

Electron localization in disordered systems (the Anderson transition)

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According to modern ideas there is a sharp boundary between the localized and extended states in the electron spectra of disordered systems (amorphous semiconductors, doped crystalline semiconductors, etc.). The mathematical description of the electron states near this boundary is a very complicated problem which is not yet completely solved. The purpose of this review is to describe, in the simplest possible way, without going into the mathematical problems, the basic physical ideas that have been put forward in this field. The Anderson and Lifshitz models are considered in detail and the criteria for localization are discussed. Examples are given of systems in which it is possible to observe experimentally the transition from localized to extended states that occurs when certain parameters are varied. The concept of minimum metallic conductivity and the properties of the wave functions near the boundary of the localized states are discussed. The results of computer experiments that attempt to model a disordered system near the mobility edge are described. The difficulties that arise in attempts to give a mathematical description of such a system, and the basic ideas of such a description, are discussed in the form of a conversation with an unsophisticated partner.

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1. INTRODUCTION

The developments with which we shall be concerned in this review arose from a paper by Anderson,¹ entitled "Absence of diffusion in certain random lattices". This paper appeared in 1958 and was somewhat ahead of its time. The rapidly growing interest in amorphous semiconductors in the mid 1960's placed the problem of the electron states of disordered systems in the forefront of the physics of condensed media. In this period, the ideas put forward by Anderson were evaluated in full measure.

For definiteness, we shall discuss first a crystal into which an impurity has been introduced, creating an electron state with energy E_0 in the gap. It is customary to say that, for a finite concentration of impurities of the same kind, an impurity band, having a finite energy width, arises in place of the impurity level. For the reader, the word "band" will bring to mind the Krönig-Penney model, which illustrates beautifully the smearing out of a level into a band. In this case, the states are characterized by a wave vector and their properties differ little from those of plane waves. In the case of a random distribution of impurities, however, the system does not have the translational symmetry that is assumed in the Krönig-Penney model. Anderson showed that, because of this, in a number of

of cases the impurity band does not possess the most important property of crystalline bands—an electron placed at one of the impurity centers does not spread out over all the centers from which the band is constructed. Its wave function remains localized. At low impurity concentrations all the states are found to be localized. When the concentration is increased an energy band in which the states are extended appears in the impurity band. The transition that occurs from extended to localized states on variation of the energy, impurity concentration, or other parameters, has become known as the Anderson transition.

It appears to us that the theory of the Anderson transition is not complete at the present time, and it is not our purpose to give a review of the methods developed in connection with this problem. We notify the reader in advance that our list of references is not complete. The purpose of the review is to attempt to describe, in the simplest possible way, using practically no mathematical apparatus, the basic ideas that have been put forward in connection with the Anderson transition. It seems to us that such an account could be useful for experimental physicists studying this question, and also for theorists wishing to form an idea of the problem.

The plan of the review is as follows. In Sec. 2 we use the tight-binding method and discuss the proper-

ties of the narrow bands that are formed by periodically arranged impurity centers situated at large distances from each other. The band structure that arises in this standard treatment is unstable. The electron-electron interaction leads to splitting of the band, as a result of which the occupied band and empty band are found to be separated by a gap (the Mott transition). This section has an introductory character. Subsequently we confine ourselves to the one-electron approximation and discuss the question of electron localization in the Anderson and Lifshitz models. In Sec. 3 the Anderson model is formulated, the causes that lead to electron localization are explained, and a simple estimate of the localization criterion is given. In Sec. 4 it is shown that electron states are also localized in the Lifshitz model (randomly arranged short-range centers). In Sec. 5 some systems in which the Anderson transition is observed are discussed. In Sec. 6 the properties of the electron states in the neighborhood of the Anderson transition are considered. Finally, in Sec. 7 the theoretical difficulties arising in the description of the Anderson transition are discussed.

2. NARROW BANDS AND THE MOTT TRANSITION

We begin this section with an auxiliary problem, which we shall subsequently cast aside. We shall suppose that the impurities in the crystal are not distributed randomly but form a regular crystal lattice (impurity sublattice), with a period much greater than that of the underlying crystal lattice. By the tight-binding method we obtain the energy spectrum and wave functions of the electrons in the impurity band. This model permits us to develop the terminology used in the following sections. In addition, we briefly discuss here the question of the role of electron-electron interaction under the conditions of a narrow allowed band.

