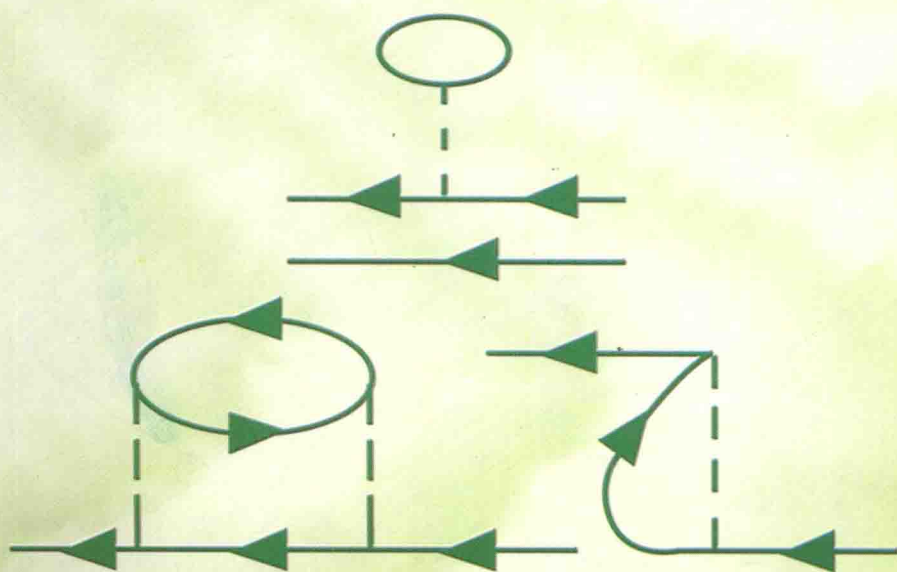


# GREEN'S FUNCTIONS FOR SOLID STATE PHYSICISTS

固态物理学家的格林函数



S. DONIACH & E. H. SONDHEIMER

Imperial College Press

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# **GREEN'S FUNCTIONS FOR SOLID STATE PHYSICISTS**

**A REPRINT VOLUME WITH ADDITIONAL MATERIAL ON  
THE PHYSICS OF CORRELATED ELECTRON SYSTEMS**

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# **GREEN'S FUNCTIONS FOR SOLID STATE PHYSICISTS**

## Preface to the Imperial College Press edition.

A lot has happened in the field of condensed matter physics since the original edition of "Green's functions for Solid State Physicists" was published in 1974. Nevertheless, the book has helped introduce several generations of condensed matter physics graduate students to the very powerful ideas of quantum many body theory and some of their applications, particularly those in the physics of itinerant magnetism and superconductivity that have nowadays come to be called "the correlated electron problem".

In preparing for the reprint edition, two new chapters have been added to the original text to provide an introduction to the recent developments in this branch of condensed matter physics. Chapter 11 focuses on the understanding of the Kondo problem which grew out of the exact solutions developed in the mid 1970's. The accompanying growth of experimental work culminating in the discovery of the heavy fermion superconductors gave substance to the idea that Coulomb repulsion between electrons in a narrow band metal can actually lead to attraction between the electrons and resulting instabilities at low temperatures to either a superconducting or an antiferromagnetic state.

Then in 1986, the discovery by Bednorz and Mueller of high  $T_c$  superconductivity in the cuprate compounds provided a bombshell in the field of correlated electron systems. For the first time it was possible to have materials in a superconducting state at temperatures well above that of liquid nitrogen. Nevertheless, in spite of more than 10 years of very intensive research by physicists in many countries, the mechanism of high  $T_c$  superconductivity remains a mystery at the fundamental level. Chapter 12 offers an introduction to some of the basic theoretical ideas of the physics of the cuprate compounds.

Although the theoretical concepts leading to the understanding of superconductivity, which resulted from the fundamental work of Bardeen, Cooper and Schrieffer in the 1950's, still provide some of the theoretical underpinnings for high  $T_c$ , there are still many aspects of the properties of these materials which do not fit in with the elementary quasiparticle ideas of Fermi liquid theory. Consequently it has become clear that new physical concepts need to be developed to explain these properties. A brief introduction to the physics of one-dimensional metals is included

at the end of chapter 11 to serve as a basis for some of the new ideas in the physics of two-dimensional metals which may be applicable to high  $T_c$ . Their application in two dimensions is briefly introduced at the end of chapter 12.

The final chapter on understanding high  $T_c$  cannot be written at this time. Nevertheless it is our hope that this reprint edition, with the new material, will serve as an introduction and stimulus to the next generation of condensed matter physicists who seek to work on this challenging class of problems.

