Mathematics Monograph Series 18

Mathematical Theory of Elasticity of Quasicrystals and Its Applications

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（准晶数学的弹性理论及应用）

SCIENCE PRESS
Beijing

Responsible Editor: Chen Yuzhuo

Published by Science Press
16 Donghuangchenggen North Street
Beijing 100717, P. R. China

Printed in Beijing

ISBN 978-7-03-025669-0

Preface

This monograph is devoted to the development of a mathematical theory of elasticity of quasicrystals and its applications. Some results on elastodynamics and plasticity of quasicrystals are also included to document preliminary advances in recent years.

The first quasicrystal was observed in 1982 and reported in November 1984. At that time several physical and mathematical theories for quasicrystal study already existed. Soon after the discovery, the theory of elasticity of quasicrystals was put forward. Based on Landau-Anderson symmetry-breaking, a new elementary excitation - the phason - was introduced in addition to the well known phonon. The phason concept was suggested in the 1960's in incommensurate phase theory. Group theory and discrete geometry e.g. the Penrose tiling provide further explanations to quasicrystals and their elasticity from the standpoint of algebra and geometry. The phonon and phason elementary excitations form the basis of the theory of elasticity of this new solid phase. Many theoretical (condensed matter) physicists have spent a great deal of effort on constructing the fundamental physical framework of the theory of elasticity of quasicrystals. Applications of group theory and group representation theory further enhance the physical basis of the description. On the basis of the physical framework and by extending the methodology of mathematical physics and classical elasticity, the mathematical theory of elasticity of quasicrystals has been developed. Recent studies on the elasto-/hydro-dynamics and the plasticity of quasicrystals have made preliminary but significant progress. As regards the dynamics, there are various viewpoints in the quasicrystal community, which reveal the unusual characteristics of phason dynamics. Yet the effect of the phason degrees of freedom on plastic deformation is not well understood, and the basic plastic properties of the material are virtually unknown. Because of many unsolved critical issues, the study of quasicrystals has attracted many researchers. The contex of the last few chapters in this book is a probe of the fascinating research area.

As this book is focused on the mathematical theory of elasticity of quasicrystals, it does not include in-depth discussions on the physics of the phason degrees of freedom and the physical nature of the phason variables. These research subjects are important to the quasicrystal study.

I sincerely thank the National Natural Science Foundation of China and the Alexander von Humboldt Foundation of Germany for their support over the years. I also thank Professors Fanghua Li (Institute of Physics in the Chinese Academy of

Science), Longan Ying (School of Mathematics of Peking University), Dihua Ding (Department of Physics, Wuhan University), Jiann-Quo Tarn (Cheng Kung University / Zhejiang University), Weiqiu Chen (Zhejiang University), Qingping Sun (Hong Kong Science and Technology University), U. Messerschmidt (Max Planck Institut fuer Mikrostruktur Physik, Halle), H.-R. Trebin (Institut fuer Theoretische und Angewandte Physik, Universitaet Stuttgart), and K. Edagawa (University of Tokyo) for their helpful discussions. Last but not least, I thank my co-workers and former and present students, especially Professor Xianfang Li (Central South University), for their help and contributions.

Tianyou Fan
January 2010, Beijing

Contents

Chapter 1
Crystals

This book discusses mainly elasticity and defects of quasicrystals, however quasicrystals have inherent connection with crystals. This chapter provides the basic knowledge on crystals which may be beneficial to study quasicrystals and relevant topics.

1.1 Periodicity of crystal structure, crystal cell

Based on X-ray diffraction patterns, it is known that a crystal consists of particles (i.e., collections of ions, atoms and molecules) which are arranged regularly in space. The arrangement is a repetition of the smallest unit, called a unit cell, resulting in the periodicity of a complete crystal. The frame of the periodic arrangement of centres of gravity of particles is called a lattice. Thus, the properties of corresponding points of different cells in a crystal are the same. The positions of these points can be defined by the radius vectors $\boldsymbol{r}$ and $\boldsymbol{r}'$ in the coordinate frame $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$, and $\boldsymbol{a}, \boldsymbol{b}$ and $\boldsymbol{c}$ are three non-mutually co-linear vectors, respectively (the general concept on vector refering to Chapter 2). Hence we have

$$\boldsymbol{r}' = \boldsymbol{r} + l\boldsymbol{a} + m\boldsymbol{b} + n\boldsymbol{c}, \tag{1.1-1}$$

in which $\boldsymbol{a}, \boldsymbol{b}$ and $\boldsymbol{c}$ are the basic translational vectors describing the particle arrangement in a complete crystal, and l, m and n are arbitrary integers. If the physical properties are described by function $f(\boldsymbol{r})$, the above invariance can be expressed mathematically as

$$f(\boldsymbol{r}') = f(\boldsymbol{r} + l\boldsymbol{a} + m\boldsymbol{b} + n\boldsymbol{c}) = f(\boldsymbol{r}). \tag{1.1-2}$$

