Bravais lattice sites in the plane closest to the base plane formed by translating the origin by $n_1\mathbf{a}_1 + n_2\mathbf{a}_2$.

Primitive cell

A *primitive cell* is a geometric shape, consistent with the group $\mathcal{G}_T$, that perfectly (i.e. without gaps and overlaps) tiles the whole space if translated

by the vectors of the group $\mathcal{G}_T$. There is a continuum of options of choosing a primitive cell. A natural (and still infinite) class of primitive cells comes with the parameterization (2), where each primitive set $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$ yields a *primitive parallelepiped* (parallelogram in 2D) build on the vectors of the given set. All primitive cells associated with the group $\mathcal{G}_T$ have one and the same volume V_c. Indeed, the primitive cell always contains exactly one point of the Bravais lattice; otherwise there would be either gaps or overlaps when tiling the space by translating the primitive cell with the vectors of the $\mathcal{G}_T$. The invariance of V_c with respect to the choice of the primitive cell follows then from a simple observation that the total number of the points of the Bravais lattice in a certain large volume $V \gg V_c$ is given by the ratio V/V_c (with the accuracy controlled by the small parameter $V_c/V \ll 1$). In other words, V_c is nothing but the inverse density of the points of the Bravais lattice.

With the parameterization (2), the explicit expression for V_c is given by the mixed scalar product of the primitive translation vectors.

$$V_c \,=\, |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)| \qquad\qquad (d = 3)\,. \tag{3}$$

The 2D analog of Eq. (3) is

$$V_c = |\mathbf{a}_1 \times \mathbf{a}_2| = |\mathbf{a}_1||\mathbf{a}_2| \sin\varphi \qquad\qquad (d = 2)\,, \tag{4}$$

where φ is the angle between the two primitive translation vectors. Equation (3)/(4) is not only necessary, but also a sufficient condition for three/two translation vectors to form a primitive set in 3D/2D. This is obvious from the necessary and sufficient condition of having exactly one site of Bravais lattice per primitive parallelepiped/parallelogram.

Along with primitive parallelepipeds/parallelograms, a popular choice of the primitive cells is the Wigner-Seitz construction (which is a type of Voronoi cell[1]), illustrated in K-Fig. 4 (here and below 'K-Fig.' stands for corresponding figure in the 8th edition of Kittel text). The Wigner-Seitz primitive cell is especially convenient in the cases when crystal structure features extra symmetries in addition to the translation group. The Wigner-Seitz primitive cell then readily reflects those symmetries, while the primitive parallelepipeds/parallelograms tend to hide them. For an illustration, see Fig. 1.

[1]For any discrete set of point sites—not necessarily forming a regular (crystal) structure—a Voronoi cell contains exactly one site, along with all the points in the plane/space for which the given site is closer than any of the rest of the sites.

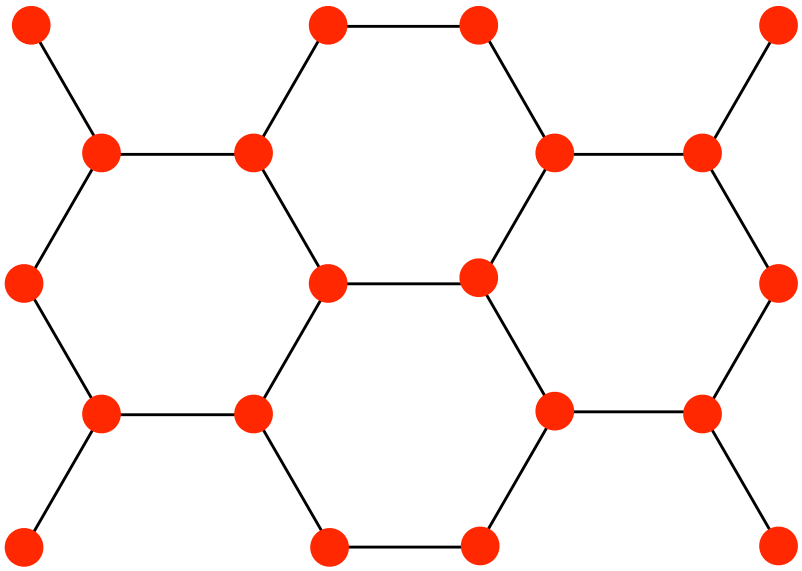

Figure 2: Honeycomb lattice. The bonds are to guide an eye. The lattice sites correspond to the vertices of hexagons tiling the plane. The lattice is not inversion-symmetric with respect to the lattice points, and thus is not a Bravais lattice. Q1: What is the Voronoi cell of this lattice? Q2: Why, in this case, the Voronoi cell is *not* the Wigner-Seitz cell?

