

INTRODUCTION TO

THE THEORY OF

DISORDERED SYSTEMS

Il'ya M. Lifshits • Sergei A. Gredeskul • Leonid A. Pastur

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INTRODUCTION TO THE THEORY OF DISORDERED SYSTEMS

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Le hasard est la réserve de Dieu. Le Tout-Puissant ne fait donner sa réserve qu'en des circonstances graves, surtout depuis qu'il a vu les hommes assez sagaces pour étudier et prévoir les chances d'après la nature et les éléments régulièrement organisés

Or, Dieu aime ou doit aimer à déjouer les combinaisons de ces orgueilleux . . . avec les éléments qui leur sont incommes, ou dont ils ne peuvent prévoir l'intervention.

Cette théorie, comme on le voit, renferme de spécieux arguments, et fournir de brillantes thèses

ALEXANDRE DUMAS, *Les Quarante-Cinq*

(Chance is what God keeps in reserve. The Almighty resorts to it only in important circumstances, particularly now that the sagacity of human beings is such that they are able to see into the future while observing nature and comprehending its laws

Yet God likes to disrupt the designs of the arrogant and does so by means of the unknown, the intrusion of which humans do not perceive.

This theory, if buttressed by cogent arguments, might serve as the basis of brilliant philosophical theses)

PREFACE

In recent decades the physical community and scientists in related fields have shown an increasing interest in the structure and properties of disordered condensed systems. The reasons for this are twofold: the advances of solid-state physics and its numerous applications, and the fact that disordered systems (crystals with impurities, liquid metals, amorphous substances, and the like) are, in a way, systems of a generic nature, while ordered structures such as the perfect crystal lattice are, strictly speaking, idealized objects. But the existing theory of ordered condensed systems depends to a great extent on the notion of the ideal structure of such systems and therefore cannot be applied to disordered systems without substantial modifications. Indeed, we know how important the notion of translational symmetry is to the electron theory of metals or the dynamical theory of the crystal lattice. It enables us to describe the low-lying levels of a macroscopic system in terms of various quasi-particles characterized by quasi-momentum and a dispersion law. The corresponding classification of states has a simple and universal structure and produces a transparent statistical description of elementary excitations and the mechanism of the kinetic phenomena associated with these excitations. In particular, the notions of quasi-particle collisions and the mean free path are introduced in kinetics with respect to the changes in the particle quasi-momentum, and the entire terminology is based mainly on these notions.

The energy spectrum of the low-lying states of a disordered condensed system is more complicated. In the first place there are branches in the spectrum that correspond to the single-particle picture, that is, resemble quasi-particles. But since no translational symmetry is present, the systematics of even the single-particle states proves to be more difficult than in the case of ordered systems, and the spectrum structure is more diversified. For instance,

besides states whose amplitude has the same order of magnitude over the bulk of the crystal (similar to the Bloch functions in an ordered system) there are also localized states. If the system is strongly disordered, the fraction of localized states is considerable (for example, in one dimension all states are localized) and greatly influences the kinetic phenomena.

Besides quasi-particles there may be other types of excitations in disordered systems. For instance, correlation effects prove to be important in a system of interacting electrons in a random impurity field. Here two states with closely lying energy levels correspond to two different ways in which the electrons are distributed over the impurity sites, and the behavior of the density of single-particle states differs from that in the single-particle picture, namely, there appears a so-called Coulomb gap (see Shklovskii and Efros, 1979).

Excitations that exist due to local rearrangement of the particles constituting the frame of a solid may also play an important role. These excitations are connected with the quantum transitions of the entire system between configurations that differ only in the positions of a small number of frame particles. If the energies corresponding to these configurations are close and the energy barrier separating them is not too high, then the transition time is small compared with the characteristic observation time, and hence the excitations of this type are in equilibrium. One of the important consequences of the existence of the simplest of such excitations, two-level excitations, is the linear behavior of the low-temperature specific heat of amorphous substances (see Anderson, *et al.*, 1972).

