Symmetry and Condensed Matter Physics

A Computational Approach

对称和凝聚态物理学中的计算方法

Michael El-Batanouny and Frederick Wooten

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Symmetry and Condensed Matter Physics

Unlike existing texts, this book blends for the first time three topics in physics: symmetry, condensed matter physics, and computational methods, into one pedagogical textbook. It includes new concepts in mathematical crystallography; experimental methods capitalizing on symmetry aspects; nonconventional applications such as Fourier crystallography, color groups, quasi-crystals and incommensurate systems; and concepts and techniques behind the Landau theory of phase transitions.

The textbook adopts and develops a computational approach to the application of group theoretical techniques to solving symmetry-related problems. This dramatically alleviates the need for intensive calculations, even for the simplest systems, usually found in the presentation of symmetry. Writing computer programs helps the student achieve a firm understanding of the underlying concepts, and sample programs, based on Mathematica®, are presented throughout the book.

Containing over 150 exercises, this textbook is ideal for graduate students in condensed matter physics, materials science, and chemistry. Solutions and computer programs are available online at www.cambridge.org/9780521828451.

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This book is dedicated to my loving wife Gloria, to the memory of my parents Maurice and Hayat, and to my sister Nagwa. (ME)

Preface

Pedagogical presentation and analysis of the symmetry aspects of physical systems in terms of group theoretical concepts and methodology has been evolving over the past six or seven decades, since the pioneering textbooks by Weyl and Wigner first appeared. This constantly evolving pedagogy has resulted in over a hundred textbooks on the subject. The impetus behind these efforts has stemmed from the general recognition of the invaluable role that the application of such methodology plays in determining and predicting the properties of a physical system.

Symmetry concepts provide a very useful means for systematizing the description of a physical system in terms of its energy and momentum, and other relevant physical quantities. Furthermore, the incipient methodologies furnish a very efficient framework for classifying its physical states, and a crucial machinery for simplifying the intervening numerical applications of physical laws. By means of the irreducible representations of its symmetry group, one can classify physical states and particles in a logical way and establish selection rules, which predict restrictions on possible transitions between different physical states. The use of symmetry also simplifies numerical calculations, for example, in solving the Schrödinger equation for condensed matter systems. Moreover, from the symmetry properties of a physical system, one can make conclusions about the values of measurable physical quantities, and, conversely, one can trace a symmetry group of a system from observed regularities in measured quantities. There is also an intimate connection between symmetry, invariance and dynamical laws.

Despite all these merits, the application of symmetry methods has been seriously hampered by the need for painstaking and tedious calculations, even when dealing with the simplest group symmetries. This drawback has led many students and practitioners in the area of condensed matter physics to shy away from learning the fundamentals of this invaluable discipline.

In the recent past, a number of new ideas, techniques and approaches have emerged that have yet to be incorporated in textbooks on symmetry. We believe that the adoption of these novel aspects within a new pedagogical approach would dramatically simplify existing instructional procedures, remove the cumbersome calculational barriers that tend to severely limit the scope of examples and exercises, and provide a conduit for elucidating and unifying seemingly diverse aspects under one umbrella. We attempt to implement such an approach in this book, and present the necessary tools for its application in diverse areas in condensed matter physics.

One of the novel features characterizing this book and setting it apart from others is that it adopts and develops at the outset a computational approach to the theory of finite groups and its applications in physics. A computational approach to group theory has several significant advantages. First, it eliminates traditional difficulties encountered in problem solving. Second, it provides an alternative pedagogical process whereby a student would learn the material through writing computer programs: A logical prerequisite for program writing is that the student must have acquired a detailed understanding of the material at hand!

The modern basis for computational methods in group and representation theories dates from the 1960s, with the development of computer algorithms for generating permutation groups and studying their structure, and with the introduction of John Dixon's method for the *exact* calculation of "characters" of finite groups, which can be easily implemented on a computer. Currently, there are at least two computational systems that are well suited for the analysis of symmetry groups: GAP and MAGMA; they can be accessed through the web. However, here we shall follow the methods proposed by Stig Flodmark and Esko Blokker. These authors, recognizing the importance and utility of Dixon's method, developed computer algorithms and programs to implement Dixon's exact character method, and to use the results to construct the corresponding unitary irreducible matrix representations.