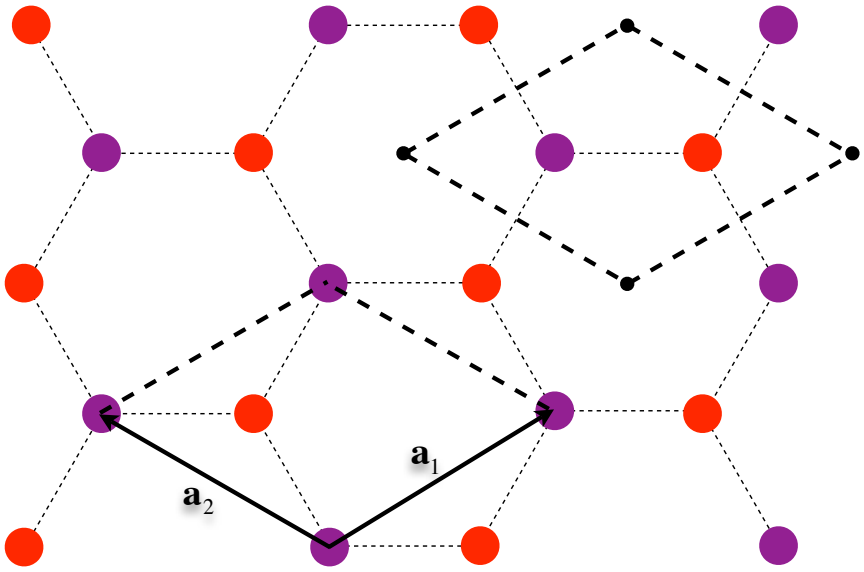

Figure 3: Using two colors, we see that the honeycomb lattice is a *bipartite* lattice formed by superimposing two identical hexagonal lattices, each of which can be taken as a Bravais lattice of the honecomb lattice. This allows one to readily construct a primitive set of translation vectors by considering one of the two hexagonal lattices. The dashed parallelogram shows an alternative choice of the Bravais lattice and, correspondingly alternative primitive cell. In this case, Bravais lattice consists of the centers of the hexagons. Note that with this choice of the primitive cell, (i) the symmetry between the two hexagonal sub-lattices is clearly seen; (ii) the basis consists of two adjacent Voronoi cells of two nearest lattice cites.

Basis of crystal structure. Non-Bravais lattices

The primitive cell can be viewed as a set of potentially non-equivalent spatial points forming the crystal structure. The word 'potentially' expresses the reservation that in addition to the translation symmetry a crystal structure can feature some extra symmetries rendering different points within a primitive cell equivalent. The crystal structure is then unambiguously fixed by specifying the values of relevant functions (say, density distributions) within the primitive cell. A primitive cell with specified functions within it is called the *basis* of crystal structure.

In many cases we are interested in some special *points* within the crystal structure, say, the maxima of the density distributions (these maxima are often loosely referred to as positions of corresponding atoms). A crystal structure of discrete points is called crystal lattice, or just a lattice. A Bravais lattice is the simplest example of a crystal lattice. It is a minimal crystal lattice corresponding to a given group $\mathcal{G}_T$. Clearly, not any lattice is a Bravais lattice. For a lattice to be a Bravais lattice it is necessary and sufficient to have exactly one lattice point per primitive cell. Correspondingly, if the primitive cell contains two or more lattice points, it is a non-Bravais lattice.

In the next sub-section, we will be discussing extra symmetries of crystal structure. Here we introduce one of them which proves extremely helpful for identifying non-Bravais lattices of identical points. The *inversion symmetry* is the symmetry with respect to changing the sign of all the coordinates with respect to a certain origin (called the center of inversion). All the Bravais lattices are inversion-symmetric with respect to inversions against the lattice points, because for any translation vector $\mathbf{T}$, the vector $-\mathbf{T}$ is also a translation vector (the group property). Hence, if a lattice is not inversion-symmetric with respect to *each* of its points, it is guaranteed to be a non-Bravais lattice!

