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Phase Transitions and Crystal Symmetry

相变和晶体对称性

Y.A.Izyumov V.N.Syromyatnikov

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国外物理名著系列序言

对于国内的物理学工作者和青年学生来讲，研读国外优秀的物理学著作是系统掌握物理学知识的一个重要手段。但是，在国内并不能及时、方便地买到国外的图书，且国外图书不菲的价格往往令国内的读者却步，因此，把国外的优秀物理原著引进到国内，让国内的读者能够方便地以较低的价格购买是一项意义深远的工作，将有助于国内物理学工作者和青年学生掌握国际物理学的前沿知识，进而推动我国物理学科研和教学的发展。

为了满足国内读者对国外优秀物理学著作的需求，科学出版社启动了引进国外优秀著作的工作，出版社的这一举措得到了国内物理学界的积极响应和支持，很快成立了专家委员会，开展了选题的推荐和筛选工作，在出版社初选的书单基础上确定了第一批引进的项目，这些图书几乎涉及了近代物理学的所有领域，既有阐述学科基本理论的经典名著，也有反映某一学科专题前沿的专著。在选择图书时，专家委员会遵循了以下原则：基础理论方面的图书强调“经典”，选择了那些经得起时间检验、对物理学的发展产生重要影响、现在还不“过时”的著作(如狄拉克的《量子力学原理》)。反映物理学某一领域进展的著作强调“前沿”和“热点”，根据国内物理学研究发展的实际情况，选择了能够体现相关学科最新进展，对有关方向的科研人员和研究生有重要参考价值的图书。这些图书都是最新版的，多数图书都是2000年以后出版的，还有相当一部分是当年出版的新书。因此，这套丛书具有权威性、前瞻性和应用性强的特点。由于国外出版社的要求，科学出版社对部分图书进行了少量的翻译和注释（主要是目录标题和练习题)，但这并不会影响图书“原汁原味”的感觉，可能还会方便国内读者的阅读和理解。

“他山之石，可以攻玉”，希望这套丛书的出版能够为国内物理学工作者和青年学生的工作和学习提供参考，也希望国内更多专家参与到这一工作中来，推荐更多的好书。

杨国桢

中国科学院院士

中国物理学会理事长

Phase Transitions and Crystal Symmetry

Preface

About half a century ago Landau formulated the central principles of the phenomenological second-order phase transition theory which is based on the idea of spontaneous symmetry breaking at phase transition. By means of this approach it has been possible to treat phase transitions of different nature in altogether distinct systems from a unified viewpoint, to embrace the aforementioned transitions by a unified body of mathematics and to show that, in a certain sense, physical systems in the vicinity of second-order phase transitions exhibit universal behavior.

For several decades the Landau method has been extensively used to analyze specific phase transitions in systems and has been providing a basis for interpreting experimental data on the behavior of physical characteristics near the phase transition, including the behavior of these characteristics in systems subject to various external effects such as pressure, electric and magnetic fields, deformation, etc.

The symmetry aspects of Landau's theory are perhaps most effective in analyzing phase transitions in crystals because the relevant body of mathematics for this symmetry, namely, the crystal space group representation, has been worked out in great detail. Since particular phase transitions in crystals often call for a subtle symmetry analysis, the Landau method has been continually refined and developed over the past ten or fifteen years. A general survey of the various trends in the evolution of Landau's theory in the past two decades is presented at the end of §1. The object of the present book is to provide an exhaustive account of the current state of Landau's theory of phase transitions as applied to crystals. The particular physical nature of a phase transition itself is of no fundamental importance, since the various (structural, magnetic, ferroelectric, and other) transitions are described in terms of a unified scheme based on the mathematical foundations of the theory of space group representations.

A special challenge to the authors was the exposition of methods that permit analysis of phase transitions in crystals of arbitrary complexity. In keeping with this goal, efficient techniques are handled and developed in this book allowing one to determine the principal characteristic of a system undergoing a phase transition, that is, the order parameter, from a knowledge of the symmetry groups of the initial and final phases, or to enumerate all the symmetry-allowed phases that are likely to arise as a result of a second-order phase transition from the initial phase. Methods are presented of constructing polynomial expansions of the thermodynamic potential in powers of a multi-component order parameter. The exposition of the general theory and methods is illustrated with numerous examples of typical phase transitions of different nature, so that the reader may learn independently to apply this material in practice. This is facilitated also by a number of tables compiled by the authors, which furnish in compact form the necessary information related to irreducible representations of space groups.

Some chapters of the book deal with the analysis of phase diagrams in the space of thermodynamic-potential parameters and in the space of generalized thermodynamic forces. Consideration is given to the most important thermodynamic potential types, and the analysis performed in the book shows what kind of physical effects may be expected to occur in specific, more complicated, cases and what devices should be invoked to accomplish such an analysis.

Along with the exposition of general methods, the book provides an overview of recent developments in a number of new branches of the physics of phase transitions, such as transitions to incommensurate phases, and the branch concerned with the role of fluctuations.