We develop the underlying ideas, algorithms and methodology for such calculations in the first seven chapters. The reader is first exposed to the relevant conceptual aspects, then introduced to corresponding computational algorithms, and instructed in methods for implementing these algorithms into programs and subroutines. We find that *Mathematica*, because of its capability to handle symbolic and combinatorial manipulations, provides a natural and convenient environment for the development of such programs. So, the main instructions in the computational approach will be based on the language of *Mathematica*. However, every student will be encouraged to develop programs in any language he or she is comfortable with. Our versions of all the *Mathematica*-based computational programs will be posted on a website, together with data files relevant to space- and point-groups.

Our work is intended to make the computational approach to group theory available to a wider audience. It is aimed at students in the physical sciences: physics, chemistry, materials science and, possibly, some disciplines in engineering. We also have in mind the working professional who would like to learn the subject or who already knows it but is unfamiliar with the modern computational approach.

In addition to adopting computational techniques, we introduce and develop several concepts that have, at best, been marginally treated in textbooks on symmetry, to date.

We develop the ideas of group actions on systems and their decomposition into orbits and strata. We demonstrate and stress the fundamental relevance of the study of the corresponding orbit space and of the set of strata to physical problems. For example, we demonstrate how the notions of the *star of the wavevector*, which appears in the theory of representations of space-groups, of *Wyckoff positions*, which are encountered in crystallography, and of images of the order-parameter of a phase transition are all manifestations of orbits. Thus, we inadvertently apply these concepts to different domains of condensed matter physics, without realizing that they are actually decompositions into orbits and strata made under different names, and, in fact they should be unified under one umbrella. Thus, linear representations, which are engendered by group action on a basis set, are just a particular case of group actions. Group actions are introduced in Chapter 6. Subsequently, their use and appearance are stressed when appropriate.

In Chapter 6, we also introduce the concept of symmetry-projection operators and develop the computational tools for their construction, using their hermiticity and idempotency properties to cast the corresponding matrices into the form of a simple eigenvalue problem.

In Chapter 8, we introduce the notions of subgroups, cosets, normal subgroups, product groups, Kronecker products, and Clebsch–Gordan series; and end by presenting techniques for determining the Clebsch–Gordan coefficients. In Chapter 9, we explore the processes of induction and subduction of irreducible representations (Irreps) and the concept of compatibilities relating these Irreps.

In Chapter 10, we present a long and comprehensive exposé of crystallography. The novel feature of this chapter is the detailed presentation of concepts in mathematical crystallography. These include a detailed discussion of arithmetic holohedries and classes, as well as Bravais classes, classification of space-groups with respect to affine conjugations, site-symmetries, and Wyckoff positions and sets. Another unique feature of this chapter is a section on Fourier crystallography, which is one of the two methods used to study the symmetries of quasi-crystals in Chapter 18. In Chapter 11, we develop the machinery for determining the Irreps of symmorphic and nonsymmorphic space-groups.

In Chapter 12, we introduce time-reversal symmetry, and discuss the concepts of double-groups. We include in this chapter a long section on color, or Shubnikov, groups and another section detailing the construction of corepresentations. The section on the color groups includes dichromatic (black and white) point-groups, lattices and space-groups. It also discusses the extension of these concepts to polychromatic symmetries. Another section on crystal-field theory is presented and extended to cover the case of dichromatic symmetry. We end this chapter with a detailed discussion of the manifestation of time-reversal symmetry in transport properties, which is elegantly cast in the Onsager reciprocity relations.

The remaining chapters, 13–18, are dedicated to applications in diverse fields of condensed matter physics. We have extended the applications beyond the usual topics taken up in most texts on the subject. In Chapter 13 we develop the theory of tensors, present techniques for the construction of symmetry-adapted tensors, and finally present a catalog of the different material tensors. We end this chapter with an exposé of tensor fields and their relation to symmetry projection operators.

Chapter 14 develops the basic principles of the electronic structure of solids and methods for computation. The final section presents how the special features of the electronic structure of magnetically ordered systems can be viewed and classified in terms of corepresentations. Chapter 15 develops methods for computing and classifying the dynamical properties of solids and solid surfaces.

Chapter 16 is dedicated to the discussion of symmetry-based experimental techniques such as neutron and atom scattering, angle-resolved photoemission, and Raman spectroscopy.

The Landau theory of phase transitions is discussed in detail in Chapter 17. Applications to commensurate–incommensurate and magnetic phase transitions are given. A long section is devoted to methods of construction of the *Landau free energy*, including ones based on the theory of invariant polynomials, group action, and order-parameter image groups.