This is called the translational symmetry or long-range translational order of a crystal, because the symmetry is realized by the operation of translation.

Formula (1.1-1) represents a kind of translational transform, while (1.1-2) shows that the lattice is invariant under transformation (1.1-1). The collection of all translational transform remaining lattice invariant constitutes the translational group.

1.2 Three-dimensional lattice types

Cells of lattice may be described by a parallel hexahedron having lengths of its three sides $\boldsymbol{a}, \boldsymbol{b}$ and $\boldsymbol{c}$ and angles α, β and γ between the sides. According to the relationship of length of sides and angles there are seven different forms observed for the cells, which form seven crystal systems given in Table 1.2-1.

Table 1.2-1 Crystals and the relationship of the length of sides and angles

Crystal system	Characters of cell
Triclinic	$\boldsymbol{a} \neq \boldsymbol{b} \neq \boldsymbol{c}, \alpha \neq \beta \neq \gamma$
Monoclinic	$\boldsymbol{a} \neq \boldsymbol{b} \neq \boldsymbol{c}, \alpha = \gamma = 90° \neq \beta$
Orthorhombic	$\boldsymbol{a} \neq \boldsymbol{b} \neq \boldsymbol{c}, \alpha = \beta = \gamma = 90°$
Rhombohedral	$\boldsymbol{a} = \boldsymbol{b} = \boldsymbol{c}, \alpha = \beta = \gamma \neq 90°$
Tetragonal	$\boldsymbol{a} = \boldsymbol{b} \neq \boldsymbol{c}, \alpha = \beta = \gamma = 90°$
Hexagonal	$\boldsymbol{a} = \boldsymbol{b} \neq \boldsymbol{c}, \alpha = \beta = 90°, \gamma = 120°$
Cubic	$\boldsymbol{a} = \boldsymbol{b} = \boldsymbol{c}, \alpha = \beta = \gamma = 90°$

Among each crystal system there are certain classes of crystals that are classified based on the configuration such that whether the face centre or body centre contains lattice point. For example, the cubic system can be classified as three classes: the simple cubic, body centre cubic and face centre cubic. According to this classification, the seven crystal systems contain 14 different lattice types, called Bravais cells as shown in Fig. 1.2-1.

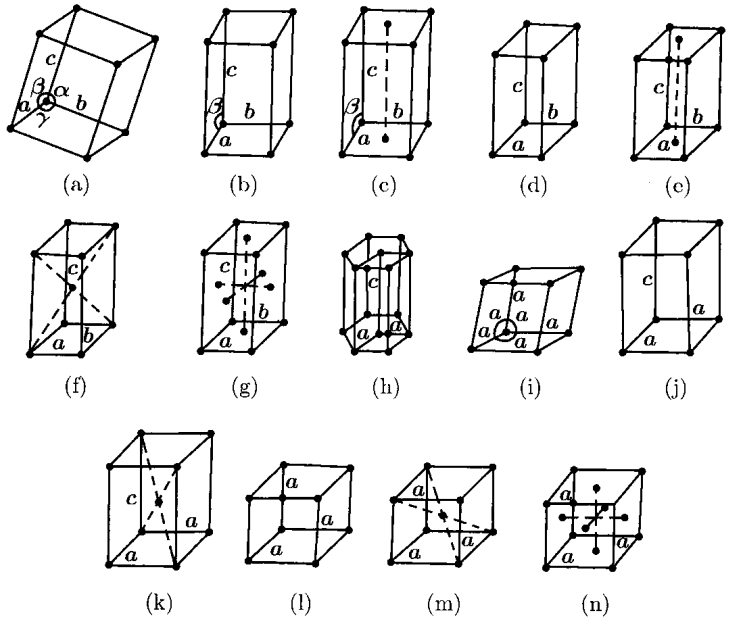

Fig. 1.2-1 The 14 Crystal cells of three-dimension
(a) Simple triclinic, (b) Simple monoclinic, (c) Button centre monoclinic, (d) Simple orthorhombic, (e) Button centre orthorhombic, (f) Body centre orthorhombic, (g) Face centre orthorhombic, (h) Hexagonal, (i) Rhombohedral, (j) Simple tetragonal, (k) Body centre tetragonal, (l) Simple cubic, (m) Body centre cubic, (n) Face centre cubic.