The potential created by the impurity sublattice has the form

$$V(\mathbf{r}) = \sum_j U(\mathbf{r} - \mathbf{r}_j), \quad (2.1)$$

where the sum is taken over all sites of the impurity sublattice, and $U(\mathbf{r})$ is the potential of a single impurity center. The problem will be solved in the framework of the effective-mass method. We suppose that we know the wave functions φ_n and energy levels E_n corresponding to the solution of the Schrödinger equation with the potential of one impurity center:

$$\left[-\frac{\hbar^2}{2m} \Delta + U(\mathbf{r}) \right] \varphi_n = E_n \varphi_n, \quad (2.2)$$

where m is the effective mass. For simplicity we confine ourselves to the case of a normal band, i.e., a nondegenerate band with an isotropic and quadratic spectrum.

We shall assume in the following that the width of the impurity band is much smaller than the spacings between the levels E_n , and consider the neighborhood of one of these levels (E_0). It is well known that a wavefunction corresponding to the potential (2.1) must be constructed in the form of a superposition of functions $\varphi(\mathbf{r} - \mathbf{r}_j)$ satisfying (2.2):

$$\Psi = \sum_j a_j \varphi(\mathbf{r} - \mathbf{r}_j), \quad (2.3)$$

$$\sum_j |a_j|^2 = 1. \quad (2.4)$$

This approximation should be good if the localization length a of the function $\varphi(\mathbf{r})$ is small compared with the period b_0 of the impurity sublattice. Indeed, the principal contribution to the energy is given by those regions of space in which the wavefunction $\Psi(\mathbf{r})$ is large, and these points, as can be seen from (2.3), are very close to the impurity centers, i.e., within the sphere of influence of one impurity, in which Eq. (2.2) is valid. Thus, the expression (2.3) should be close to the solution of the Schrödinger equation with the potential (2.1). The coefficients a_j must be found from the minimum-energy condition.

Since the wave functions $\varphi(\mathbf{r} - \mathbf{r}_j)$ corresponding to different sites are not orthogonal, the expectation value of the energy is not a quadratic form in the coefficients a_j . However, if $a \ll b_0$, the overlap between neighboring states is small. In this case we can confine ourselves to the first approximation in the expansion of the expectation value of the energy in a^2/a_{j+m} . For the part of the energy depending on $a^* a_{j+m}$ we obtain

$$E = \sum_{j,m} a_j^* a_{j+m} I(m). \quad (2.5)$$

The quantity $I(m)$ is called the energy overlap integral (or simply the overlap integral). We shall not give explicit expressions for it. We note only that under the conditions of interest to us it is very small, since it contains the factor $e^{-b_0/a}$ (for nearest neighbors).

It is easy to see that the set a_j that minimizes (2.5) under the condition (2.4) has the form $a_j = \mathcal{N}^{-1/2} e^{i\mathbf{k} \cdot \mathbf{r}_j}$ (\mathcal{N} is the total number of sites of the impurity sublattice). Substituting this expression into (2.5), we obtain

$$E = \sum_{\mathbf{m} \neq 0} e^{i\mathbf{k} \cdot \mathbf{m}} I(\mathbf{m}). \quad (2.6)$$

Since the quantity $I(\mathbf{m})$ falls off exponentially with increase of $|\mathbf{m}|$, in (2.6) it makes sense to confine ourselves to nearest neighbors. The actual expressions depend on the form of the lattice. For example, for a simple cubic lattice we obtain

$$E = 2I(b_0) (\cos k_x b_0 + \cos k_y b_0 + \cos k_z b_0). \quad (2.7)$$

The energy width V_b of the allowed band is equal to $12|I(b_0)|$ for the simple cubic lattice and $8|I(b_0)|$ for the simple square lattice. In these cases the rule $V_b = 2Z|I(b_0)|$ holds, where Z is the number of nearest neighbors. For small k , from (2.7) we obtain

$$E = 6I(b_0) - I(b_0) k^2 b_0^2. \quad (2.8)$$

The quantity $\hbar^2/2Ib_0^2$ in formula (2.8) plays the role of the electron mass in the band that is formed. With increase of the distance between nearest neighbors the width of the allowed band decreases exponentially ($I(b_0) \sim e^{-b_0/a}$). In this case the mass becomes exponentially large. This prompts the thought that in the case of interest to us, namely, that of low impurity concentrations, i.e., large values of b_0 , the band properties in the familiar sense are fictitious. Nevertheless, we shall see shortly that for an arbitrarily narrow band the electron wave function is a modulated plane wave and the electron can move without being scattered.

