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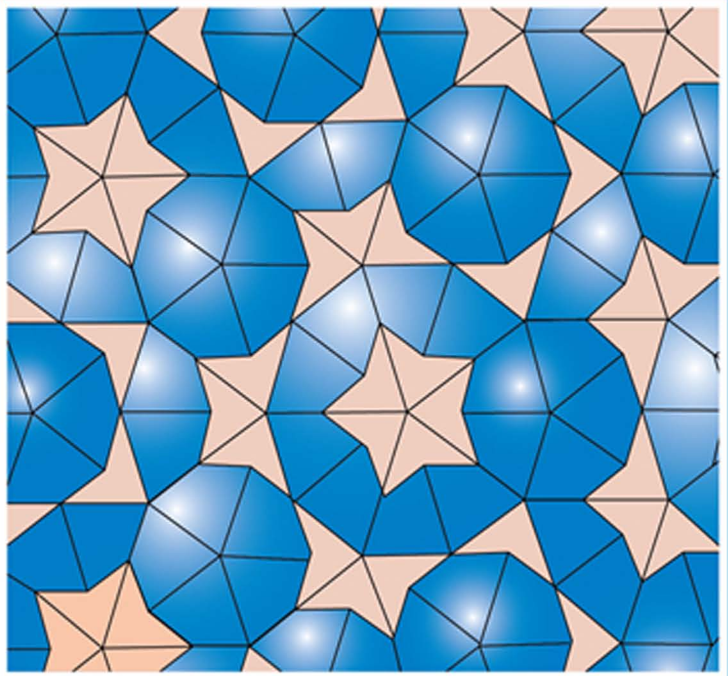
——数学模型和解

GENERALIZED DYNAMICS OF SOFT-MATTER QUASICRYSTALS
——Mathematical Models and Solutions

范天佑　著



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内 容 简 介

The monograph systematically introduces the mathematical models and solutions of generalized dynamics of soft-matter quasicrystals (SMQ). The solutions obtained demonstrate the distribution, deformation and motion of the matter and explore the interactions among phonons, phasons and fluid phonon through some fundamental SMQ samples.

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Preface

As well-known quasicrystals with 12-fold symmetry observed since 2004 in liquid crystals, colloids, polymers and nanoparticles have received a great deal of attention. In particular, 18-fold symmetry quasicrystals in colloids were discovered in 2011. More recently the quasicrystals with 12-fold symmetry were also found in giant surfactants. The formation mechanisms of these kinds of quasicrystals are connected closely with self-assemble of spherical building blocks by supramolecules, compounds, block copolymers and so on and are quite different from that of the metallic alloy quasicrystals. They can be identified as soft-matter quasicrystals exhibiting natures of quasicrystals with soft-matter characters. Soft matter lies in the behaviour of intermediate phase between solid and simple fluid, while the nature of quasicrystals exhibits importance of symmetry as they are highly ordered phase. These features are very complex yet extremely interesting and attractive. Hence, they have raised a great deal of attention of researchers in physics, chemistry and materials science.

All the observed soft-matter quasicrystals so far are two-dimensional quasicrystals. It is well-known that two-dimensional quasicrystals consist of only two distinct types, one being 5-, 8-, 10- and 12-fold symmetries, the other being 7-, 9-, 14- and 18-fold according to the symmetry theory. Therefore, two terminological phrases can be defined such as the first and second kinds of two-dimensional quasicrystals respectively. The two-dimensional solid quasicrystals observed so far belong to the first kind only, while soft-matter quasicrystals discovered up to now can be in both kinds. This may imply that many new types of soft-matter quasicrystals in addition to those with 12- and 18-fold symmetries may be observed in the near future. Hence, the interdisciplinary studies on soft-matter quasicrystals present great potential and hopeful research topics.

However, some difficulties exist in studying those new phases due to the complexity of their structures and lack of fundamental experimental data including the material constants to date. Furthermore, the theoretical studies are also difficult. For example, the symmetry groups of soft-matter quasicrystals observed or possibly to be observed have not yet been well investigated although there are some work being done (the details are not to be included in the book). In conjunction with this issue, the study on constitutive laws for phonons and phonon-phason coupling is still difficult.