Finally, Chapter 18 addresses the fundamental aspects of the symmetry of quasi-crystals and incommensurate systems. The symmetries of these systems are developed along two tracks. First, the concepts of hyperspace symmetries and their projection onto the natural lower-dimensional spaces are presented. Second, the application of the techniques of Fourier space crystallography, developed in Chapter 10, are discussed.

The main emphasis, throughout this book, is on exposing the *conceptual* building blocks of this mathematical theory of symmetry. Consequently, we frequently skip over long detailed mathematical proofs which can be found in a multitude of textbooks. Instead, we point the reader to references where such proofs are clearly presented. Moreover, in contrast to previous texts on the subject, the different aspects of group theory are presented wherever they are needed rather than being lumped into one single exposé. This has the merit of associating a certain aspect of the theory with a tangible physical attribute. Thus, for example, we defer the introduction of cosets and invariant subgroups till we discuss space-groups, where they find immediate application.

Our interest throughout is in clarity and simplicity rather than elegance. We have striven to meet the needs of the beginner who must work through the gory details of many simple examples, much as we ourselves did in trying to learn the subject matter. We do not wish to hide these details in compact mathematical notation.

Contents

1

Symmetry and physics

1.1 Introduction

The application of *group theory* to study physical problems and their solutions provides a formal method for exploiting the simplifications made possible by the presence of symmetry. Often the symmetry that is readily apparent is the symmetry of the system/object of interest, such as the three-fold axial symmetry of an NH_3 molecule. The symmetry exploited in actual analysis is the symmetry of the Hamiltonian. When alluding to symmetry we usually include geometrical, time-reversal symmetry, and symmetry associated with the exchange of identical particles.

Conservation laws of physics are rooted in the symmetries of the underlying space and time. The most common physical laws we are familiar with are actually manifestations of some universal symmetries. For example, the homogeneity and isotropy of space lead to the conservation of linear and angular momentum, respectively, while the homogeneity of time leads to the conservation of energy. Such laws have come to be known as universal conservation laws. As we will delineate in a later chapter, the relation between these classical symmetries and corresponding conserved quantities is beautifully cast in a theorem due to Emmy Noether.

At the day-to-day working level of the physicist dealing with quantum mechanics, the application of symmetry restrictions leads to familiar results, such as selection rules and characteristic transformations of eigenfunctions when acted upon by symmetry operations that leave the Hamiltonian of the system invariant.

In a similar manner, we expect that when a physical system/object is endowed with special symmetries, these symmetries forge conservation relations that ultimately determine its physical properties. Traditionally, the derivation of the physical states of a system has been performed without invoking the symmetry properties, however, the advantage of taking account of symmetry aspects is that it results in great simplification of the underlying analysis, and it provides powerful insight into the nature and the physics of the system. The mathematical framework that translates these symmetries into suitable mathematical relations is found in the theory of groups and group representations. This is the subject we will try to elucidate throughout the chapters of this book.

Let us begin with a tour de force, exploring the merits of invoking symmetry aspects pertinent to familiar but simple problems. We start by reminding ourselves of the trivial example of using symmetry, or asymmetry, to simplify the evaluation of an integral.

Consider

$$\int_{-b}^{+b} \sin x \, dx = 0.$$

We *know* this to be true because $\sin x$ is an odd function; $\sin(-x) = -\sin(x)$. In evaluating this integral, we have taken advantage of the asymmetry of its integrand. In order to cast this problem in the language of symmetry we introduce two mathematical operations: I, which we will identify later with the operation of inversion, and which, for now, changes the sign of the argument of a function, i.e. $I\,f(x) = f(-x)$; and E, which is an identity operation, $E\,f(x) = f(x)$. This allows us to write

$$\int_{-b}^{+b} \sin x \, dx = \int_{0}^{b} (E + I)\, \sin(x)\, dx = \int_{0}^{b} \big(1 + (-1)\big)\, \sin(x)\, dx = 0.$$

Figure 1.1 shows schematically the plane of integration, with $\oplus$ and $\ominus$ indicating the sign of the function $\sin x$.

We may introduce a more complicated integrand function $f(x, y)$, and carry the integration over the equilateral triangular area shown in Figure 1.2.

