

**Part I**

**ATOMIC STRUCTURE**

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# 1. The Idea of Crystals

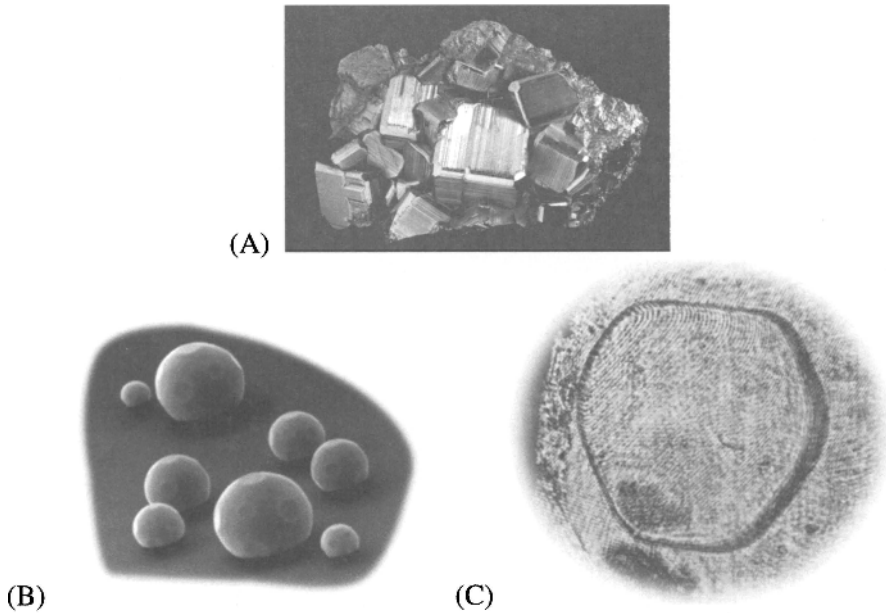
## 1.1 Introduction

*From the point of view of the physicist, a theory of matter is a policy rather than a creed; its object is to connect or co-ordinate apparently diverse phenomena, and above all to suggest, stimulate and direct experiment.*  
—Thomson (1907), p. 1

The goal of condensed matter physics is to understand how underlying laws unfold themselves in objects of the natural world. Because the complexity of condensed matter systems is so enormous, the number of atoms they involve so great, and the possibility of solving all underlying equations in full detail so remote, the laws of greatest importance are principles of symmetry.

A first step is to describe how atoms are arranged. As a mental image of arrangement, the idea of the *crystal* has emerged out of an obscure class of minerals to dominate thought about all solids. Here is symmetry with a vengeance. A small group of atoms repeats a simple pattern endlessly through the stretches of a macroscopic body. The most precise experiments and the most detailed theories of solids are all carried out in perfect crystals. Yet the world is neither a collection of crystals, nor a collection of solids wishing to be crystals but falling short of perfection. Principles of symmetry more general than crystalline order still function in structures bearing no resemblance to the perfect lattice, while a rigid insistence upon considering only solids in crystalline form would force one to abandon most naturally occurring substances and technologically important materials. Nevertheless, the science of condensed matter physics begins with the crystal, its single most important structural idea.

In Greek, the word *κρύσταλλος* originally referred to ice. In the middle ages, the word “crystal” first referred to quartz, and later to any solid whose external form consisted of flat faces intersecting at sharp angles (Figure 1.1). The first law of *crystal habit*, discovered by Steno (1671), and illustrated in Figure 1.2, states that corresponding faces of quartz always meet at the same angle. The second law of crystal habit (see Problem 9 in Chapter 2), discovered by Haüy (1801), states that if one takes three edges of a crystal as coordinate axes and then asks where the planes of other faces intersect these axes, the three intersection points are always rational multiples of one another. Haüy explained this law by assuming, as many other scientists had done since around 1750, that crystals were built of vast numbers of identical units, perhaps small polyhedra, stacked together in a regular fashion.



**Figure 1.1.** (A) Naturally occurring crystals of iron pyrite, showing the intersection of flat faces at definite angles that characterizes the external appearance of all crystals. (Courtesy of J. Sharp, University of Texas.) (B) Small equilibrium crystals of gold at  $1000^\circ\text{C}$ , roughly  $5\ \mu\text{m}$  in diameter, showing alternating smooth and faceted surfaces. [Source: Heyraud and Métois (1980), p. 571.] (C) Equilibrium crystal of solid  $^4\text{He}$  at  $0.8\ \text{K}$ . (Courtesy of S. G. Lipson, Technion; see Lipson (1987).)