In spite of these problems, there are potential efforts to undertake the study of these topics. For example, the soft-matter quasicrystals as a new ordered phase are connected with broken symmetry or symmetry breaking, like those discussed in solid quasicrystals. Thus, the elementary excitations such as phonons and phasons are important issues in the study of quasicrystals based on the Landau phenomenological theory. For soft-matter quasicrytals, furthermore, another elementary excitation, i.e., the fluid phonon must be considered besides phonons and phasons. According to the Landau school, liquid acoustic wave *is fluid* phonon (refer to Lifshitz EM and Pitaevskii LP, *Statistical Physics, Part 2*, Oxford: Butterworth-Heinemann, 1980). This is suitable for describing the liquid effect of soft-matter quasicrystals, which can be seen as complex liquids or structured liquids. The elementary excitations—phonons, phasons and fluid phonon—and their interactions constitute the main feature of the new phase. They will be discussed as a major issue in the book. The concept of the fluid phonon is introduced in the study of quasicrystals for the first time. Related to this, the equation of state should also be introduced. With these two key points and in reference to the hydrodynamics of solid quasicrystals, the dynamics of soft-matter quasicrystals can be established, but with an important distinction compared with that of solid quasicrystals. The present hydrodynamics cannot be linearized due to the nonlinearity of equation of state. To overcome the difficulty arising from other aspects in theory, we can draw from study of solid quasicrystals (For example, Lubensky TC, *Symmetry, elasticity and hydrodynamics in quasiperiodic structures*, in Introduction to Quasicrystals, ed by Jaric MV, Boston: Academic Press, 199–289, 1988; Hu CZ et al, *Symmetry groups, physical property tensors, elasticity and dislocations in quasicrystals*, Rep. Prog. Phys., 63(1), 1–39, 2000; Fan TY, *Mathematical Theory of Elasticity of Quasicrystals and Its Applications*, Beijing: Science Press/Heidelberg: Springer-Verlag, 1st edition, 2010, 2nd edition, 2016). This shows that the theory of solid quasicrystals is a basis for the present discussion, which provides an initial glimpse from the viewpoint of quantitative analysis into the rich phenomena of soft-matter quasicrystals.

Some applications are given by describing the distribution, deformation and motion of soft-matter quasicrystals. The mathematical principle and its applications require the assistance of other areas of knowledge, a part of which is briefly listed in the first six chapters of the book (for more details, refer to Chaikin J and Lubensky TC, *Principles of Condensed Matter Physics*, New York: Cambridge University Press, 1995), and the others are introduced in the due computation. The computational results are preliminary and very limited so far, but verify partially the mathematical model, and explored in certain degree to distinguish the dynamic behaviour between soft-matter and solid quasicrystals. In addition, the specimens and flow modes adopted in the computation might be intuitive, observable and verified easily. However, it does not mean that they belong to the most important samples.

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Tian-You Fan
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注：本书采用全英文撰写，书中的表达方式与国际通用习惯保持一致。

Notations

$\mathbf{r}$	Radius vector
D	Domain
S	Boundary of domain
S_u	Boundary part at which the displacements are given
S_t	Boundary part at which the tractions are given (or S_σ at which the applied stresses are given**)**
ρ	Mass density (g/cm^3)
p	Fluid pressure (Pa=N/m^2)
$\mathbf{u}$	Phonon-type displacement field (cm)
$\mathbf{w}$	Phason-type displacement field (or second phason displacement field only for quasicrystals with 7-, 9-, 14- and 18-fold symmetry) (cm)
$\mathbf{V}$	Fluid velocity field (or fluid phonon field) (cm/s)
$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$	Phonon strain tensor
$w_{ij} = \frac{\partial w_i}{\partial x_j}$	Phason strain tensor (or second phason strain tensor only for quasicrystals of the second kind)
$\dot{\xi}_{ij} = \frac{1}{2}\left(\frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i}\right)$	Fliud phonon deformation rate tensor (1/s)
σ_{ij}	Phonon stress tensor (Pa)
H_{ij}	Phason stress tensor (or second phason stress tensor only for quasicrystals of the second kind) (Pa)
σ'_{ij}	Viscous stress tensor (Pa)
$p_{ij} = -p\delta_{ij} + \sigma'_{ij}$	Fluid phonon stress tensor (Pa)

C_{ijkl}	Phonon elastic coefficient tensor (Pa)
K_{ijkl}	Phason elastic coefficient tensor(or second kind phason elastic coefficient tensor only for quasicrystals for second kind of quasicystals) (Pa)
R_{ijkl}	Phonon-phason coupling elastic coefficient tensor (u–w coupling elastic coefficient tensor) (Pa)
η	First viscosity coefficient of fluid (0.1Pa • s=Poise)
η / ρ	First kinetic viscosity coefficient of fluid (cm^2/s)
ζ	Second viscosity coefficient of fluid(0.1Pa • s=Poise)
ζ / ρ	Second kinetic viscosity coefficient of fluid (cm^2/s)
Re	Reynolds number
$\Gamma_{\mathbf{u}}$	Phonon dissipation coefficient (m^3 • s/kg)
$\Gamma_{\mathbf{w}}$	Phason dissipation coefficient (or the second kind phason dissipation coefficient only for quasicrystals of the second kind) (m^3 • s/kg)
$\mathbf{v}$	First phason-type displacement field (only for second kind quasicrystals) (cm)
$v_{ij} = \dfrac{\partial v_i}{\partial x_j}$	First phason strain tensor (only for second kind quasicrystals)
τ_{ij}	First phason stress tensor (only for the second kind quasicrystals) (Pa)
r_{ijkl}	Phonon-first phason coupling elastic coefficient tensor (or u–v coupling elastic coefficient tensor only for the second kind quasicrystals) (Pa)
Γ_v	The first kind phason dissipation coefficient of quasicrystals (m^3 • s/kg)