An important[2] example of non-Bravais lattice is the honeycomb lattice, see Figs. 2 and 3.

Extra symmetries of crystal structure

In addition to the translation group $\mathcal{G}_T$, there can exist other symmetry

[2] And extremely popular nowadays because of *graphene* (Nobel Prize 2010).

operations that carry a given crystal structure into itself.[3] The most typical of those operations is a rotation about an axis. The *crystallographic restriction theorem* states that only a few special rotation angles (modulo 2π) are consistent with discrete translation symmetry: $2\pi/2$, $2\pi/3$, $2\pi/4$, and $2\pi/6$. Corresponding axes are conveniently denoted by the symbols 2, 3, 4, and 6. The proof of the theorem is very simple in the case when the rotation axis is perpendicular to one of the translation vectors (which is automatic in 2D). This is also the case for any rotation that carries the Bravais lattice into itself, since it implies the existence of two sites of Bravais lattice in a line perpendicular to the rotation axis.

Let R be the operator of the rotation by the angle θ that carries the crystal structure into itself. Without loss of generality we assume that $\theta \neq \pi$, since were are not going to rule out the case $\theta = \pi$. The existence of the translation vector perpendicular to the rotation axis then guaranties the existence of a plane of the sites of Bravais lattice perpendicular to the rotation axis. Let $\mathbf{a}$ be the shortest translation vector in this plane. Clearly, the pair $(\mathbf{a}, R\mathbf{a})$ of shortest translation vectors forms a primitive set in this plane, and the vector $R^2\mathbf{a}$ can be represented as

$$R^2\mathbf{a} \,=\, nR\mathbf{a} + m\mathbf{a}\,, \tag{5}$$

where n and m are some integers. [At this point one can notice that Eq. (5) applies also to the case $\theta = \pi$, since in this case $R\mathbf{a} = -\mathbf{a}$.]

Writing (5) in Cartesian components—with the x-axis along $\mathbf{a}$ and the z-axis being the axis of rotation—we get

$$\begin{bmatrix} \cos 2\theta & \sin 2\theta \\ -\sin 2\theta & \cos 2\theta \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = n \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} + m \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \tag{6}$$

which yields a system of two constraints:

$$\begin{cases} (2\cos\theta - n)\cos\theta = m + 1\,, \\ \quad 2\sin\theta\cos\theta = n\sin\theta\,. \end{cases} \tag{7}$$

From the second constraint we see that either $\sin\theta = 0$ or $\cos\theta = n/2$ (in both cases the first constraint is then easily met by an appropriate choice of m). This proves the statement. (The proof for a general case can be found at http://en.wikipedia.org/wiki/Crystallographic_restriction_theorem.)

[3] The symmetry of the crystal structure can be naturally lower than the symmetry of corresponding Bravais lattice, since Bravais lattice is the minimal possible crystal structure with corresponding translation group.

The group of rotations about a given l-fold axis ($l = 2, 3, 4, 6$) is an example of a *point group*. The crystallographic point group or crystal class is the mathematical group comprising the symmetry operations that carry a crystal into itself while leaving at least one point unmoved. The other point symmetry operations are: *reflection*, which reflects the structure across a reflection plane; *inversion*, which changes the sign of the coordinate of each point with respect to a center of symmetry or inversion point (in 2D, inversion is the same as the angle-π rotation, and the inversion symmetry is thus the same as the 2-fold axis with the same center); *improper rotation*, which consists of a rotation about an axis followed by an inversion. Rotation axes (proper and improper), reflection planes, and centers of symmetry are collectively called symmetry elements. In 3D, there are 32 possible crystal classes. Each one can be classified into one of the seven crystal systems.

The *space group* of the crystal structure is composed of the translational symmetry operations in addition to the operations of the point group. Apart of the group $\mathcal{G}_T$ of pure translation which each crystal structure has by definition, space groups can include *screw axes*, which rotate a point around an axis while translating parallel to the axis and *glide planes*, which reflect a point through a plane while translating it parallel to the plane. In 3D, there are 230 distinct space groups. The 2D analogs of space groups are called *wallpaper groups* (or plane crystallographic groups); there are 17 distinct groups in 2D.