The band formed by the impurities is not more than half filled, since each impurity gives (or takes away) one electron and the band is doubly degenerate in the spin. Thus, it turns out that, if the impurities could really be assumed to be periodically arranged, the conduction due to the impurity electrons should be metallic in character for arbitrarily small impurity concentrations.

This statement is incorrect even with the stipulation of a relatively periodic arrangement of the impurities. The point is that in the above deduction we used the one-electron approximation. This approximation, which works satisfactorily in the calculation of the broad allowed bands of metals, turns out to be inadmissible in the case of narrow bands. As can be seen from (2.3), the electron wave function near each site differs little from the site function $\varphi(\mathbf{r})$. We shall estimate now the interaction energy of two electrons with different spins, situated at one site. This turns out to be of the order of $U_0 \approx e^2/a$. If the magnitude of U_0 is small compared with the width V_b of the allowed band, the change in the wave functions as a result of the electron interaction will be insignificant. This is the situation in good metals. In the case of interest to us, however, the quantity V_b is exponentially small and considerably smaller than U_0 . Let the impurity-sublattice constant b_0 be infinitely large. Then at each site there are two electron levels. An electron can have energy E_0 or $E_0 + U_0$, depending on whether or not there is another electron at the site. For a finite value of b_0 , both levels are spread out into bands, with width of the order of $I(b_0)$ (Fig. 1). The number of places in each of these bands is half as many as in the band (2.6), and is equal to the number of sites. (In the lower band, there cannot be a site with two electrons.) The lower band will be filled, and the upper band empty. Thus, if $I(b_0) \ll U_0$, our substance will be an insulator. With decrease of b_0 , at a certain point A the width of the gap vanishes and an insulator-metal transition, customarily called the Mott transition, occurs. The question of the character of this transition and of the behavior of the electrical conductivity at the transition point remain open up to now.

For a quantitative study of the Mott transition one uses, as a rule, the Hubbard model. In this maximally simplified model it is assumed that the electrons repel each other only if they are at the same site. The Hubbard Hamiltonian has the form

$$\mathcal{H} = \sum_{j, m \neq 0} I(m) a_{j, \sigma}^{\dagger} a_{j+m, \sigma} + \frac{U_0}{2} \sum_{j, \sigma} n_{j, \sigma} n_{j, \sigma} \quad (2.9)$$

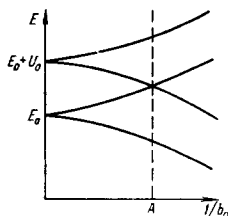


FIG. 1. Electron bands as a function of the period b_0 of the impurity sublattice. To the left of the point A we have an insulator, and to the right a metal.

where $n_{j, \sigma} = a_{j, \sigma}^{\dagger} a_{j, \sigma}$ is the occupation-number operator for the state on site j with spin σ . This Hamiltonian is obtained from (2.5) by adding a term describing the repulsion of electrons situated on the same site and having different spins.

The Hubbard model permits an exact solution only in the one-dimensional case.² The result contradicts the qualitative arguments given above. In the one-dimensional case the gap in the spectrum is preserved for all values of $I(b_0)/U_0$, i.e., the one-dimensional model is always an insulator. It is customary, however, to assume that this is an exceptional property of one-dimensional systems, and that this fact does not throw a shadow on the qualitative picture described above, so long as this refers to two- and three-dimensional systems.

A review of the theory developed in connection with the Mott transition is not part of our purpose. An account of these questions can be found in the book by Mott³ or in the review by Khomskii.⁴ We have given a picture of the Mott transition only because in real systems a situation usually arises in which, in the vicinity of the Anderson transition, we cannot neglect the electron-electron interaction, as a result of which the transition has features of an Anderson transition and features of a Mott transition. Theoretically, of course, these two phenomena are strictly distinct. The Anderson transition exists in the one-electron approximation, and in the following sections we return to this approximation. It is necessary only to bear in mind that, when speaking of a narrow impurity band, we shall always have in mind the lower Hubbard band (see Fig. 1). The broadening of this band, which can be due both the quantum overlap and to spreading of the levels as a result of a fluctuating classical field, will be assumed to be small compared with its distance U_0 from the second band. Therefore, when studying the structure of the impurity band at zero temperature we shall assume that there can be only one electron at each site. As we have seen, this follows not from the Pauli principle, which permits the presence of two electrons in one orbital state, but from the charge restriction, which turns out to be more stringent in this case.