Contents

Chapter 1

A Brief Introduction to Soft Matter

Soft-matter quasicrystals are observed in liquid crystals, colloids, polymers and surfactants, which belong to some kinds of soft matter. Soft matter is the common title, introduced by de Gennes [1] in 1991, of liquid crystals, colloids, polymers, foams, emulsions, surfactants, biomacromolecules etc.; they are neither ideal solid nor simple fluid, but present characters of both solid and fluid, belonging to an intermediate phase between isotropic fluid and ideal solid macroscopically. Sometimes, one calls them anisotropic fluids or structured fluids [2–5], or more exactly, anisotropic liquids or structured liquids.

The Chinese chemists argue [6] that if every atom or a molecular possesses the thermal energy $k_B T$, in an ideal solid, e.g. solid crystal, here k_B is the Boltzmann constant, T the absolute temperature, the thermal energy per unit volume $k_B T / l^3$, may characterize an entropy state of the crystal, here $l \sim 0.1$ nm is the lattice size or interatomic distance. For soft-matter systems, the structure and dynamic properties are related with mesoscopic size $l \sim 10-100$ nm (e.g. the size of long-chain of polymers, or size of self-assembly structures, etc.) and fluctuation, thermal motion and self-organization or self-assembly, which are often induced by entropy, whose thermal energy per unit volume may be denoted by $k_B T / l^3$. Apparently, at room temperature, the thermal energy per unit volume of soft matter is of 6–9 order of magnitude lower than that of the ideal crystals, this may explain the softness of soft matter from point of view of intra-structure of materials. In contrast, the ideal solid presents very highly stiffness. This distinction between soft matter and ideal solid is significant. In some cases we have to draw some lessons from crystal study, the thermal energy per unit volume concept may provide a basis by some analogies between soft matter and ideal solid. The other differences between soft matter and conventional materials will be discussed in the following description, but there is not possible to study them in detail and in-depth in the book.

For simplicity, we here consider only the hydrodynamics of soft-matter quasicrystals. Strictly speaking only the fluidity, or the flow effect from point of view of fluid is considered apart from elasticity and interaction between fluidity and elasticity of the matter. The fluidity, elasticity and their interaction are only a part of the behaviour of soft matter, which can help us understand the deformation and motion of soft-matter quasicrystals in macroscope. In this case the micro-scale structures of the matter have not been concerned. Although the meso-scale structures are important for soft matter, it has not been concerned in general in our presentation apart from some special exceptions. In this sense, the modelling on hydrodynamics of soft matter and soft-matter quasicrystals is a macro- and continuum-medium study, with low-frequency and long-wavelength characters, which have been discussed in solid quasicrystals, and can be extended to the present study.

Among various kinds of soft-matter systems, liquid crystals are typical and relatively well studied, and their material constants are more detailed. The phenomenological, i.e. from macroscopic and continuum point of view, understanding of liquid crystals provides us some insights, which are beneficial and useful for studying the mechanical behaviour of soft-matter quasicrystals. For example, in some cases, the Newton’s fluid law can approximately be used, and the Hooke’s elasticity law can also be used, but the deformation is comparatively complex, which consists of bulk deformation and deformation induced by curvature variation for liquid crystals. For the bulk deformation the conventional Hooke’s law still holds, and for the deformation due to curvature one needs some additional expressions, which are not related with the discussion in this chapter and omitted here, except in Chap. 12, there we have to mention the quantity arising from curvature of smectic A liquid crystals, which is very interesting. Because of the intermediate phase between simple fluid and ideal solid, the soft matter presents many behaviour different from those of isotropic liquids and ideal crystals. For example, in ordinary liquid, and in nematic liquid crystals, there is only one acoustic wave speed, i.e., longitudinal wave sound speed. In solid crystals and amorphous solids, there are three acoustic wave speeds under the linear deformation, i.e. $c_1 = \sqrt{\frac{\lambda + 2\mu}{\rho}}$ (or $c_1 = \sqrt{\frac{L + 2M}{\rho}}$), $c_2 = c_3 = \sqrt{\frac{\mu}{\rho}}$ (or $c_2 = c_3 = \sqrt{\frac{M}{\rho}}$), refer to the discussion in Chap. 10 of the book [7]. For smectic A liquid crystals, there is only one nonzero displacement component, belonging to one-dimensional crystals, or saying, their elastic deformation is in anti-plane state, or longitudinal shear state. If it is pure solid, it has only one acoustic wave speed $\sim \sqrt{\frac{E}{\rho}}$ where E is the elastic modulus and ρ is the mass density; if it is pure fluid, there is only one acoustic speed $\sim \sqrt{\frac{\partial p}{\partial \rho}}$, where p is the fluid pressure. For smectic A liquid crystals there are both acoustic wave speeds $\sim \sqrt{\frac{E}{\rho}}$ and $\sim \sqrt{\frac{\partial p}{\partial \rho}}$ and the former often depends upon the angular between wave vector $\mathbf{k}$ and the normal vector $\mathbf{n}$ of the layer of the smectic A liquid crystal. From this example, we can see that the soft matter presents behaviour different from those of simple fluid and ideal solid. Because soft matter present some very complicated nonlinear behaviour, whose spectra and dispersion relations cannot be easily determined, so the wave speeds. Some time one introduces $\sqrt{\frac{\lambda + 2\mu}{\rho}}$, $\sqrt{\frac{\mu}{\rho}}$ and $\sqrt{\frac{\partial p}{\partial \rho}}$ (in some cases we denote $\sqrt{\frac{\partial p}{\partial \rho}} = c_4$ for simplicity) to describe wave speeds propagating in soft matter, this is only a coarse approximation, and the realistic wave speeds in the matter present differences with those in magnitude and nature, and relevant mechanism is not so clear. In the succeeding introduction to computations, we will partly reveal these questions.