Sometimes one is interested in the symmetry of the Bravais lattice only. Since not any crystal lattice is a Bravais lattice, we can expect that the number of distinct symmetry groups of Bravais lattices is smaller than the total number of crystallographic groups. And this is indeed the case. In 2D there are only 5 distinct symmetry groups (often referred to as symmetry *types*) of Bravais lattices. That is only 5 out of 17 wallpaper groups are relevant to the symmetries of 2D Bravais lattices. One of the five lattice types is generic, it is called *oblique* (a.k.a. *parallelogram*) Bravais lattice. The other four—*square, hexagonal, rectangular*, and *centered rectangular* (a.k.a. *rhombic*, or *isosceles triangular*), see K-Fig. 7—are special, they feature extra symmetries.

The square lattice (symmetry group *p4m*) has two rotation centres of order 4, and reflections in 4 distinct directions (horizontal, vertical, and diagonals).

The hexagonal lattice (symmetry group *p6m*) has one rotation centre of order 6, two rotation centres of order 3, and three of order 2. It has also reflections in 6 distinct directions.

The rectangular lattice (symmetry group *pmm*) has reflections in two

perpendicular directions (parallel or perpendicular to the sides of the primitive rectangle), and four rotation centres of order 2 located at the intersections of the reflection axes.

The centered rectangular (a.k.a. rhombic, or isosceles triangular) lattice (symmetry group *cmm*) has reflections in two perpendicular directions (parallel to diagonals of the primitive rhombus), and a rotation of order 2 whose centre is not on a reflection axis. It also has two order-2 rotations whose centres are on a reflection axis.

In 3D there are only 14 symmetry types of Bravais lattices (only 14 out of 230 space crystallographic groups are relevant to the 3D Bravais lattices), see Fig. 5. The *triclinic* is the generic 3D type, an analog of of the oblique lattice in 2D, the other 13 feature some extra symmetries. In 3D, along with lattice types there are also lattices *systems*. The idea of systems is to group the lattice types sharing certain similarity. There are 7 Bravais lattice systems: *triclinic, monoclinic, orthorombic, tetragonal, trigonal, cubic, hexagonal*. Three out of the 7 systems—triclinic, trigonal, and hexagonal—are just synonyms to corresponding Bravais lattice. The other four systems contain two and more Bravais lattices each. A very simple and important cubic system contains three Bravais lattices: *simple cubic* (*sc*), *body-centered cubic* (*bcc*), and *face-centered cubic* (*fcc*), see Fig. 5.

Close-packed structures

An important class of lattices is formed by close-packed identical spheres. A macroscopically large system of identical spheres is called close-packed if it maximizes the *packing fraction* defined as the ratio of the volume occupied by the spheres to the total volume of the system. The statement that the maximal packing fraction equals $\pi/(3\sqrt{2}) \approx 0.74048$ has been know for a long time as *Kepler conjecture*. In 1998 Thomas Hales, following an approach suggested by Fejes Tóth (1953), announced his proof of the Kepler conjecture (by exhaustion involving checking of many individual cases using complex computer calculations). Hales' proof is very close to being accepted as a theorem.

There are infinitely many (!) ways to achieve the Kepler's packing fraction. One starts with a close-packed layer (2D hexagonal lattice) of identical spheres, see K-Fig. 19, and observes that there are two equivalent ways of putting the next layer on top of the previous one. Correspondingly, a close-packed 3D structure of the layers can be described as a *periodic*, or *non-periodic* sequence of three letters, A, B, and C, characterizing three distinct types of the layers. (The only restriction on the sequence is that two ad-