Today the physics of disordered systems constitutes a wide and highly diversified part of the physics of the condensed state. For this reason the topics discussed in works devoted to various aspects of the theory of disordered systems are so diverse and the number of works so great that it is very difficult to give a coherent exposition of the ideas and results of these works, at least in a book of reasonable size. The present monograph makes no attempt of this kind. It is devoted to the one-body approximation in the theory of disordered systems.

The point is that, just as in the case of ordered systems, even a one-body approximation enables us to formulate a number of basic concepts, perceive many of the characteristic features of disordered systems, and study various interesting phenomena. The scope of problems studied within the framework of this approximation is rather extensive and at present constitutes a highly developed part of the theory. This book, therefore, endeavors to give an exposition of the general and well-established facts of the one-body theory of disordered systems.

We will mainly be analyzing the structure of the energy spectrum and the quantum states of such systems, that is, our most important task will be to study the density of states and the space-time correlation functions, in terms of which we express the basic thermodynamic and kinetic characteristics within the framework of the one-body approximation. However, the choice of subject matter for the realization of the stated program is obviously subjective.

This is true also of the literature cited, which in no way can be considered complete.

The widely used versions of the one-body approximation are the motion of a particle in a random field and of a system of coupled oscillators in an aperiodic structure. The first is important in describing the behavior of an excess electron in a solid, while the second is important in explaining the vibrational spectrum, the spin-wave spectrum, and the exciton spectrum in condensed media. The reader must bear in mind, however, that the results obtained via such models are much less universal than in the ordered case. In a periodic structure the translational and point symmetries alone provide considerable model-independent information about the systematics of quantum states and the quasi-particle spectrum, while in disordered systems there are many more possibilities. But certainly these models are of considerable generality, and many of the laws which they obey are of a fundamental nature. For instance, in the regions of the spectrum that are neighborhoods of the spectrum singularities (genuine spectrum boundaries, one-impurity levels, or the boundaries of a "bare" spectrum when the system is only slightly disordered), the quantum states allow a simple and transparent systematics (see Lifshits, 1964), which considerably narrows the possibilities mentioned above. Much of the present monograph is devoted to studies of these regions.

In Chapter 1 we give briefly the description of the one-body models most widely used in the book and, in general, in the theory of disordered systems. We also discuss the general properties inherent in such systems: the spatial homogeneity on the average and the disappearance of statistical correlations between the disorder parameters at points far apart. One of the most important consequences of these properties is the fact that specific extensive quantities (such as the density of states and the conductivity) are self-averaged, that is, such quantities in a macroscopically large system are always nonrandom. The abovementioned properties also explain a number of general properties of the spectrum, such as the nonrandomness of the boundaries, the fact that the discrete spectrum is dense, and the criteria for the localization and delocalization of states. Moreover, in this chapter we present the widely accepted qualitative picture of the spectrum structure and the behavior of various correlation functions in disordered systems. This picture employs, among other things, quasi-classical reasoning and the ideas used in percolation theory.

Chapters 2 and 3 are devoted to one-dimensional problems. In the theory of disordered systems, just as in other fields of theoretical physics, one is able to move quite far ahead in studying one-dimensional models. The fact that here the space is assumed to be one-dimensional enables one to write closed dynamical equations (that is, equations valid in each realization) for quantities that determine the properties of the system under investigation. The structure of these equations is always such that they can be used as a basis for deriving other, nonrandom equations (of the Fokker-Planck and Smoluchowski types) for the probability densities of the corresponding quantities. In some cases one

is able to solve these equations in closed form; when this is not possible, a study of the dynamics of the system (that is, the properties of individual random equations) for characteristic regions of the spectrum makes it possible to predict the structure of the solutions of the respective nonrandom equations and, starting from this, to develop an approximate method for finding these solutions.