Apart from the above mentioned 14 Bravais cells with three-dimensional lattices, there are 5 Bravais cells of two-dimensional lattice, we do not go any further.

1.3 Symmetry and point groups

In Section 1.1 we have discussed the translational symmetry of crystals. Here we point out that the symmetry reveals invariance of crystals under translational transformation

$$\boldsymbol{T} = l\boldsymbol{a} + m\boldsymbol{b} + n\boldsymbol{c}. \tag{1.3-1}$$

Formula (1.3-1) is referred to as an operation of symmetry, which is a translational operation. Apart from this, there are rotation operation and reflection (or mapping) operation, they belong to so-called point operation. A brief introduction on the rotation operation and orientational symmetry of crystals is given below.

By rotating about an axis through a lattice, the crystal always returns to the original state since the rotational angles are $2\pi/1, 2\pi/2, 2\pi/3, 2\pi/4$ and $2\pi/6$ or integer times of these values. This is the orientational symmetry or the long-range orientational order of a crystal. Because of the constraint of translational symmetry, the orientational symmetry holds for $n = 1, 2, 3, 4$ and 6 only, which is neither equal to 5 nor more greater than 6 where n is the denominator of $2\pi/n$ (e.g. a molecule can have five-fold rotation symmetry, but a crystal cannot have this symmetry because the cells either overlap or have gaps between them when $n = 5$, Fig. 1.3-1 is an example). The fact constitutes the following fundamental law of crystallography:

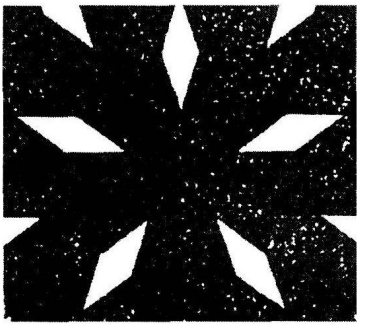

Fig.1.3-1 There is no five-fold rotational symmetry in crystals

Law of symmetry of crystals Under rotation operation, n-fold symmetry axis is marked by n. Due to the constraint of translational symmetry, there are axes $n = 1, 2, 3, 4$ and 6 exist only, neither 5 nor number greater than 6 exists.

In contrast to translational symmetry, rotation is a point symmetry. Other point symmetries are: plane of symmetry, the corresponding operation is mapping, marked by m; centre of symmetry, the corresponding operation is inversion, marked by I; rotation-inversion axis, the corresponding operation is composition of rotation and inversion, when the inversion after rotation $2\pi/n$, marked by $\bar{n}$.

For crystals, the point operation consists of eight independent ones only, i.e.,

$$1, 2, 3, 4, 6, \quad I = (\bar{I}), \quad m = \bar{2}, \bar{4}, \tag{1.3-2}$$

which are the basic symmetric elements of point symmetry.

The rotation operation is also denoted by $C_n, n = 1, 2, 3, 4, 6$.

The mapping operation can also be expressed by σ. The horizontal mapping by m_h and S_h, the vertical one by S_v.

The mapping-rotation is a composite operation, denoted by S_n, which can be understood as

$$S_n = C_n\sigma_h = \sigma_h C_n.$$

The inversion can be understood as

$$I = S_2 = C_2\sigma_h = \sigma_h C_2.$$

Another composite operation—rotation-inversion $\bar{n}$ is related to S_n, e.g. $\bar{1} = S_2 = I$, $\bar{2} = S_1 = \sigma, \bar{3} = S_6, \bar{4} = S_4, \bar{6} = S_3$.

So that (1.3-2) can be redescribed as

$$C_1, C_2, C_3, C_4, C_6, I, \sigma, S_4. \tag{1.3-3}$$

The collection of each symmetric operation among these eight basic operations constitutes a point group, the collection of their composition forms 32 point groups listed in Table 1.3-1.