3. THE ANDERSON MODEL

In Sec. 2 we assumed that the impurities form a perfect lattice. The ideality of the impurity sublattice can be violated in several ways. The simplest way is to assume that the arrangement of the impurities is random. We shall return to this latter, but consider now another, more developed and also practically important, variant of disordering. We suppose that the impurities are situated at the sites of a regular lattice, but that the electron levels at all the sites are different. We shall denote each level by ϵ_j , assigning it the site index. Thus, we obtain a system of periodically arranged potential wells of different depths (Fig. 2). The Hamiltonian of such a system in the site representation is obtained from (2.5) by adding a term representing the sum of the energies of the electrons situated at the isolated sites:



FIG. 2. Potential wells in the Anderson model.

$$\mathcal{H} = \sum_j \varepsilon_j a_j^\dagger a_j + \sum_{j, m \neq 0} I(m) a_j^\dagger a_{j+m}. \quad (3.1)$$

The energies ε_j are assumed to be random quantities, with no correlation between them. In other words, the probability that a certain site has a given energy does not depend on the energies of the other sites. We shall assume the energy distribution to be constant in a certain interval W . The distribution function $P(\varepsilon)$ has the form

$$P(\varepsilon) = \begin{cases} 1/W, & |\varepsilon| < W/2 \\ 0, & |\varepsilon| > W/2. \end{cases} \quad (3.2)$$

The model formulated was proposed by Anderson¹ and bears his name. Unfortunately, the Anderson model does not permit an exact solution. Despite the enormous number of papers on the problem of the Anderson transition, a good mathematical description of this phenomenon does not yet exist. Nevertheless, a qualitative understanding of it, based on comparatively simple physical concepts, undoubtedly does exist and inspires confidence. As we shall see, it is also confirmed by computer experiments. Primarily, it is the qualitative picture of the phenomenon that we shall discuss.

The fundamental problem that is raised in the consideration of the Anderson model is to determine whether the electron wave functions are localized in the neighborhood of a certain site or whether they extend over the whole system. In both cases the wave function near each impurity is similar to the site wave function, so long as the overlap is small. It is important to understand whether a coherent state is formed that consists of a superposition of an infinite number of site functions, occurring with approximately equal weight, and extends over a macroscopic distance. The alternative variant is that the site functions appear in the superposition with a weight that decreases exponentially with the distance from a certain site. Such a state is said to be localized near this site. If all states are localized, the conductivity of the system at zero temperature is equal to zero.

The problem of how to formulate the condition for localization in mathematical language is far from trivial. Several different criteria for localization are used. Anderson¹ used the following criterion. We suppose that at time zero the electron wave function coincided with the site function corresponding to the site i . This function is not an eigenfunction of the Hamiltonian (3.1), and will change with time. By solving the Schrödinger equation we find the modulus squared $|\Psi_i(t)|^2$ of the wave function at site i at large times t . If the states are not localized, the initial wave packet spreads out over the whole system. Therefore, in an infinite system, $\lim_{t \rightarrow \infty} |\Psi_i(t)|^2 = 0$. If there is no spread of the levels, and we have the ideal band structure considered in the preceding section, the spreading of the wave packet occurs over a time of the order of \hbar/V_b . But if the true wave functions are localized, spreading does not occur at all: With time, the wave function acquires "tails" with

exponentially small amplitudes at neighboring sites and will be concentrated in approximately the same region of space as at the initial time. Therefore, $\lim_{t \rightarrow \infty} |\Psi_i(t)|^2$ will turn out to be a finite quantity. This is the Anderson criterion.

Other localization criteria have also been proposed. Bell and Dean⁵ considered the quantity

$$B_\alpha = \int |\Psi_\alpha(\mathbf{r})|^4 d\mathbf{r} / \left[\int |\Psi_\alpha(\mathbf{r})|^2 d\mathbf{r} \right]^2, \quad (3.3)$$

where Ψ_α is a stationary wave function of the Hamiltonian (3.1) in the coordinate representation. It is easy to understand that for extended states the quantity B_α tends to zero like $1/\mathcal{N}$, where \mathcal{N} is the total number of sites in the system, while for localized states the quantity B_α is nonzero and does not depend on the size of the system.

Herbert and Jones⁶ considered the criterion for localization to be the asymptotic behavior of the site-off-diagonal matrix element G_{0n} of the Green function in the site representation at large values of the distance R_{0n} . It is natural to suppose that this quantity falls off like R_{0n}^{-1} for extended states, and like $\exp[-R_{0n}/a(E)]$ for localized states, where $a(E)$ is a certain localization length (see Sec. 6).