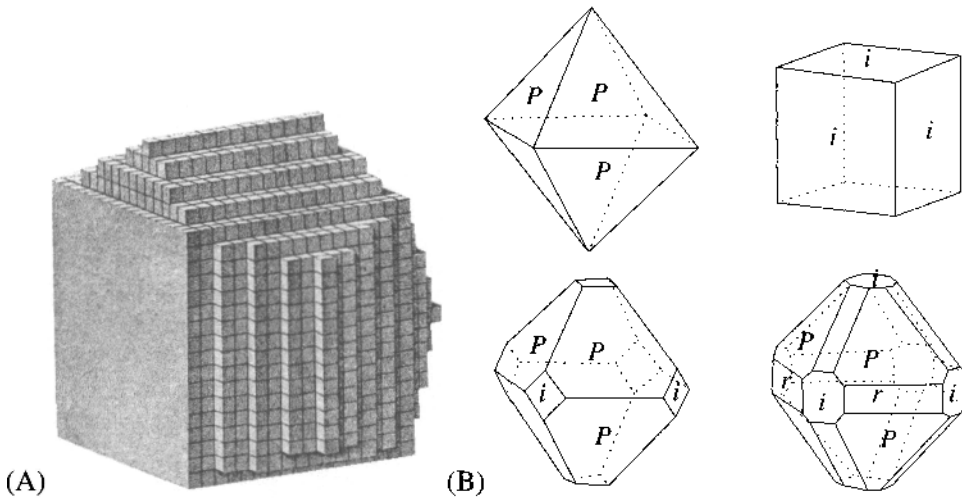
Figure 1.2(A) shows one of his diagrams, the earliest published image of crystalline arrangement.

As the nineteenth century progressed, an elaborate mathematical theory of symmetry developed, showing that observed symmetries of natural crystals could be identified with the symmetries of regular lattices. The complete enumeration of all possible classes of crystals was completed in 1890, waiting for the discovery of X-ray scattering two decades later that would make it possible to specify crystals down to atomic detail.

### 1.1.1 Why are Solids Crystalline?

Crystalline order is the simplest way that atoms could possibly be arranged to form a macroscopic solid. Small basic units of atoms repeat endlessly, one placed next to the other, so the whole solid can be described completely by studying a small number of atoms. It is remarkable that this simple structural model can be used to understand so much.

Why are low-energy arrangements of atoms so often periodic? No one really knows. A simple explanation is that if there is some optimal neighborhood for each atom, then the lowest energy state for a large number of atoms gives this same neighborhood to every atom. One might try to check this idea by imagining how

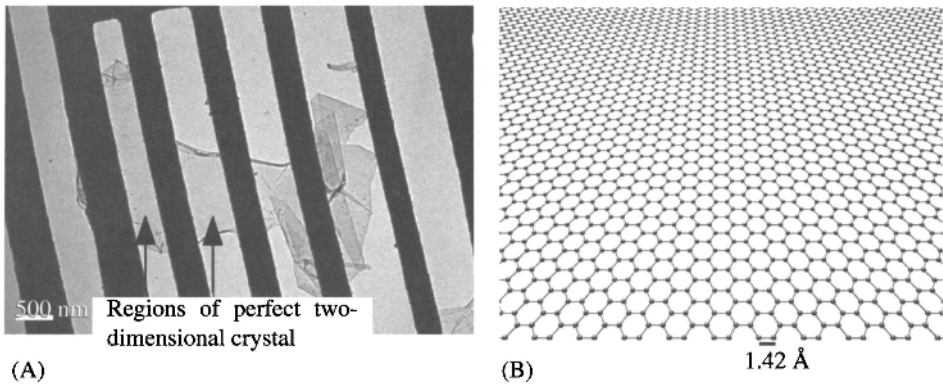


**Figure 1.2.** (A) The first published picture of the structure of a crystal. [Source: Haüy (1801).] (B) The first law of crystal habit states that when various crystals can be oriented so that their faces can be placed in one-to-one correspondence, with all corresponding faces parallel, then all angles between the faces are the same. The sketches of red copper oxide (Cyprus oxide,  $\text{Cu}_2\text{O}$ ) are taken from Haüy (1801), Plate 71. A comprehensive catalog of such diagrams was compiled by Groth (1906–1919).

the energy of a collection of atoms depends upon their relative locations, writing down an energy functional, and then minimizing the functional with respect to all atomic positions (Problem 5). Such a calculation is a serious oversimplification, mainly because it ignores most of the complexities of quantum mechanics, but even in this context there is no theorem to prove that periodic arrays provide ground states. Nevertheless, for almost all the elements and for a vast array of compounds, the lowest energy state is crystalline. The only exception among the elements is helium, which remains liquid at zero temperature and standard pressure.