In Chapter 2 we use this approach to study the density of states for many one-dimensional systems, and most of the results are exact.

More complex characteristics (than the density of states) of one-dimensional disordered systems are considered in Chapter 3. The main consequence of the absence of translational invariance in disordered systems is the presence of a macroscopically large number of localized states in such systems. This feature, which constitutes the main difference between disordered and ordered systems, leads to a radical change in the kinetic properties. Such effects manifest themselves most strongly in one-dimensional systems, where even a weak random potential leads to localization of all the states of the system; as a result the diffusion coefficient and the dc conductivity vanish (we are speaking, of course, of the one-body approximation). In this respect one-dimensional systems are essentially disordered; therefore, the methods of solid-state physics usually prove to be invalid for studying such systems.

However, by employing the method of Fokker-Planck equations, which exploits the intrinsic features of one-dimensional topology and is developed in Chapter 2, we are able to study in detail the structure of states of one-dimensional systems (the localization range of wave functions, the nature of the spectrum, etc.) and their kinetic properties (the density-density correlation function and conductivity). More complete results are obtained in the quasi-classical energy range, where in analyzing the equations one can use a variant of the method of averaging over the "fast" variable.

In Chapter 4 we consider the behavior of the density of states and the wave functions in multidimensional disordered systems near the special boundaries of the spectrum (we call these fluctuation boundaries). In the neighborhood of these boundaries the spectrum exists only because there are low-probability fluctuations of the random parameters of the system, due to which the density of the states in this neighborhood is, as a rule, exponentially small. The calculation of the leading term of the exponent constitutes the main part of this chapter. Note that for many disordered systems the fluctuation region of the spectrum is not exhausted by the neighborhood of the boundary in the restricted sense. Generally speaking, the fluctuation region can be divided into several segments, in each of which, when calculating the density of states and the wave functions, we can replace the initial random potential with an effective potential in such a manner that each segment is included in the genuine fluctuation boundary of the appropriate effective potential. The presence of additional small parameters in the problem often makes these regions rather broad.

In contrast to fluctuation regions, an effective analysis of the spectral region of a disordered system where the density of states is essentially nonzero (for one, the region that lies in the spectrum of the initial translationally invariant part of the total Hamiltonian) is possible only when there are some small parameters characterizing the disorder of the system. The impurity concentration is one such parameter. The smallness of this parameter is taken into account by expanding the various averaged values in powers of the concentration, and this does not assume that the impurity potential is small. The applicability of this method is broadened considerably when we go over to its modifications, which are described and used in Chapters 5 and 6.

Chapter 5 provides a description of the general structure of concentration expansions and gives examples of simple applications. It also discusses various ways of constructing modified self-consistent forms of the expansions. These lead to expressions that contain, in addition to the characteristics of the translationally invariant part of the Hamiltonian, only the first power in concentration and are, in essence, analogous to the Hartree-Fock approximation in many-body theory. These expressions prove to be useful in studies dealing with the extended states that lie quite far from the boundaries. Here such expansions retain their meaning at concentrations that are not too low, take on the character of interpolations, and illustrate the qualitative aspects in the changes in the system properties. In addition, in this chapter we give a description of models for which the above-noted approximations prove to be asymptotically exact in a certain sense.

In Chapter 6 we discuss the impurity band that appears due to the broadening of a local impurity level. The structure of the quantum states and the behavior of the density of states in this region can be diverse, depending on the impurity concentration and the separation between the initial-spectrum boundary and the local level. At a low impurity concentration the energy levels and the states in the impurity band allow for a simple and graphic systematics. The wave functions usually prove to be localized at one or two impurities, although the corresponding energy levels depend on the position of other impurity centers. The density of states and spatial correlation functions calculated within the framework of this systematics are, in the leading terms in the concentration, of a universal nature (that is, are represented within a certain scale by functions that are concentration-independent). States localized at a greater number of impurity centers result from considerably less probable configurations, and their relative contributions to the density of states and correlation functions depend on the concentration.