Finally, in Sec. 6 we consider in detail yet another criterion, proposed by Edwards and Thouless.

The most important characteristic of the impurity band is the density of states. This is defined as the number of levels in a small energy interval, divided by this interval and by the volume of the system. It should be borne in mind that in a macroscopic system the density of states is a continuous function of the energy in a certain interval, even if we are speaking of the impurity band, which is a set of discrete levels. Thus, the density of states does not contain information permitting us to distinguish a true band from a set of discrete levels that are unconnected with each other and randomly dispersed in energy space.

The Anderson model contains one dimensionless parameter W/I , where I is the overlap integral for neighboring sites. Anderson's result, confirmed by a large number of later investigations, is as follows. For sufficiently large values of W/I all states are localized. There exists a critical value (W_c/I) , at which extended states first appear at the center of the band. With further decrease of W/I the region of extended states increases, encompassing almost the whole band (Fig. 3). It is curious that all this does not apply to a one-dimensional system. As Mott and Twose have shown, in a one-dimensional system the states are always localized.⁷⁻¹³ The situation here is analogous to the sit-

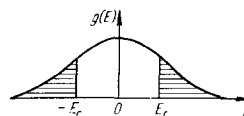


FIG. 3. Density of states in the Anderson model. The localized states are shaded. The energies E_c and $-E_c$ separating the regions of localized and extended states are the mobility edges.

uation with the Mott transition, mentioned in the preceding section. We see that the inclusion of arbitrarily weak fluctuations of the site energies, like inclusion of the electron-electron interaction, inevitably transforms a one-dimensional conductor into an insulator.

Both the Anderson transition and the Mott transition are variants of the metal-insulator transition. As we have seen, the basic difference between them is that the Anderson transition is connected with disorder of the system while the Mott transition also occurs in a perfect periodic structure. In addition, it is necessary to bear in mind that the Mott transition arises as a consequence of the electron-electron interaction, while in the theory of the Anderson transition the motion of one electron is considered.

In order to comprehend Anderson's result, we shall consider the auxiliary problem of two wells of different depths, positioned at a large distance apart. This quantum-mechanical problem is easily solved. Let the energies of the electrons in each of the wells when the other well is disregarded be ε_1 and ε_2 , respectively, and let the wave functions be φ_1 and φ_2 . If the wells are identical, then $\varepsilon_1 = \varepsilon_2$ and two states arise, with the wave functions

$$\Psi_I = \frac{1}{\sqrt{2}}(\varphi_1 + \varphi_2), \quad \Psi_{II} = \frac{1}{\sqrt{2}}(\varphi_1 - \varphi_2). \quad (3.4)$$

The difference in the energies of these states is equal to $E_I - E_{II} = 2I$, where I is the overlap integral. It is important to note that, however far apart these wells are, and whatever the overlap integral is, in both states the electron belongs to each of the wells to an equal extent, i. e., it can be found in either of them with equal probability. The character of the solution changes little, if $|\varepsilon_1 - \varepsilon_2| \ll I$. In the opposite limiting case $|\varepsilon_1 - \varepsilon_2| \gg I$ the picture is completely different. As before, there are two states:

$$\Psi_I = C_1\varphi_1 + C_2\varphi_2, \quad \Psi_{II} = C_3\varphi_1 + C_4\varphi_2. \quad (3.5)$$

However, in the state I the energy E_I is close to the energy ε_1 , and the wave function is close to φ_1 . The ratio $C_2/C_1 \approx I/|\varepsilon_1 - \varepsilon_2|$, and decreases exponentially with increase of the distance between the wells. On the other hand, in the state II the energy E_{II} is close to the energy ε_2 , and the wave function Ψ_{II} is close to φ_2 . Thus, in this case collectivization of the electron does not occur. Each state is essentially the state of an electron in one of the wells.

This example helps us to understand the essence of the Anderson transition.¹⁾ We shall consider a certain energy band of width Δ , symmetric about zero, with Δ of the order of the overlap integral I . The sites whose energies fall in this band will be called resonance sites, and the sites with energies outside the band—nonresonance sites. The point of this definition is that an electron state is collectivized between two resonance sites if these sites are nearest neighbors. Further, we shall say that two resonance sites are connected with each other if they are nearest neighbors or if there is

a third resonance site which is a nearest neighbor of both of them. Two resonance sites are also connected with each other if they are joined by a chain of connected resonance sites. An aggregate of sites connected with each other will be called a cluster. Corresponding to these clusters will be electron states in which the modulus squared of the wave function is of the same order at all the sites belonging to the cluster and small everywhere outside the cluster. As the next step, we exclude all the non-resonance sites from consideration. This step is dubious. The Anderson Hamiltonian (3.1) connects only neighboring sites. But two resonance sites can also have a common electron state in the case when there is a nonresonance site between them. However, the effective overlap integral in this case will be not of order I but of order I^2/W . If I/W is small, the connection through the nonresonance site will lead to collectivization of the states in a band considerably narrower than the one we are considering, and this can be neglected. Having discarded the nonresonance sites, then, we find that the characteristic size of the wave function is determined by the size of the clusters of connected resonance sites.