Equilibrium lattice structure are functions of temperature and pressure. Even at temperatures where vibrations about a particular state are small, the entropy associated with the vibrations may be enough to cause the ions to switch from one configuration to another. This switch is possible because the differences in energy between different crystalline configurations can be very small: according to Table 11.9, as little as one part in  $10^4$ . Examining a source such as Emsley (1998) shows that most elements change crystal structure several times before they melt. In some cases, more than one crystalline form of an element or compound may be stable at a given temperature and pressure; such compounds are *allotropic*. Carbon at room temperature is stable both as graphite and as diamond, while tin comes as gray tin or white tin, the first of which is a semiconductor and the second of which is a metal. Only one of these states can be a true equilibrium state, yet the time to transform spontaneously from one to the other is so immense that this possibility may safely be neglected.

Even should it eventually be proved that the lowest energy state of assemblages



**Figure 1.3.** (A) Two dimensional crystal of carbon just one atom thick, in the form of *graphene*, hanging freely from a metal scaffold [Source: Meyer et al. (2007), p. 60]. (B) Theoretical image of the honeycomb lattice of graphene at the atomic scale. The spheres represent carbon atoms, and the rods indicate attractive bonds between nearest neighbors.

of atoms really is crystalline, it does not follow that perfect crystalline structures will always appear in nature or provide the greatest interest for study. The world is largely constructed of solids whose crystalline order is defective, or absent altogether.

## 1.2 Two-Dimensional Lattices

A *crystal* is a solid where the atoms are arranged in the form of a *lattice*. A lattice is an arrangement of points where the same pattern repeats over and over again. If one were to move from place to place over a lattice taking photographs it would be impossible to tell one part of the lattice from another. Two-dimensional lattices are much easier to picture and understand than their three-dimensional counterparts. Therefore, all the central definitions for lattices will first be introduced in a two-dimensional setting. Two-dimensional lattices are not mathematical fictions. They naturally occur as surfaces and interfaces of three-dimensional crystals, and sometimes are created free-standing in their own right (Figure 1.3).

### 1.2.1 Bravais Lattices

The simplest type of lattice is called a *Bravais lattice*. In a Bravais lattice the neighborhood of each and every point is exactly the same as the neighborhood of every other point. In two dimensions, the location of every point in such a lattice can be described in the form

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2, \quad n_1 \text{ and } n_2 \text{ are integers.} \quad (1.1)$$

where the two-dimensional vectors  $\vec{a}_i$  are called *primitive vectors* and must be linearly independent. The choice of primitive vectors is not unique—one makes choices that are as simple as possible or that have some nice symmetry to them.

**Example: Hexagonal Lattice.** To create a hexagonal lattice, take

$$\vec{a}_1 = a(1 \ 0) \quad a \text{ is the lattice spacing illustrated in Figure 1.4.} \quad (1.2a)$$

$$\vec{a}_2 = a \begin{pmatrix} 1 & \sqrt{3} \\ 2 & 2 \end{pmatrix}. \quad (1.2b)$$

To illustrate that this choice is not unique, one can equally well choose

$$\vec{a}'_1 = a \begin{pmatrix} -1 & \sqrt{3} \\ 2 & 2 \end{pmatrix} \quad (1.3a)$$

$$\vec{a}'_2 = a \begin{pmatrix} 1 & \sqrt{3} \\ 2 & 2 \end{pmatrix}. \quad (1.3b)$$

One way to make a mistake is to choose a set of vectors that is not linearly independent. For example, trying to build the hexagonal lattice out of the three vectors

$$\vec{a}''_1 = a(1, 0) \quad (1.4a)$$

$$\vec{a}''_2 = a \begin{pmatrix} -1 & \sqrt{3} \\ 2 & 2 \end{pmatrix} \quad (1.4b)$$

$$\vec{a}''_3 = a \begin{pmatrix} 1 & \sqrt{3} \\ 2 & 2 \end{pmatrix} \quad (1.4c)$$

would constitute an error since  $\vec{a}''_1 = \vec{a}''_3 - \vec{a}''_2$ .

## 1.2.2 Enumeration of Two-Dimensional Bravais Lattices

In two dimensions there are five Bravais lattices, shown in Figure 1.4.