Table 1.3-1 32 Point groups of crystals

Sign	Meaning of sign	Point group	Number
C_n	Having n-fold axis	C_1, C_2, C_3, C_4, C_6	5
I	Symmetry central	$I(i)$	1
$\sigma(m)$	Mapping	$\sigma(m)$	1
C_{nh}	Having n-fold axis and horizontal symmetry plane	$C_{2h}, C_{3h}, C_{4h}, C_{6h}$	4
$C_{n\nu}$	Having n-fold axis and vertical symmetry plane	$C_{2\nu}, C_{3\nu}, C_{4\nu}, C_{6\nu}$	4
D_n	Having n-fold axis and n 2-fold axes, they are perpendicular to each other	D_2, D_3, D_4, D_6	4
D_{nh}	Meaning of h is the same as before	$D_{2h}, D_{3h}, D_{4h}, D_{6h}$	4
D_{nd}	d means in $D_n$there is a symmetry plane dividing the angle between two 2-fold axes	D_{2d}, D_{3d}	2
S_n	Having n-fold mapping-rotation axis	$S_4, S_6 = C_{3i}$	2
T	Having four 3-fold axes and three 2-fold axes	T	1
T_h	Meaning of h is the same as before	T_h	1
T_d	Meaning of d is the same as previous	T_d	1
O	Having three 4-fold axes which perpendicular to each other and six 2-fold axes and four 3-fold axes	O, O_h	2

Note: $T = C_{3'}D_2$ means the composition between operations $C_{3'}$ and D_2, where suffixes $3'$ denotes a 3-fold axis.

$O = C_{3'}C_4C_{2''}$ means the composition between operations $C_{3'}$, C_4 and $C_{2''}$, where $3'$ represents a 3-fold axis, $2''$ represents a 2-fold axis.

The concept and sign of point groups will be used in the subsequent chapters.

1.4 Reciprocal lattice

The concept of the reciprocal lattice will be concerned in the subsequent chapters, here is a brief introduction.

Assume that there is relation between the base vectors $\boldsymbol{a}_1, \boldsymbol{a}_2$ and $\boldsymbol{a}_3$ of a lattice (L) and the base vectors $\boldsymbol{b}_1, \boldsymbol{b}_2$ and $\boldsymbol{b}_3$ for another lattice (L_R)

$$\boldsymbol{b}_i \cdot \boldsymbol{a}_j = \delta_{ij} = \begin{cases} 1, & i = j, \\ 0, & i \neq j, \end{cases} \qquad i, j = 1, 2, 3, \tag{1.4-1}$$

such that the lattice with the base vectors $\{\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3\}$ is the reciprocal lattice L_R of crystal lattice L with the base vectors $\{\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3\}$. Between $\boldsymbol{b}_i$ and $\boldsymbol{a}_j$ there exist the relationship

$$\boldsymbol{b}_1 = \frac{\boldsymbol{a}_2 \times \boldsymbol{a}_3}{\Omega}, \quad \boldsymbol{b}_2 = \frac{\boldsymbol{a}_3 \times \boldsymbol{a}_1}{\Omega}, \quad \boldsymbol{b}_3 = \frac{\boldsymbol{a}_1 \times \boldsymbol{a}_2}{\Omega}, \tag{1.4-2}$$

where $\Omega = \boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)$ is the volume of lattice cell.

Denote

$$\Omega^* = \boldsymbol{b}_1 \cdot (\boldsymbol{b}_2 \times \boldsymbol{b}_3),$$

then

$$\Omega^* = \frac{1}{\Omega}.$$

The position of any point in the reciprocal lattice can be expressed by

$$\boldsymbol{G} = h_1 \boldsymbol{b}_1 + h_2 \boldsymbol{b}_2 + h_3 \boldsymbol{b}_3 \tag{1.4-3}$$

in which $\boldsymbol{G}$ called the reciprocal vector and

$$h_1, h_2, h_3 = \pm 1, \pm 2, \cdots$$

Points in the lattice can be described by $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$ as well as by $\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3$.

In a similar fashion the concept of the reciprocal lattice can be extended to the higher dimensional space, e.g. six-dimensional space, which will be used in the discussion in Chapter 4.

The brief introduction above provides a background for reading the subsequent text of the book. Further information on the crystals, the diffraction theory, and the point groups can be found in books[1, 2]. We will recall the concepts in the following text.

1.5 Appendix of Chapter 1: Some basic concepts

Some basic concepts will be described in the following chapters, with which most of physicists are familiar. For the readers of non-physicists, a simple introduction is provided as follows; the details can be found in the relevant references.