Sebastian Doniach  
Stanford, California  
Winter 1998

## Preface

During the last 15 years the Green's function methods of quantum field theory have become generally recognized as a powerful mathematical tool for studying the complex interacting systems of solid state physics. In writing this elementary account we have tried to show the method in action, so that—without bothering about lengthy formal preliminaries—we use it from the start to discuss physical problems. The idea is to show in practice how the mathematics—in the form of the analytic properties of the Green's function in the complex energy plane—accounts for the physical effects (level shifts, damping, instabilities) characteristic of interacting systems. We concentrate on general physical principles and do not discuss experiments in detail, but we have included introductions to topics of current research interest such as the Mott metal-insulator transition and the singularities (x-ray, Kondo) associated with transient perturbations in an electron gas. We hope that the reader will feel compensated for any loss in generality of treatment by being kept in contact with real problems.

In the first three chapters the Green's function technique is illustrated on the exactly solvable example of the harmonic vibrating lattice. We go on to discuss scattering by random impurities in a gas of non-interacting fermions and show how to calculate the electrical conductivity of a metal. We then turn to the interacting fermi gas, devoting particular attention to magnetic instabilities. We finish with a short chapter on superconductivity. Two appendices deal briefly with second quantization and the fluctuation-dissipation theorem. We have also included a historical note on George Green. We have omitted several important subjects such as classical liquids, liquid helium, critical phenomena, and the details of the Landau theory of fermi liquids. Our choice of topics has been determined by our tastes and interests and should not be taken as canonical.

The book grew out of a course of intercollegiate graduate lectures given by S.D. in the University of London. We hope that it will appeal to beginning graduate students in theoretical solid state physics, as a first



introduction to more comprehensive or more specialized texts, and also to experimentalists who would like a quick, if impressionistic, view of the subject. A basic knowledge of solid state physics and quantum mechanics, at undergraduate honors or first-year graduate level, is assumed.

We are indebted to a number of colleagues for their interest and helpful comments. We are particularly grateful to Dr. W. G. Chambers for showing us the treatment given in Appendix 1, and to the chairmen of our departments for facilitating consultation at close quarters.

S. DONIACH  
E. H. SONDEIMER

## Introduction

# The Theory of Condensed Matter

The science of condensed matter (thermodynamics, hydrodynamics, etc.) is in many ways much older than that of the atomic constituents. However, it is only in the last two or three decades that a systematic mathematical formulation of the many-body problem—with the  $10^{23}$  or so degrees of freedom needed to describe a macroscopic sample—has become developed so that the properties of the simplest classes of condensed matter can be related back quantitatively to the properties of the constituent atoms.

There are two fundamental classes of properties possessed by condensed matter which belong essentially to its many-body character and do not occur for the individual constituent degrees of freedom. One is the existence of propagation—the notion of a sound wave, the transport of electronic charge in metals, the propagation of light in insulators; the other is the occurrence of phase transitions by which the matter changes its fundamental symmetry—for classical systems melting and freezing, for quantum systems phenomena such as magnetism, superconductivity and superfluidity. Both classes of effects involve phenomena of long range, spreading over distances much greater than the effective range of the basic atomic forces which mediate them.

What is the nature of the mathematical construction which links the atomic to the condensed description of matter? Its formulation takes on many guises, but the essential feature is that, even when the individual atomic interactions may be treated, in some sense, as “weak,” the properties of the condensed system can only be treated correctly by taking them into account in infinite order. The most elementary example of such an infinite-order process leads to the occurrence of propagation through the “handing on” of excitation energy from one atom to the next. We shall see in Chaps. 1–3 that a natural formalism with which to set up the theory of the propagation phenomenon is the Green’s function

approach, which in a classical system reduces to the theory of correlation functions.

For a single degree of freedom the Green's function, or inverse differential operator, gives the amplitude of the degree of freedom at time  $t$ , given its amplitude at some previous time  $t'$ . This may refer either to a localized degree of freedom (e.g., a single atomic oscillator) or to a non-localized system (e.g., the amplitude of an electron wave function at position  $\mathbf{x}$  at time  $t$ , given that at position  $\mathbf{x}'$  at time  $t'$ ). The many-body effects are then embodied in the repeated emission of Huyghens wavelets as the electron propagates through the medium, giving rise to an infinite series of multiply scattered waves which sums to provide the Green's function for an electron interacting with the medium (which may consist of other electrons). In this way one can obtain the response of complex interacting systems to simple forms of excitation without having to find the full eigenvalue spectrum, a task which is generally neither practicable nor of physical interest. The relation between the Green's function formalism and scattering theory will be studied in Chaps. 4 and 5.

A major simplification which occurs for homogeneous many-body systems is that the low-lying excited states with energies near the ground state can often be simply described in terms of the resulting propagating modes. Because of their mode-like nature (with rather well-defined excitation energy  $\omega_{\mathbf{k}}$  as a function of the propagation wave-vector  $\mathbf{k}$ ) the quanta of these elementary excitations are referred to as quasiparticles. The Green's function approach to the theory of elementary excitations is developed in Chaps. 1-6 through the study of a series of specific examples drawn from solid state physics. We shall see how the Green's function determines the excitation spectrum through its analytic properties in the complex energy plane. We also show how the excitations produced by applied external fields can be formulated in terms of Green's functions, leading to general expressions for measured quantities such as electrical conductivities and magnetic susceptibilities. An important property of Green's functions is that they are related, via the fluctuation-dissipation theorem, to time correlation functions which determine scattering cross-sections and which also give the averages needed to discuss properties of the ground state of the system (or, at finite temperature, the thermal equilibrium state). These relationships are illustrated a number of times in the text.