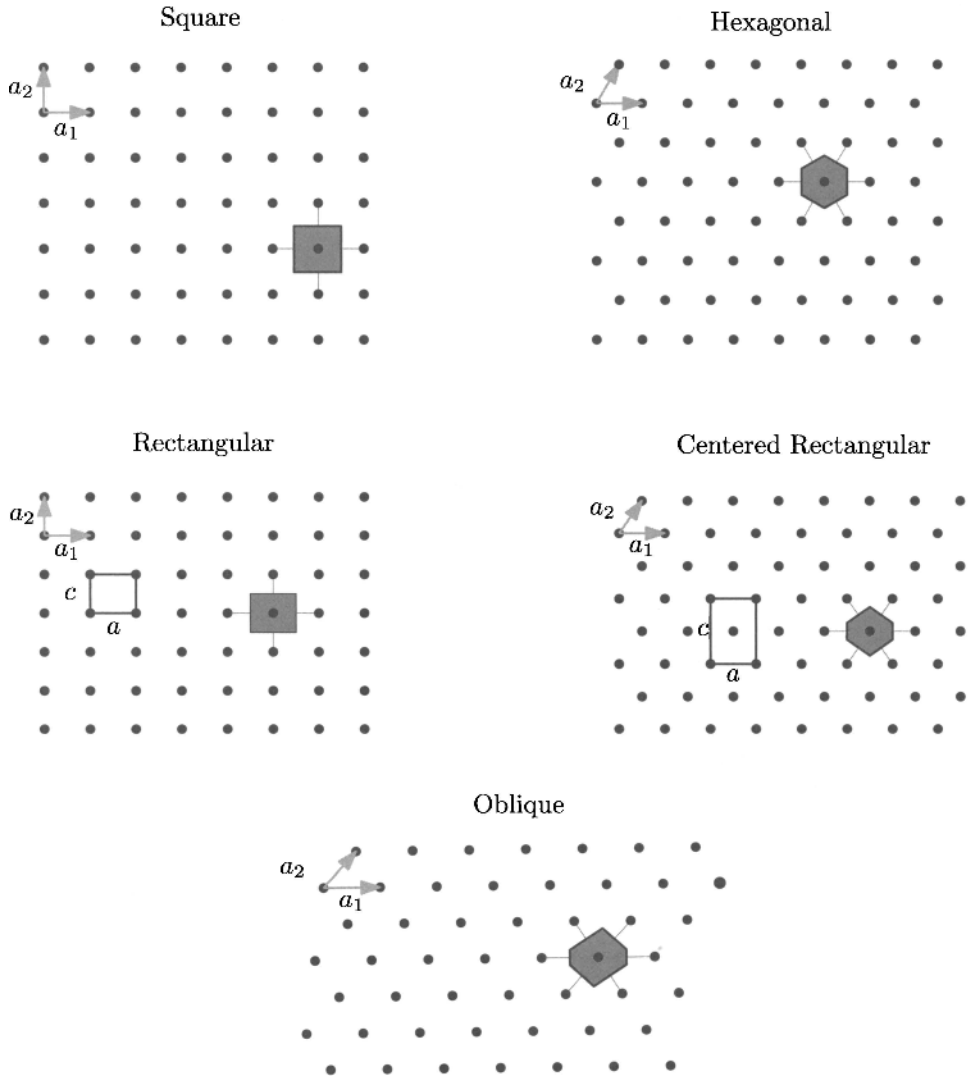
**Square Lattice:** The *square lattice* is symmetric under reflection about both  $x$  and  $y$  axes and with respect to  $90^\circ$  rotations.

**Rectangular Lattice:** When compressed along one axis, the square lattice loses the  $90^\circ$  rotational symmetry and becomes the *rectangular lattice*.

**Hexagonal Lattice:** The *hexagonal* (or *triangular*) lattice is invariant under reflections about the  $x$  and  $y$  axes as well as with respect to  $60^\circ$  rotations.

**Centered Rectangular:** The *centered rectangular lattice* results from a compression of the hexagonal lattice and loses the  $60^\circ$  rotational symmetries.

**Oblique Lattice:** Finally, an arbitrary choice of  $\vec{a}_1$  and  $\vec{a}_2$  with no special symmetry results in an *oblique lattice*. This lattice still possesses inversion symmetry,  $\vec{r} \rightarrow -\vec{r}$ .



**Figure 1.4.** The five two-dimensional Bravais lattices. Note that the centered rectangular lattice can be built by repetition of the structure in the hollow box, which shows how it obtains its name. The figure also shows Wigner–Seitz cells for each lattice. One constructs them by choosing some point  $O$  in the lattice and then drawing the perpendicular bisector of the line between  $O$  and each of its neighbors. The Wigner–Seitz cell is the region surrounding  $O$  contained within all these perpendicular bisectors.



### 1.2.3 Lattices with Bases

It is important to emphasize that the neighborhoods of all particles must be identical under translation in order for a structure to qualify to be a Bravais lattice. Most lattices occurring in nature are not Bravais lattices, but are lattices with a basis. Lattices of this type are constructed by beginning with a Bravais lattice, but putting at each lattice site an identical assembly of particles, rather than a single rotationally invariant particle.