1.5.1 *Concept of phonon*

In general, the course of crystallography does not contain the contents given in this section. Because the discussion here is dependent on quasicrystals, especially with the elasticity of quasicrystals, we have to introduce some of the simplest relevant arguments.

In 1900, Planck put forward the quantum theory. Soon after Einstein developed the theory and explained the photo-electric effect, which leads to the photon concept. Einstein also studied the specific heat c_v of crystals by using the Planck quantum theory. There are some unsatisfactory points in the work of Einstein although his formula explained the phenomenon of $c_v = 0$ at $T = 0$, where T denotes the absolute temperature. To improve Einstein's work, Debye[3] and Born et al. [4,5] applied the quantum theory to study the specific heat arising from lattice vibration in 1912 and 1913 respectively, and got a great success. The theoretical prediction is in excellent agreement to the experimental results, at least for the atom crystals.

The propagation of the lattice vibration is called the lattice wave. Under the long-wavelength approximation, the lattice vibration can be seen as continuum elastic vibration, i.e., the lattice wave can be approximately seen as the continuum elastic wave. The motion is a mechanical motion, but Debye and Born assumed that the energy can be quantized based on Planck's hypothesis. With the elastic wave approximation and quantization, Debye and Born successfully explained the specific heat of crystals at low temperature, and the theoretical prediction is consistent with the experimental results in all range of temperature, at least for the atomic crystals. The quanta of the elastic vibration, or the smallest unit of energy of the elastic wave is named phonon, because the elastic wave is one of acoustic waves. Unlike photon, the phonon is not an elementary particle, but in the sense of quantization, the phonon presents natural similarity to that of photon and other elementary particles, thus can be named quasi-particle. The concept created by Debye and Born opened the study on lattice dynamics, an important branch of solid state physics. Yet according to the view point at present, the Debye and Born theory on solid belongs to a phenomenological theory, though they used the classical quantum theory.

Landau[6] further developed the phenomenological theory and put forward the concept of elementary excitation. According to his concept, photon and phonon etc.

belong to elementary excitations. In general one elementary excitation corresponds to a certain field, e.g. photon corresponds to electro-magnetic wave, phonon corresponds to elastic wave, etc. The phonon concept is further extended by Born[5]; he pointed out the phonon theory given by Debye corresponds to the vibration as molecule as a whole body, which is called phonetic frequency vibration modes, or the phonetic branch of phonon. In this case the physical quantity phonon describing displacement field deviated from the equilibrium position of particles (atoms, or ions, or molecules) at lattice is also called as phonon field, or briefly phonon. Macroscopically it is the displacement vector $\boldsymbol{u}$ of elastic body (if the crystal is regarded as an elastic body). But Born emphasized that there is another vibration in crystals with compound lattice, i.e., the relative vibration between atoms within a molecule, which is called photonic frequency vibration modes, or photonic branch of phonon. For this branch the phonon cannot be understood simply as macroscopic displacement field. But our discussion here is confined to the frame work of continuum medium, with no concern with the photonic branch, so the phonon field is the macro-displacement field in the consideration.

In many physical systems (classical or quantum systems) the motion presents the discrete spectrum (the energy spectrum or frequency spectrum, which corresponds to the discrete spectrum of an eigen-value problem of a certain operator from the mathematical point of view), the lowest energy (frequency) level state is called ground state, and that beyond the ground state is called excited state. The so-called elementary excitation induces a transfer from the ground state to the state with the smallest non-zero energy (or frequency). Strictly speaking, it should be named lowest energy (or frequency) elementary excitation.

The solid state physics was intensively developed in 1960~70's, then evolved into the condensed matter physics. The condensed matter physics is not only extending the scope of solid state physics by considering the liquid state and micro-powder structure, but also developing the basic concepts and principles. Modern condensed matter physics is established as a result of the construction of its paradigm, in which the symmetry-breaking is in a central place, which was contributed by Landau[6] and Anderson[7] and other scientists.

Considering the importance of the concept and principle of symmetry-breaking in development of elasticity of quasicrystals, we give a brief discussion here.

It is well known that for a system with a constant volume, the equilibrium state thermodynamically requires the free energy of the system

$$F = E - TS \tag{1.5-1}$$

be minimum, in which E is the internal energy, S is the entropy and T is the absolute temperature.