The phase transition phenomenon can also be reached via the elementary excitation concept. For some quantum systems this may be studied at zero temperature by seeing how an excited state, of lower symmetry than the ground state, becomes degenerate with the ground state as the interaction strength is increased. This "softening" of the excitation energy will show up as a singularity of the Green's function at the instability point of the system. In classical systems this singular behavior reduces to the Ornstein-Zernike theory of the two-particle correlation function. In Chaps. 7-10 we discuss the instability phenomenon in the context of the magnetic and superconducting instabilities of the interacting electron system. We also show how, once in the state of lower symmetry, the system acquires a new spectrum of elementary excitations which are no longer unstable.

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## Chapter 1

### Lattice Dynamics in the Harmonic Approximation

We start our exploration of the Green's function approach by considering the problem of a lattice of interacting vibrating atoms. Within the harmonic approximation this represents perhaps the simplest type of many-body problem. By transforming to normal-mode coordinates the hamiltonian can be reduced to that of a set of independent oscillators and can thus be diagonalized exactly. But such exact closed solutions can only be obtained in quantum mechanics in exceptional cases, and it is therefore worth studying this problem by means of a more general formalism which can also be applied to more complicated cases, such as the important but much more difficult problem of the lattice dynamics of an *anharmonic* crystal. This is one reason for studying the harmonic problem by means of Green's functions. Another is that the Green's function approach provides a unified systematic method for calculating various quantities of physical interest. Thus we shall see that it gives the ground state energy of the system, or—more generally—the free energy at non-zero temperature, from which the thermodynamic properties such as the specific heat can be obtained.

In addition to these equilibrium properties, Green's functions also provide information on the excitation energies of a system. For example, scattering processes correspond to excitations in which one particle is added to the system, and we shall consider the scattering of thermal neutrons by the lattice vibrations as an example of this. There is also an important class of excitations in which the particle number is conserved; the theory of linear response to an externally applied field describes such excitations and, as we shall see in later chapters, provides expressions for dielectric response functions, electrical conductivities and magnetic susceptibilities in terms of appropriately defined Green's functions. Green's functions thus make it possible to evaluate measurable thermodynamic and transport properties by studying the response of a system to simple perturbations. This approach is particularly important for



interacting many-particle systems, where the complete set of wave functions and energy levels is highly complex but is not in fact needed for studying properties related to experiment.

In the first three chapters we use the harmonic lattice as an exactly soluble example to study and compare the principal methods for calculating Green's functions. The physical phenomena produced by the interaction between atoms in this case are the propagating modes—excitation energy is handed on from one atom to the next so as to produce traveling sound waves (quantized as phonons). We shall find later that in more complicated cases also there exist excitations which take the form of sets of coupled oscillators—plasmon excitations in the case of an electron gas with Coulomb interactions (Chap. 6), and spin waves in the case of an insulating magnet (Chap. 8). Thus the phonon Green's function serves also as a prototype for studying a number of other interacting systems of interest in solid state physics.

## 1.1 THE GROUND STATE ENERGY

We consider the hamiltonian

$$H = \sum_i \frac{\mathbf{p}_i^2}{2M} + \frac{1}{2} \sum_{i \neq j} V(\mathbf{X}_i - \mathbf{X}_j), \quad (1.1.1)$$

which describes a simple lattice composed of  $N$  identical interacting atoms of mass  $M$  situated at the points  $\mathbf{X}_i$  ( $i = 1, 2, \dots, N$ ). It is assumed that the potential energy  $V$  is a two-body potential which depends only upon the relative positions of pairs of atoms. We write  $\mathbf{X}_i = \mathbf{R}_i + \mathbf{u}_i$ , where  $\mathbf{R}_i$  is an undisplaced lattice point and the lattice displacement  $\mathbf{u}_i$  is assumed to be small. In the harmonic approximation  $V$  is expanded in powers of the  $\mathbf{u}_i$  as far as second-order terms. Since the expansion is about the equilibrium configuration the coefficients of the linear terms are zero, and the expansion is

$$H = \sum_i \frac{\mathbf{p}_i^2}{2M} + \frac{1}{2} \sum_{i \neq j} \sum_{\alpha\beta} \frac{1}{2!} (u_i^\alpha - u_j^\alpha)(u_i^\beta - u_j^\beta) \nabla^\alpha \nabla^\beta V, \quad (1.1.2)$$

where  $u_i^\alpha$  is a cartesian component of  $\mathbf{u}_i$ .

To separate out the interaction between different atoms we rewrite