**Example: Honeycomb Lattice.** The *honeycomb lattice*, shown in Figure 1.5, is a lattice with a basis. One can construct it by starting with a hexagonal lattice with primitive vectors of Eq. (1.2) and then decorating every lattice point with basis particles at

$$\vec{v}_1 = a \begin{pmatrix} 0 & \frac{1}{2\sqrt{3}} \end{pmatrix} \quad (1.5a)$$

$$\vec{v}_2 = a \begin{pmatrix} 0 & -\frac{1}{2\sqrt{3}} \end{pmatrix}. \quad \text{The basis vectors are being described in Cartesian coordinates.} \quad (1.5b)$$

Another way to describe basis vectors is in terms of a non-Cartesian coordinate system, where the coordinates refer to multiples of the primitive vectors:

$$\vec{v}_1 = (1/6 \ 1/6) \quad \text{Since } \vec{a}_1/6 + \vec{a}_2/6 = a \begin{pmatrix} \frac{1}{2\sqrt{3}} & 0 \end{pmatrix} = \vec{v}_1. \quad (1.6a)$$

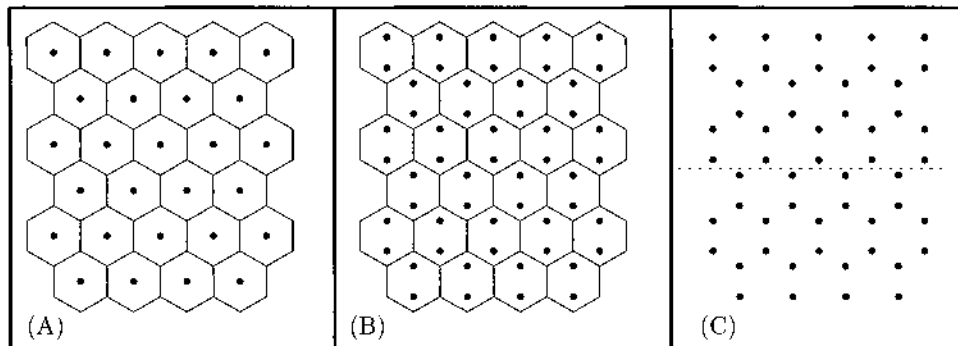
$$\vec{v}_2 = (-1/6 \ -1/6). \quad (1.6b)$$

The left- and right-hand particles in each cell find their neighbors off at different sets of angles. Notice, however, that the neighborhood of every particle is identical if one is allowed to rotate it through  $\pi/3$  before making comparisons. While this fact does not make the honeycomb lattice a Bravais lattice, it means that the qualitative arguments explaining why one expects crystalline ground states for interacting particles work just as well for lattices with bases as they do for true Bravais lattices.

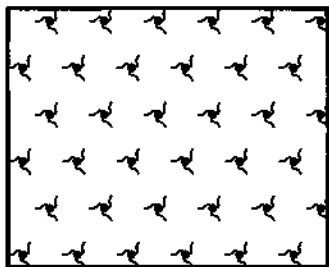
**Selective Destruction of Symmetry by a Basis.** Once one decorates a lattices with a basis, its symmetries change. Adding a basis does not automatically destroy the rotational and reflection symmetries of the original lattice; in general, these symmetries can be destroyed selectively by adding basis elements of various types. For example, if one builds a triangular lattice and then decorates it as shown in Figure 1.6, the rotational symmetries of the original triangular lattice are preserved, but the reflection symmetries are gone.

### 1.2.4 Primitive Cells

Because lattices are created by repeating small basic units over and over throughout space, the full information of a crystal can be contained in a small region of space. Such a region, chosen to be as small as it can be, is called a *primitive unit cell*. For example, for the square lattice, a square can be used as a primitive cell, as shown in Figure 1.7 (A).

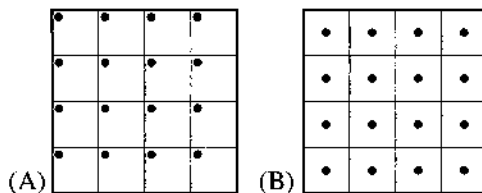


**Figure 1.5.** One may construct the honeycomb lattice by beginning with a hexagonal lattice (A), and replacing the single point in the center of each cell with a pair of points, as shown in (B). The honeycomb lattice is more obviously visible in (C). Because the top and bottom particles in each cell do not have identical neighborhoods, the honeycomb lattice is a lattice with a basis, and not a Bravais lattice. The dotted line is a glide line; the lattice is invariant when translated horizontally by  $a/2$  and reflected about this line, but is not invariant under either operation separately.



**Figure 1.6.** A triangular lattice decorated with chiral molecules so as to lose reflection symmetries.

**Figure 1.7.** Two primitive cells for the square lattice: one cell has a particle at the corner, while the other has a particle at the center.



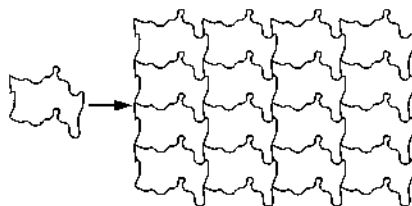
Primitive cells are not unique, as one can see by comparing Figures 1.7(A) and 1.7(B). However all different choices must have exactly the same area. The reason is that in a Bravais lattice the primitive cell contains exactly one particle, while the primitive cells put end to end fill the crystal; therefore the volume of the primitive cell is exactly the inverse of the density of the crystal. Cells are free to have rather peculiar shapes, as in Figure 1.8, just so long as they fit together properly. In two dimensions, one says they form a *tiling* or a *tessellation*.