For liquid crystals, the dynamic viscosity describing fluid effect $\eta = 0.1\ \text{Pa} \bullet \text{s} = 1\ \text{Poise}$, which is the dynamic viscosity coefficient, sometime, the kinetic viscosity coefficient η / ρ will also be used. Note that the unit is cm^2/s rather than Poise; and the elastic modulus describing the bulk deformation $E = 10^8\ \text{erg/cm}^3 = 10^7\ \text{Pa} = 10\ \text{MPa}$; and the Poisson's ratio ν may be negative unlike that for solid; these quantities are very fundamental and useful for us, and we can draw them as the basic material constants for soft-matter quasicrystals within the discussion, and are frequently used in our computation. Although liquid crystals do not completely represent other kinds of soft matter, their viscosity is quite large (for about larger 100 times than that of water), and meantime with a certain elasticity. In general, for simple fluid one has not considered its elasticity; while for ideal solid one does not consider its viscosity (at least which is not so important). In the introductions in the following chapters, when we carry out the analysis and computation on deformation and motion of soft-matter quasicrystals, the experiences and data accumulated in the study of liquid crystals are good references for us. Apart from these, some data, e.g. the phonon dissipation coefficient Γ_{u} and phason dissipation coefficient Γ_{w} for soft-matter quasicrystals, are not available, which we have to draw relevant values from solid quasicrystals as a reference.

Another important feature of motion of soft matter is that it presents usually small Reynolds number Re. According to the definition, $Re=\dfrac{\rho Ua}{\eta}$, in which a represents the characteristic size of the matter or flow field. Because the characteristic velocity U is small and the viscosity coefficient η is great, in general, the Reynolds number is small, i.e., $Re=10^{-4}\sim 1$. In this case the force due to viscosity is greater than that due to inertia. We can take the Stokes assumption omitting the inertia terms in the equation of motion in some time, like that done in the classical fluid dynamics. This simplifies the equations, but which are still very complicated, the analytic solution, even if an approximate analytic solution, is not available and not like that in the classical fluid dynamics, there one has obtained quite lot of approximate analytic solutions. Although the equations in the classical fluid dynamics are complex, which are much simpler than those in hydrodynamics of soft matter. It should be pointed out that the Stokes approximation in the two-dimensional case leads to the famous Stokes paradox—there will be no solution. Oseen [8] deeply analyzed the Stokes paradox physically. To overcome the paradox, the Stokes approximate equations must be modified, they should be replaced by Oseen approximate equations and leads to reasonable solutions in the two-dimensional case. The further discussion on this can refer to Sommerfeld [9], Sleozkin [10] and Kochin et al. [11]. When we discuss the soft-matter dynamics, especially the two-dimensional problems, we will touch the similar problems, and the Oseen theory is very important and useful for us. Note that [10] pointed out Oseen approximation holds for the cases $Re < 10$, which is helpful for the study of soft matter.

In summary, in the previous introduction concerning soft matter is very limited and preliminary, which only provides the most elementary knowledge for presentation and application in the current chapter. The readers are suggested to refer monographs [2–5] for a further understanding of soft matter such a great broader field with fruitful contents. The hydrodynamics and possible hydrodynamics will be introduced in the subsequent chapters.

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