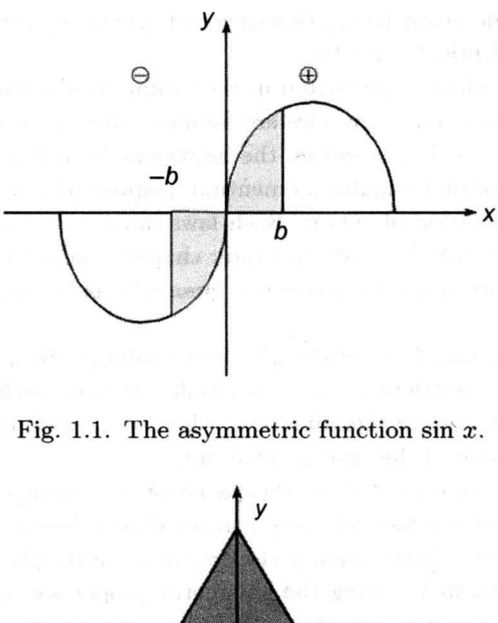

Fig. 1.1. The asymmetric function $\sin x$.

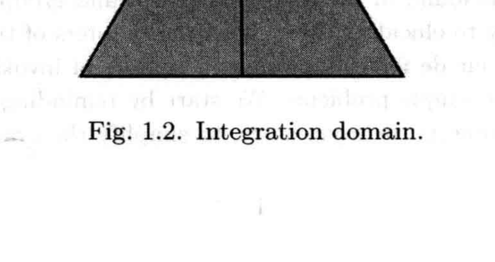

Fig. 1.2. Integration domain.

Making use of the 3-fold symmetry of the triangle, which includes rotations by multiples of $2\pi/3$, as well as reflections shown in Figure 1.3, we write the integral in the form

$$\int_{\text{triangle}} f(x,y)\,dx\,dy = \int_{\text{wedge}} \left(E + O_{(2\pi/3)} + O_{(4\pi/3)} + \sigma_1 + \sigma_2 + \sigma_3\right) \times f(x,y)\,dx\,dy,$$

where the Os represent counterclockwise rotations by the angle specified in the suffix, and the σs are defined in Figure 1.3. Now, if the function $f(x,y)$ possesses a symmetry which can be associated with that of the triangle, as for example shown in Figure 1.4, the integral vanishes.

Later, we will see how to reach similar conclusions in the case of selection rules, for example, where the situation may be much more complicated.

Next, we present a simple example to demonstrate how to invoke symmetry to simplify the solution of dynamical problems. We consider a system of two masses and three springs as illustrated in Figure 1.5. Assume both masses to be equal to m and that all springs have the force constant κ. In that case, the Hamiltonian, which is the

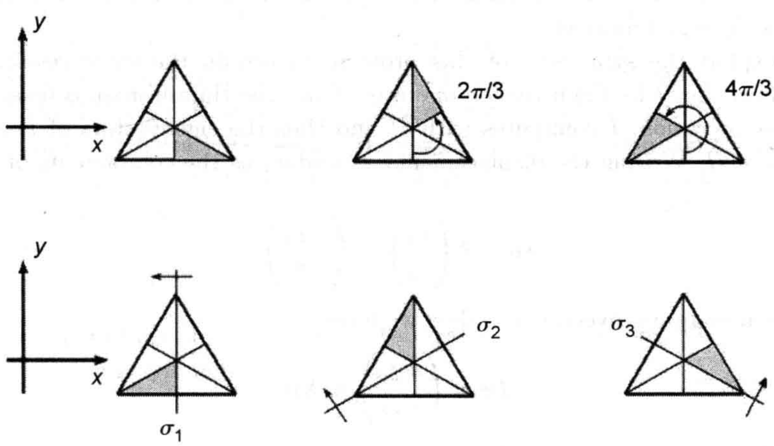

Fig. 1.3. Symmetry operations of an equilateral triangle.

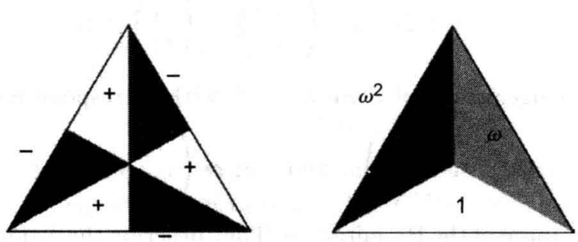

Fig. 1.4. Some possible symmetries of $f(x,y)$ on an equilateral triangle.