### 1.2.5 Wigner-Seitz Cells

It is convenient to have a standard way of constructing the primitive cell, and it is valuable to have a primitive cell invariant under all symmetry operations that

leave the crystal invariant. Such a construction is provided by the *Wigner–Seitz primitive cell*. It is built by associating with each lattice point all of space which is closer to it than to any other lattice point. Because this relation does not change under any operation that leaves the lattice invariant, the Wigner–Seitz cell displays the full symmetry of the lattice. The Wigner–Seitz cells for the symmetrical two-dimensional Bravais lattices are shown in Figure 1.4, where their construction is also described.

**Figure 1.8.** An unusual tiling of the plane, as discussed by MacGillavry (1976).



Frequently a convenient way to display the full structure of a crystal is by drawing a *nonprimitive unit cell*: one that contains several particles and that produces the full crystal upon repetition. The rectangular box used in Figure 1.4 to illustrate the construction of the centered rectangular lattice provides an example.

### 1.3 Symmetries

The word symmetry has been used casually in discussing the two-dimensional Bravais lattices, but before continuing to the three-dimensional lattices, it is best to make it a bit more precise.

One motivation for studying crystal structure from the point of view of symmetries is that these are intimately bound up with the experimental observations one is able to make. In the case of scattering, to be studied in Chapter 3, the intensities of peaks result from hosts of details, but the fact of sharp peaks is exclusively the result of lattice symmetries; to understand what a scattering experiment means, one must understand what crystalline symmetries are possible. Equally important is the fact that solutions of Schrödinger's equation in Chapter 7 for electrons in periodic crystals will only be possible when simplifications resulting from symmetry are fully employed.

#### 1.3.1 The Space Group

The general view of symmetries begins from the observation that one is interested in picking the lattice up, moving it rigidly, perhaps rotating or reflecting it, placing it back down, and finding that all the points following this operation overlap the original points. That is, problem is to find the complete set of ways that a given crystal can be transformed so that the distances between all points are preserved, and the crystal perfectly overlap itself after the transformation. Most rigid motions can be composed from simpler ones, so the real goal is to find a minimal set of transformations. Rigid motions include not only translations and rotations, which can be accomplished by twisting a body around in space, but also inversions.

Rigid motions can be described as a translation  $\vec{a}$  plus a rotation  $\mathcal{R}$ :

$$\mathbf{G} = \vec{a} + \mathcal{R}(\vec{r}, \hat{n}, \theta). \quad (1.7)$$

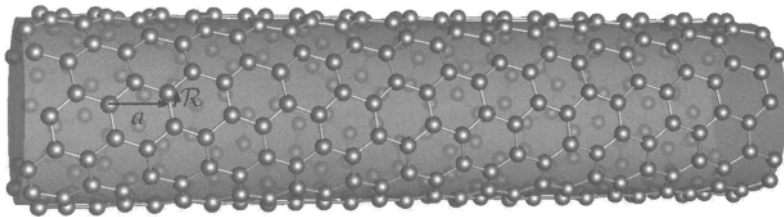
Explicit expressions for  $\mathcal{R}$  in terms of angles and rotation axes appear in books on classical mechanics such as Marion and Thornton (1988) or Goldstein (1980) under the heading of Euler angles.

$\mathcal{R}(\vec{r}, \hat{n}, \theta)$  produces a rotation through  $\theta$  around axis  $\hat{n}$  passing through point  $\vec{r}$ . Operators  $\mathcal{R}$  that invert or reflect the crystal are also allowed.

The complete set of rigid motions that take a crystal into itself is called the *space group*. It is a group (formally defined in Section 7.3) because it consists of a set of operations (rigid motions) with a natural product (perform a first rigid motion, then another—the combined result is still a rigid motion). The unit element consists of doing nothing.

### 1.3.2 Translation and Point Groups

Two subgroups of the space group deserve special mention. The *translation group* consists of translations through all lattice vectors of the form  $n_1\vec{a}_1 + n_2\vec{a}_2 \dots$ , and by definition it leaves the crystal invariant. The *point group* consists of those operations that leave the crystal invariant and which in addition map some particular Bravais lattice point onto itself. It might seem that the space group is simply a product of the point group and the translation group. This is true for Bravais lattices, but not for crystals in general, since there can exist combinations of translation and reflection or rotation that leave a crystal invariant when used together but not separately. The honeycomb lattice (Figure 1.5C) is invariant when translated horizontally by  $a/2$  and then reflected about a *glide line*. *Screw axes*, where a lattice is invariant under a combination of translation and proper rotation neither of which is itself a symmetry, first appear in three dimensions. A *nanotube* with symmetry of this type is shown in Figure 1.9.