The distribution of the energies ε_1 in the Anderson model is assumed to be constant in the interval W . For this reason, the fraction of resonance sites should be of the order of I/W . For small values of this parameter there are few resonance sites and they are distributed primarily singly. However, at a certain critical value of I/W an infinite cluster of connected resonance sites appears, i. e., paths going away to infinity are formed. The wave functions of the electron states spread out along these paths. It is this which constitutes the Anderson transition.

Percolation theory (see the review of Ref. 15) enables us to find the exact value of the quantity Δ/W_c at which an infinite cluster is formed.²⁾ For this we must equate the fraction Δ/W of resonance sites to the percolation limit $x_c(s)$ for the site problem, i. e.,

$$\frac{\Delta}{W_c} = x_c(s). \quad (3.6)$$

Values of $x_c(s)$ for various lattices (Fig. 4) are given in Table I. For the two- and three-dimensional lattices the data given in the review of Ref. 15 are used, while the data for the hyper-lattices are borrowed from the paper by Kirkpatrick.¹⁶

To estimate the critical value W_c/I it is necessary to find the relationship between the width Δ of the resonance and the overlap integral I . There is the most complicated (and controversial) aspect of the proposed estimate. The point is that the very definition of the resonance sites is not exact, since with decrease of the difference $|\varepsilon_i - \varepsilon_j|$ the collectivization of the electron states between two sites occurs gradually rather than discontinuously.

Nevertheless, the Anderson transition occurs at a fully determinate value W_c/I . Indeed, if the wave func-

¹⁾The idea of the following arguments is due to Thouless.¹⁴

²⁾The latter part of this section was written jointly with B. I. Shklovskii.

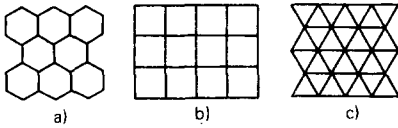


FIG. 4. Planar lattices: a) hexagonal, b) square, and c) triangular.

tion decreases exponentially from site to site, it cannot belong to an extended state. Therefore, for large values of W/I all states are localized. In an infinite system, the appearance of an extended state on decrease of W/I is a sharply pronounced critical phenomenon, corresponding to which there should be a well defined threshold value W_c/I . Therefore, the aforementioned indeterminacy in the definition of the resonance sites is evidence of the approximate character of a description that uses the concept of a resonance band.

It is possible, however, to postulate a way of estimating the width and the critical value W_c/I , based on the topological properties of an infinite cluster (see Ref. 15). Near the percolation limit an infinite cluster is a network composed of practically one-dimensional chains of resonance sites. If we neglect the difference in the energies of the resonance sites, it turns out that, because of the overlap of the wave functions along a chain, a band of width $4I$ is formed. Therefore, it is natural to assume that the width of the resonance band is $\Delta \approx 4I$. Substituting this value into (3.6), we obtain the following estimate:

$$\frac{W_c}{I} = \frac{4}{x_c(s)}. \quad (3.7)$$

For a number of lattices the value of W_c/I are known from numerical experiments on a computer. Edwards and Thouless,¹⁷ and also Licciardello and Thouless,¹⁸ have carried out experiments for two-dimensional lattices, and Weaire and Srivastava¹⁹ have done so for three-dimensional lattices and lattices of higher dimensionality. The results of these papers are collected in Table I. For comparison, the results of the estimate (3.7) are also given. Of course, the assumptions made in the derivation of (3.7) are very crude and can give rise to objections. (The most serious objection, in our opinion, is associated with the one-dimensionality of the percolation paths, and is discussed in Sec. 6.) Table I, however, shows that the estimate agrees well with the results of the numerical experiments.