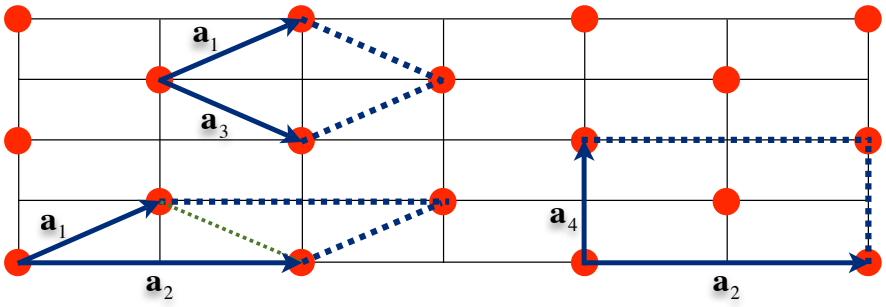

Figure 4: The centered rectangular (a.k.a. rhombic, or isosceles triangular) lattice. Solid lines show the reflection axes. The following three constraints have to be satisfied: (i) $|\mathbf{a}_4| \neq |\mathbf{a}_2|$, (ii) $|\mathbf{a}_1| \neq |\mathbf{a}_2|$, and (iii) $|\mathbf{a}_1| \neq |\mathbf{a}_4|$. Indeed, if $|\mathbf{a}_4| = |\mathbf{a}_2|$, the lattice becomes a square lattice, and if either $|\mathbf{a}_1| = |\mathbf{a}_2|$ or $|\mathbf{a}_1| = |\mathbf{a}_4|$, the lattice is a hexagonal lattice. The rectangular cell built on the vectors $\mathbf{a}_2$ and $\mathbf{a}_4$ is not primitive—it contains two sites. This cell gives the main name to the lattice. This cell is very convenient for visualizing all the symmetries of the centered rectangular lattice. The set $(\mathbf{a}_1, \mathbf{a}_3)$ defines the primitive rhombus ($|\mathbf{a}_3| = |\mathbf{a}_1|$), explaining why the lattice is also called rhombic. The primitive parallelogram build on the set $(\mathbf{a}_1, \mathbf{a}_2)$ consists of two isosceles triangles explaining the origin of yet another name of the lattice.