**Figure 1.9.** The points on this nanotube map back onto themselves after translation through  $\vec{a}$  and rotation through  $\mathcal{R}$ , but neither of these operations alone is a symmetry of the nanotube.

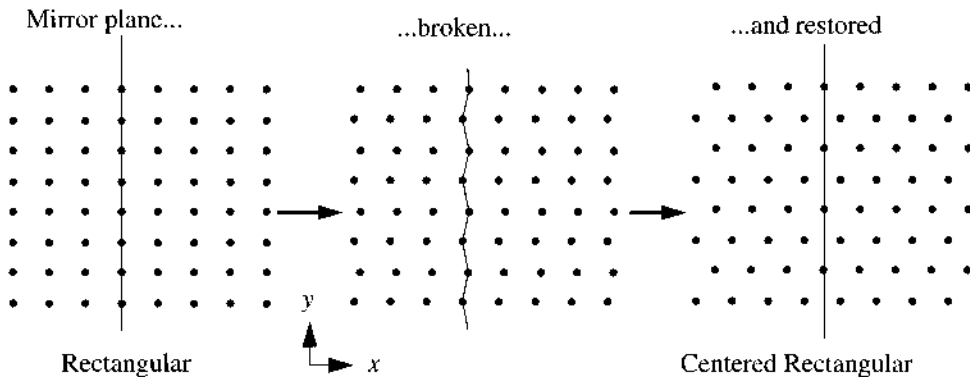
Does the point group of a lattice define the lattice? The answer is no. Different lattices can be invariant under precisely the same set of point symmetry operations. For example, the rectangular and centered rectangular lattices shown in Figure 1.4 have many symmetries in common:

**Translational symmetries:** The two crystals can be translated along arbitrary multiples of their two primitive vectors.

**Point group symmetries:** Choose any lattice point as the origin. Both rectangular and centered rectangular lattices can be reflected about the  $x$  or  $y$  axes, and each is invariant under a  $180^\circ$  rotation.

Because the rectangular and centered rectangular lattices share the same point group symmetries, they are said to belong to the same *crystal system*, but they are not the same lattice.

One might protest that the rectangular and centered rectangular lattices are obviously different because their primitive vectors are different. However, making this argument would lead one to conclude that two square lattices of different size are different as well. The correct question to ask in determining if two lattices are the same is whether one structure can be deformed continuously into the other without losing symmetries along the way. For example, if one lattice is twice the size of another, but otherwise the same, one would want to call them the same. Although centered rectangular and rectangular lattices share point group symmetries, they are different lattices and have different space groups. They are different because there exists no way to deform the first continuously into the second without temporarily destroying some symmetries, as indicated in Figure 1.10.



**Figure 1.10.** In deforming the rectangular lattice into the centered rectangular lattice, reflection symmetry about the  $y$  axis is destroyed.

A more formal expression of this same idea uses the idea of a change of coordinates. Suppose one has a first group of symmetry operations,  $G = \mathcal{R} + \vec{a}$  and a second group  $G' = \mathcal{R}' + \vec{a}'$ . Then the two groups are equivalent if there exists a single matrix  $S$  (change of coordinates) such that

$$S^{-1}\mathcal{R}S + S^{-1}\vec{a} = \mathcal{R}' + \vec{a}'. \quad (1.8)$$

In other words,  $G$  and  $G'$  must be the same up to linear changes of coordinate systems. This definition of equivalent lattices is the same as the previous one, because once one has the matrix  $S$ , then there is a family of matrices

$$S_t = (1-t) + St, \quad (1.9)$$

which varies smoothly between the unit matrix and  $S$  as  $t$  varies between 0 and 1. It generates explicitly a smooth deformation of one lattice into the other while preserving the group operations.

### 1.3.3 Role of Symmetry

Perhaps symmetry is more important for physicists to understand the world than it is for the world itself. Most of the exact statements in physics result from symmetry arguments, and often symmetry provides the only path to making any substantive statement about complicated assemblies of matter. Its importance persists in condensed matter physics, although the discipline's domain includes disordered and noisy systems. Helpful books on the formal theory of symmetry in physics include Heine (1960) and Tinkham (1964).