For $W < W_c$, then, a band of extended states appears in the electron spectrum. It is natural to ask whether, near the transition, this band is infinitesimally narrow or has a finite width from the outset. A well sub-

stantiated answer to this question does not exist. It is usually assumed (*cf.*, e.g., Ref. 18) that the band of extended states "opens out" gradually, although, in our view, there are no serious arguments in favor of this opinion. Moreover, it seems to us that the existence of arbitrarily narrow extended bands is difficult to reconcile with the concept of a minimum metallic conductivity (see Sec. 6).

4. LOCALIZATION IN THE LIFSHITZ MODEL

In the Anderson model, potential wells of different depths are located at the sites of a regular crystal lattice. We now consider the alternative (in a certain sense) model: identical potential wells, randomly located in space. In the physics literature this model is sometimes called a "model with structural disorder". We shall assume that the well potential is short-range and that the average spacing between wells is large not only in comparison with the range of the potential but also in comparison with the radius of the wave-function corresponding to one well. This model was first studied in detail by I. M. Lifshitz.^{20,21}

The fundamental question that we wish to elucidate is whether the electron states in this case are localized near the individual wells or whether they are spread out over the whole system. At first glance, it may appear that, since all the wells are identical, in the terminology of Sec. 3 they are resonance wells, and, consequently, spreading out of the wave packet should occur. However, overlap of the wave functions of neighboring wells leads to a shift in the energy levels, and since, for different wells, the nearest neighbors are at different distances, the shifts will also be different. It would seem, after this, that we should turn to the results of the preceding section. However, the Anderson model does not help us. It was assumed in the latter that the spread of the levels and the overlap have a different nature and can be specified in an arbitrary ratio. If the spread is considerably greater than the overlap, the states are localized, while if it is considerably smaller, they are extended. In the Lifshitz model the overlap and spread have the same nature and the same order of magnitude. The only small parameter in the problem is the ratio of the radius of the wave-function to the average spacing between the wells. As we shall now see, this parameter also assists in the analysis of this situation.

We shall not give a full account of the mathematical apparatus developed for this case by Lifshitz, but consider the problems of two and three potential wells. This clarifies the problem sufficiently to make it possible to explain the principal results of Lifshitz without further mathematics. These results are as follows. The electron states either turn out to be localized near individual potential wells, or belong to two closely spaced wells at once, forming a superposition of the form (3.4). Both types contain exponentially small admixtures of other states. States in which wave functions of three or more wells appear on an equal footing are not realized, since this could happen only for a strictly symmetrical arrangement of these wells. Thus,

TABLE I.

| Lattices | $x_c(s)$ | $4/x_c(s)$ | W_c/I | Lattices | $x_c(s)$ | $4/x_c(s)$ | W_c/I |
|--------------------------------|----------|------------|---------|-----------------------------|----------|------------|---------|
| Two-dimensional hexagonal | 0.70 | 5.7 | 4.3 | Simple cubic | 0.31 | 12.9 | 14.4 |
| square | 0.59 | 6.8 | 6.1 | Hypercubic four-dimensional | 0.20 | 20 | 25 |
| triangular | 0.50 | 8.0 | 9.4 | | | | |
| Three-dimensional diamond-type | 0.43 | 9.3 | 8.0 | five-dimensional | 0.14 | 28.6 | 36 |

the states in the Lifshitz model are localized. This information is sufficient for the reader to pass on to the next sections.

For the reader who is prepared to go more deeply into the Lifshitz model, its Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \sum_j U(\mathbf{r} - \mathbf{r}_j). \quad (4.1)$$

We suppose that the potential $U(\mathbf{r})$ of an individual well produces a localized state $\Psi_0(\mathbf{r})$ with energy E_0 , and that the other states formed by this well are separated from E_0 by an energy considerably greater than the displacement of the level E_0 under the influence of the other potential wells. We shall assume that $U(\mathbf{r})$ falls off much faster than $\Psi_0(\mathbf{r})$, so that the wavefunction in the sphere of influence of the potential can be assumed to be constant. Therefore, in the Schrödinger equation the term $\sum_j U(\mathbf{r} - \mathbf{r}_j)\Psi(\mathbf{r})$ is replaced by the term $\sum_j U(\mathbf{r} - \mathbf{r}_j)\tau_j$, where $\tau_j = \Psi(\mathbf{r}_j)$. Then,

$$\left(\frac{\hat{p}^2}{2m} - E\right)\Psi(\mathbf{r}) + \sum_j U(\mathbf{r} - \mathbf{r}_j)\tau_j = 0, \quad (4.2)$$

where E is the required energy, or

$$\Psi(\mathbf{r}) = \left(E - \frac{\hat{p}^2}{2m}\right)^{-1} \sum_j U(\mathbf{r} - \mathbf{r}_j)\tau_j. \quad (4.3)$$