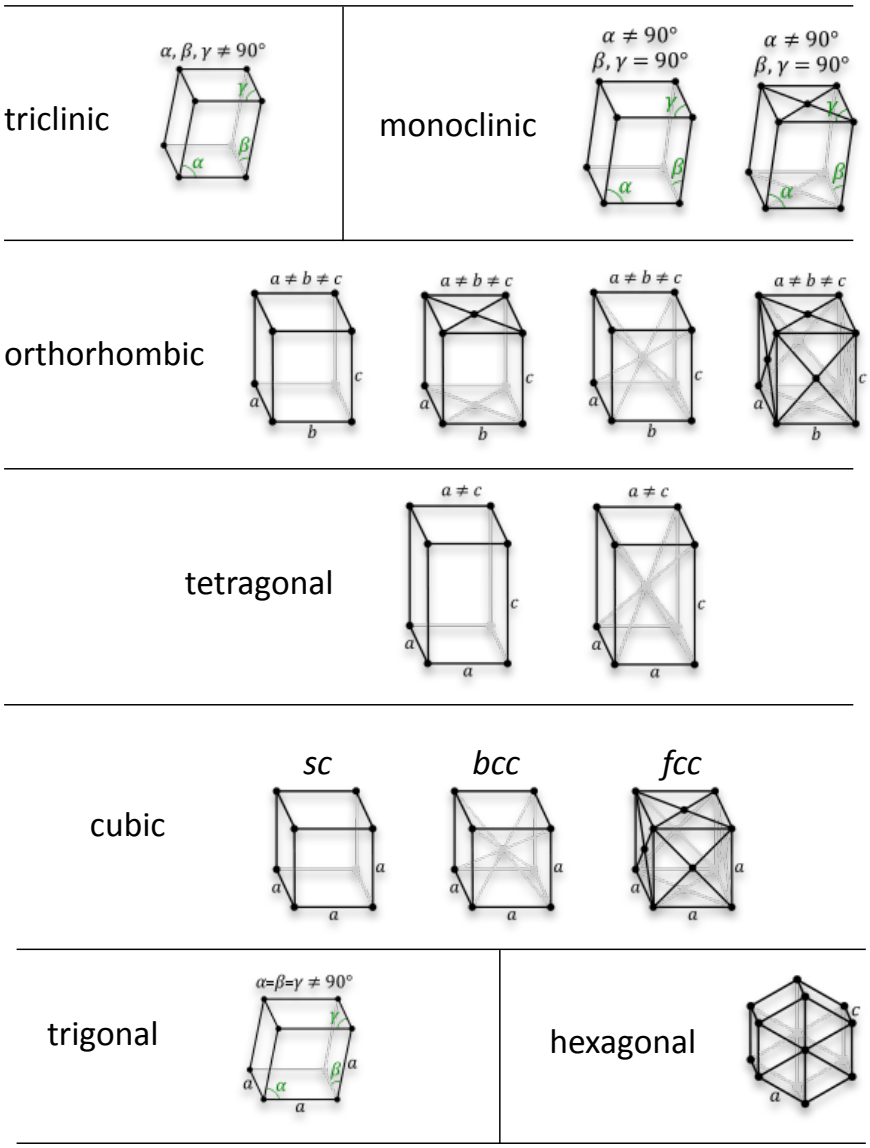

Figure 5: The 14 types of 3D Bravais lattices grouped into 7 systems.

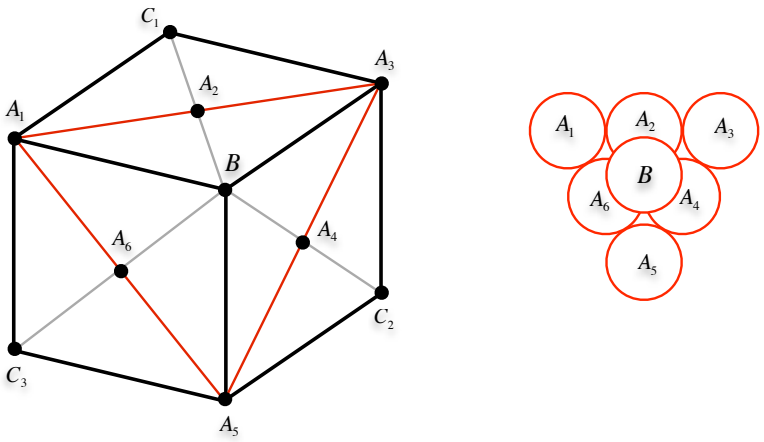

Figure 6: Revealing the $ABCABC\ldots$ close-packing layers in the *fcc* lattie. Shown are only the three "visible" faces of the cube. The diameter of the close-packed spheres equals $|A_1A_2|$. The spheres centered at the points $A_1, A_2, \ldots, A_6$ belong to a close-packed A-layer. The point B belongs to a B-layer. A straightforward—but not the shortest—way to see that the points C_1, C_2, C_3 belong to a C-type layer (rather than a B-type layer) is to consider the cubic units adjacent to the shown one. A more short and elegant way is to invoke the inversion symmetry with respect to one of the A-points. For example, the inversion with respect to the point A_2 swaps the points B and C_1, proving that the two points belong to the layers of different types.

jacent letters be different.) The two most simple and important cases are $ABAB\ldots$ and $ABCABC\ldots$. The case $ABAB\ldots$ yields the *hexagonal close-packed* (*hcp*) lattice. The *hcp* lattice consists of two hexagonal sublattices corresponding to the sets of A and B layers, respectively. Hence, the Bravais lattice of the *hcp* lattice is hexagonal, and there are two points in the primitive cell: an A-type one and a B-type one. The $ABCABC\ldots$ packing corresponds to the *fcc* lattice, see Fig. 6. It is instructive to note that the $ABAB\ldots$ packing—as opposed to the $ABCABC\ldots$ packing—features reflectional symmetry with respect to the planes of the A and B layers. On the other hand, the $ABCABC\ldots$ packing—as opposed to the $ABAB\ldots$ packing—features inversion symmetry with respect to the centers of the spheres; the inversion with respect to an A-center swaps B and C layers, etc. It is worth recalling that the mere fact that the $ABAB\ldots$ packing does not have inversion symmetry with respect to the lattice points implies that corresponding *hcp* lattice is not a Bravais lattice.

Closed-packed lattices are typical, e.g., for noble gases. Apart from helium, all solid phases of the noble gases have the *fcc* lattice. The solid ^{4}He has the *hcp* lattice, except for a small and essentially *finite-temperature* region of the *bcc* lattice, see Fig. 7.

Sodium chloride and cesium chloride structures

Sodium chloride and cesium chloride give the names to two very common two-color cubic crystal structures shown in Figs. 8 and 9. Note that in both cases applying the colors changes the type of the Bravais lattice (within the same cubic system).