Finally, in Chapter 7 we consider the problem of calculating the average transmission coefficient for a flux of particles passing through layers of a randomly nonuniform medium. The intricacy of the problem lies in the fact that since the transmission coefficient is seldom a self-averaged quantity, its physical meaning is far from obvious and special conditions are required for the average value to be realized. The chapter starts with a discussion of these

questions. Then we establish the exponential decrease of the average transmission coefficient as the thickness of the layer grows, find the probability distribution for the transmission coefficient, calculate the corresponding decrement in the over-the-barrier quasi-classical region, and discuss the connection of the transmission coefficient with the static kinetic characteristics (electrical and thermal conductivities) of disordered one-dimensional finite systems. Next we deal with sub-barrier transmission for a layer with impregnated point impurities. We show that there are two energy regions in which the transmission is essentially different: in one it is resonant, in the other nonresonant. In the more interesting resonant case the mean transmission coefficient is formed at the low-probability impurity configurations, which correspond to an almost ideal transparency of the layer.

This book (the Russian edition) was conceived in the mid 1970s and completed in 1980. For this reason it does not include recent important results obtained in the scaling-localization theory and weak-localization theory. One can get acquainted with the new branches of the theory of disordered systems initiated by these results through the reviews of Altshuler, *et al.*, (1983), and Sadovskii (1981) as well as through the Proceedings of the 16th International Conference on Low Temperature Physics LT-16 [*Physica B + C*, **107**, **108** (1981)].

I. M. LIFSHITS
S. A. GREDESKUL
L. A. PASTUR

Work on the manuscript for the English translation of the book was nearing its end when our teacher and coauthor, Il'ya Lifshits, suddenly died. It is impossible to overstate the influence of this remarkable scientist on the physics of condensed matter and, in particular, on the theory of disordered systems, one of whose creators was Il'ya Lifshits. (His first works in this field appeared at the end of the 1930s, and his last papers were published after his death.)

The scope of his interests and profoundness of his ideas can be appreciated from his publications. But all who had the pleasure of participating in scientific discussions and personal conversations with Il'ya Lifshits felt the drive of his ideas to a much greater extent. His animation and passion for science, his gentleness and readiness to help, complemented by an uncompromising attitude toward his work, all merged to make a charming and outstanding person who will always be remembered by his friends and colleagues.

S. G. and L. P.

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1 GENERAL PROPERTIES OF DISORDERED SYSTEMS

We will start our discussion of the general ideas of the theory by describing an object which in the modern theory of condensed matter is commonly known as a disordered system. When considering such a system, we must first of all bear in mind that there is a relatively rigid “frame” (e.g., the equilibrium positions of the heavy particles in the solid) that serves as a background for the faster degrees of freedom (conduction electrons, excitonic and spin excitations, or atomic vibrations). The frame may be not absolutely rigid, but its rearrangement time must be large compared to the characteristic time of a fast process (the “instantaneous frame” in a liquid may also satisfy this requirement). The disorder of a system in the sense commonly used in the theory of condensed matter is related to the aperiodic random structure of this frame. In a solid the disorder at low temperatures is the result of the nonequilibrium nature of such a structure, but its time of existence is usually very large.

Two problems prove to be effective models of excitations in a wide range of cases: the problem of the quantum-mechanical motion of a particle in a random potential field (which has its own interest), and the problem of classical wave propagation in a random medium. It is these models that will be the main objects of our study.

All disordered systems possess a number of general properties in common. The most important such property is the spatial homogeneity in the mean and the absence of any correlation between the random parameters that characterize the disorder (e.g., the random potential in the Schrödinger equation) at points that are far apart. One of the more important consequences is the self-averaging of the extensive physical quantities, which means that when these quantities, which are random in a finite system, are divided by the