### Problems

#### 1. Honeycomb lattice:

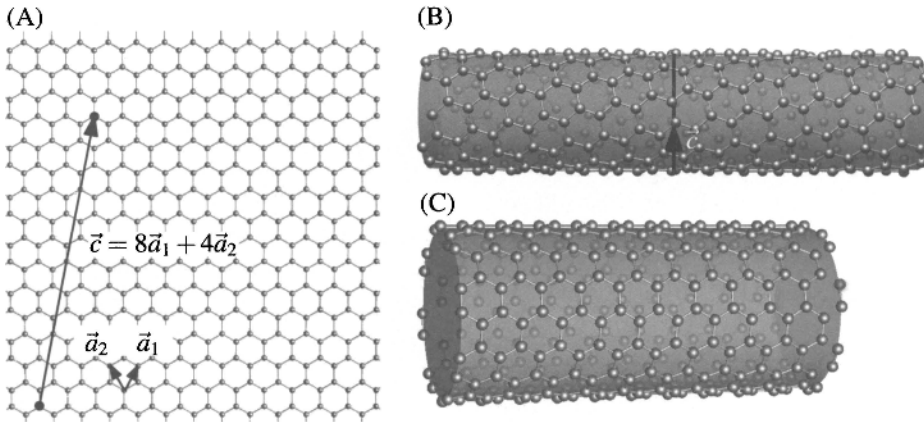
- Verify that the honeycomb lattice described by Eq. (1.5) has properly been constructed so that the distance between all neighboring points is identical.
- From Table 2.1, the lattice spacing of graphene is  $2.46\text{\AA}$ . Find the distance between nearest neighbors (Figure 1.3).
- Find the density of graphene in  $\text{gm/cm}^2$ .

#### 2. Hexagonal lattice:

- The hexagonal lattice may be viewed as a special case of the centered rectangular lattice. Referring to Figure 1.4 and to the conventional unit cell depicted there, find the ratio  $c/a$  for which the centered rectangular lattice would become hexagonal.
- Enumerate the symmetries of the hexagonal lattice, and compare them with the symmetries of the centered rectangular lattice.

3. **Nanotube structures:** To form a *single-walled nanotube*, one rolls up a single atomic layer of graphite, graphene, as shown in Figure 1.11. Referring to Figure 1.11 (A) and (B), all nanotubes can be indexed with two integers  $m$  and  $n$  where  $\vec{c} = m\vec{a}_1 + n\vec{a}_2$  and  $\vec{a}_1$  and  $\vec{a}_2$  are primitive vectors; one created in this way is an  $(m, n)$ -nanotube.

- Are all structures labeled by distinct pairs of integers  $m, n \in (-\infty, \infty)$  different from each other?
- What are the indices for the nanotube appearing in (C)?
- Suppose that the atoms of a two-dimensional crystal lie at locations  $\vec{R}$ , and that the crystal is rolled into a cylinder by pulling together two atoms separated by vector  $\vec{c}$  as shown in Figure 1.11 (A). Write down an explicit expression for locations of atoms after the sheet has been rolled into a tube.



**Figure 1.11.** How to roll a sheet of graphene into a nanotube.

#### 4. Allowed symmetry axes:

- (a) Consider a two-dimensional Bravais lattice that is left invariant after rotation by angle  $\theta$  around the origin. Suppose the lattice to have points at  $(0, 0)$  and  $(a, 0)$ . By requiring the image of  $(a, 0)$  under rotations through  $\pm\theta$  to be in the Bravais lattice, find a simple expression that implicitly specifies all possible rotation axes.
- (b) Prove that the only allowed axes are twofold, threefold, fourfold, and sixfold. In particular, it is impossible for a Bravais lattice to have a fivefold rotation axis.

#### 5. Two-dimensional ground states:

Portions of this problem are most easily carried out with the aid of a computer algebra program or brief compiled programs.

- (a) Consider a collection of particles in two dimensions whose energy is

$$\mathcal{E} = \frac{1}{2} \sum_{i \neq j} \phi(r_{ij}) \quad (1.10)$$

where

$$\phi(r) = \begin{cases} \phi_0 \exp(-r) \left( \frac{1}{r^3} - 1 \right) & \text{if } r < 1.5 \\ 0 & \text{else,} \end{cases} \quad (1.11)$$

and  $r_{ij}$  is the distance (measured, say, in  $\text{\AA}$ ) between particles  $i$  and  $j$ . Find the crystal structure in Figure 1.4 which provides a minimum energy state for this potential, and the equilibrium lattice spacing, assuming no particles are at a distance less than 1. The potential has been chosen so that only nearest neighbors interact in the ground state. Do not check all crystal structures explicitly, only the square and hexagonal lattices.

(b) Suppose that  $\phi$  is replaced by

$$\tilde{\phi}(r) = \begin{cases} \phi_0 \exp(-r) \left( \frac{1}{2r} - 1 \right) & \text{if } r < 1.5 \\ 0 & \text{else.} \end{cases} \quad (1.12)$$

Show that particles would collapse into a state of high density. It is not necessary to perform sums numerically: Consider what happens when particles are so closely spaced that they can be thought of as constituting a continuous distribution.

(c) Taking for  $\phi$

$$\phi(r) = \phi_0 \exp(-r) \left( \frac{1}{r^3} - 1 \right) \quad (1.13)$$

and assuming that the ground state is a lattice of the same symmetry as in part (a), find the equilibrium lattice spacing and energy per particle within 10%. This sum does need to be performed numerically.

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