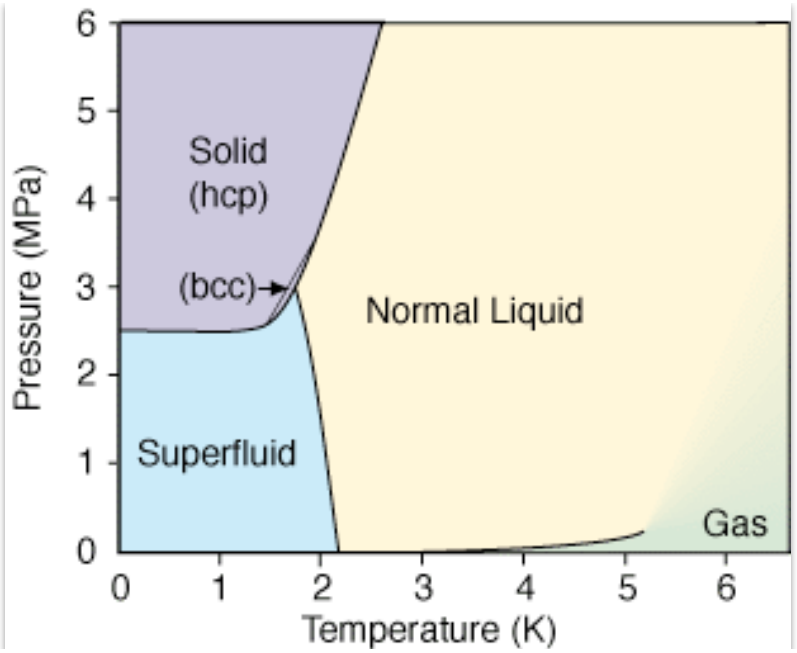

Figure 7: Phase diagram of ^{4}He.

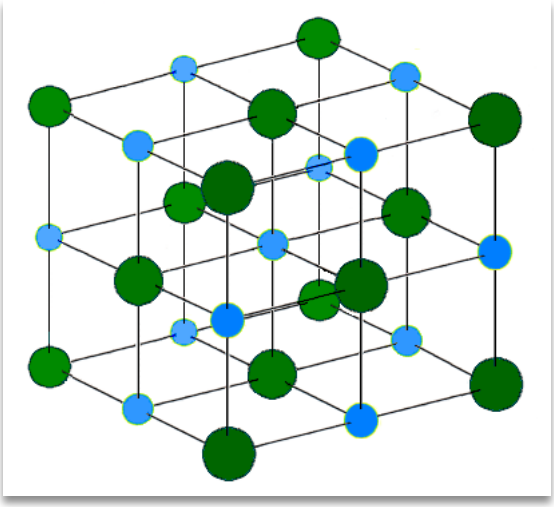

Figure 8: Sodium chloride structure. This two-color structure is obtained by alternating coloring the points of a simple cubic lattice. The Bravais lattice of the sodium chloride structure is *fcc*. The basis of the structure contains two points of different colors.

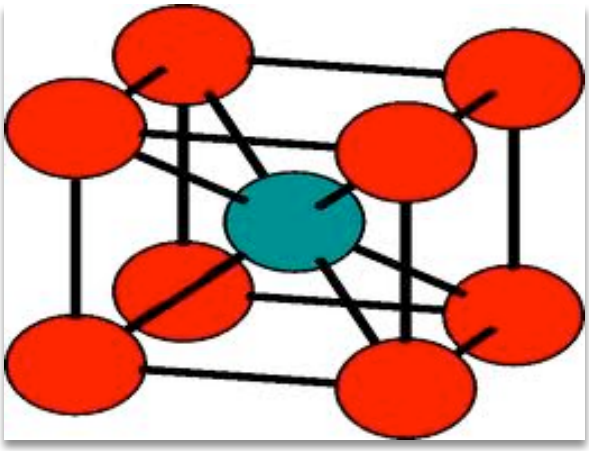

Figure 9: Cesium chloride structure. This two-color structure consists of two simple cubic sub-lattices of different colors. The two sub-lattices are translated with respect to each other by the vector $(1/2, 1/2, 1/2)$. The Bravais lattice of the cesium chloride structure is *sc*. The basis of the structure contains two points of different colors.