Thus the present book combines and gives a sufficiently detailed treatment of both major constituents of the contemporary phase transition theory — symmetry theory and fluctuation theory. By doing so, the authors have tried to show how the underlying suggestion by Landau that second-order phase transitions display a universal symmetry-governed behavior has been revived in fluctuation theory as the universality of the critical indices, which depend only on the number of components of the order parameter, that is, ultimately on symmetry again.

Taking into account the systematic and fundamental character of presentation, it is hoped that the sophisticated reader will find in the book a general and fairly exhaustive treatment of a large domain of the theory of phase transitions in crystalline systems, as well as some new techniques of symmetry analysis at a phase transition. As for the reader who has just started studying phase transition theory, he will be able to master methods of analysis and to learn how to apply these in solving particular problems. The reader who is unconcerned with the mathematical machinery of phase transition theory and wishes only to become acquainted with the most fundamental results of the theory is recommended, on reading the first introductory chapter of the book, to start reading the last four chapters.

The authors wish to express their sincere appreciation to Prof. I.E. Dzyaloshinsky for his support of the idea to write this book, for the numerous bits of advice as to the selection of the topics involved, and for the criticism and discussions that have helped to improve the text.

Preface to the English Edition

Nearly five years have passed since the Russian edition of the book appeared. In this time span some problems of the phenomenological theory of phase transitions in crystals have been the subject of intensive research and have evolved into new independent provinces. Three major areas have arisen: the theory of reconstructive phase transitions, aspects associated with the exploitation of color symmetry, and the theory of incommensurate structures.

It is these new areas of research activity that have received considerable attention in the present English edition (Chapters 8–10). Chapters 8 and 10, dealing with reconstructive transitions and color symmetry, have been written especially for the English edition. Chapter 9, devoted to incommensurate structures, has been substantially revised and enlarged.

Chapter 8 treats martensitic phase transitions from the b.c.c. to the f.c.c. and h.c.p. phases. These transitions are certainly first-order transitions and go without the group-subgroup relation. However, a decisive role in these transitions attaches to strains, from which one may construct the order parameter and use the expansion of the thermodynamic potential in powers of it, in the spirit of Landau's second-order phase transition theory. In describing the transition itself and the characteristic pretransient phenomena, an important role pertains to inhomogeneous states, which are soliton solutions of non-linear equations of elasticity theory. Chapter 8 provides a systematic review of recent developments in the problem of martensite transformations.

Chapter 10 treats a set of phase transitions whose description calls for color symmetry. Here belong transitions to incommensurate structures and quasicrystals and also phase transitions in systems described by a quantum mechanical order parameter. Traditionally, color symmetry is used to describe and classify structures. This chapter lays emphasis on the more important physical meaning of the color groups as a mathematical machinery that enables one to ascertain the role of physical interactions responsible for the occurrence of specific structures. Consideration is given also to another aspect of color symmetry, the so-called color supersymmetry — the symmetry of multidimensional lattices, in terms of which a generality of commensurate-incommensurate and melt-quasicrystal transitions is established. Section 20 contains a new subsection that deals with orientational phase transitions, and the bibliography of Chapter 1 has been supplied with fresh references.

It is hoped that the enlarged English edition of the book contains a practically complete up-to-date exposition of problems in the theory of phase transitions in crystals, which is based on the concept of the order parameter and on symmetry.

Most sincere thanks are due to Prof. A. Janner and Prof. J. Birman who have recommended including in the English edition many of the above problems, and also we would like to express our sincere gratitude to Dr. D.J. Larner who has given us an opportunity, on behalf of the D. Reidel Publishing Company, to introduce the aforementioned additions. For technical assistance in preparing the English manuscript, we would like to thank Vyacheslav Reprintsev.

Yuri Izyumov

Vladimir Syromyatnikov

Notation

G	crystal space group
G_κ	wave-vector group
$g = \{h\|\tau_h\}$	space group element with h its rotational part and τ_h its accompanying translation
$\mathbf{t}_n$	arbitrary integral translation of the crystal
$\mathbf{b}$	arbitrary reciprocal-lattice vector
$\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$	primitive reciprocal-lattice vector
κ	wave-vector
$\{\kappa\}$	wave-vector star
κ_L	star arm
l_κ	number of star arms
g_L	representative element of the decomposition of group G_κ relative to a subgroup
$d^{\kappa\nu}$	wave-vector group irreducible representation
l_ν	dimension of the representation
$D^{\{\kappa\}\nu}$	space group irreducible representation
d_p^κ	permutational representation of group
d_m^κ	mechanical representation of group
d_M^κ	magnetic representation of group
τ	irreducible representation of group G_κ according to Kovalev's tables
$\psi_\lambda^{\kappa\nu}$	irreducible-representation basis function
$C_\lambda^{\kappa\nu}$	mixing coefficients of the basis functions of an irreducible representation
η_λ or ξ_λ	order parameter component
n	number of order parameter components
ϕ	phase of the complex order parameter
Φ	thermodynamic potential

r	coefficient of a quadratic expansion term
u_p	coefficients of quartic expansion terms
δ	coupling coefficient of the concomitant and leading order parameters

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