Expanding the right-hand side in a Fourier series, we find

$$\Psi(\mathbf{r}) = \sum_j F(E, \mathbf{r} - \mathbf{r}_j)\tau_j, \quad (4.4)$$

where

$$F(E, \mathbf{r}) = \int \frac{c(\mathbf{k}) \exp(i\mathbf{k}\mathbf{r}) d\mathbf{k}}{E - (\hbar^2 \mathbf{k}^2 / 2m)}, \quad (4.5)$$

$$U(\mathbf{r}) = \int c(\mathbf{k}) e^{i\mathbf{k}\mathbf{r}} d\mathbf{k}.$$

Putting $\mathbf{r} = \mathbf{r}_i$, we obtain a system of linear homogeneous equations

$$\tau_i - \sum_j F(E, \mathbf{r}_{ij})\tau_j = 0 \quad (4.6)$$

($\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$), and the condition for solvability of this system determines the energy E .

If there is only one well, the energy level E_0 is determined by the equation

$$1 - F_0(E_0) = 0, \quad (4.7)$$

where

$$F_0(E_0) = \int \frac{c(\mathbf{k}) d\mathbf{k}}{E_0 - (\hbar^2 \mathbf{k}^2 / 2m)}. \quad (4.8)$$

The reader will find a detailed analysis of Eq. (4.7) in, e.g., the book by Kosevich.²²

The wavefunction $\Psi_0(\mathbf{r})$ of an electron in the one well is determined from (4.4):

$$\Psi_0(\mathbf{r}) = \Psi_0(0) F(E_0, \mathbf{r}). \quad (4.9)$$

At large r we can replace $c(\mathbf{k})$ by $c(0)$ in the integral (4.5) and we obtain

$$F(E_0, \mathbf{r}) = -A \frac{e^{-\alpha r}}{r}, \quad (4.10)$$

$$A = (2\pi)^3 \frac{mc(0)}{\hbar^3}, \quad \alpha^2 = -\frac{2mE_0}{\hbar^2},$$

which determines the asymptotic form of the wavefunction.

We now write the condition for solvability of the system (4.6), which determines the energy E in the potential of a large number of wells. We assume that the quantity $\varepsilon = E_0 - E$ is small compared with the distance to the next single-well level, and perform the expansion in (4.8). For the diagonal terms of (4.6), making use of (4.7) we obtain

$$1 - F_0(E) = B\varepsilon, \quad (4.11)$$

where

$$B = \int \frac{dk c(k)}{(E(k) - E_0)^2}.$$

For the nondiagonal terms we make use of the formula (4.10), since the average distance between cells is $N^{-1/3} \gg \alpha^{-1}$. As a result, we obtain the following equation for the energy ε :²¹

$$\text{Det} \left[\varepsilon \delta_{ij} + \lambda \frac{e^{-\alpha r_{ij}}}{r_{ij}} (1 - \delta_{ij}) \right] = 0, \quad (4.12)$$

where $\lambda = A/B$. For the case of two wells separated by a distance r , this is easily solved:

$$\varepsilon_{1,2} = \pm \lambda \frac{e^{-\alpha r}}{r}. \quad (4.13)$$

The wave functions have the form

$$\Psi_{1,2} = \frac{1}{\sqrt{2}} [\Psi_0(\mathbf{r} - \mathbf{r}_1) \pm \Psi_0(\mathbf{r} - \mathbf{r}_2)], \quad (4.14)$$

where $\Psi_0(\mathbf{r})$ is determined by (4.9). Thus, the electron states belong to both wells in equal measure, and the shift of the levels decreases exponentially with the distance between the wells.

We now consider three wells, lying on a straight line as shown in Fig. 5. We shall assume the distance r_{12} to be fixed and see how the energies of the levels vary as a function of r_{23} . We represent each of the three roots of Eq. (4.12) in the form

$$\varepsilon = \varepsilon_0 s^2, \quad (4.15)$$

where ε_0 is a power function of r_{12} and r_{23} , in which we shall not be interested—we concentrate our attention on the exponential dependence. The dependence of s on $x_{23} = \alpha r_{23}$ for each root of Eq. (4.12) is depicted in Fig. 5. If $r_{23} > r_{12}$, the states are classified as follows. Two states are collectivized between the wells 1 and 2, and have the wavefunctions (4.14). Their energies are determined by (4.13), and $s = x_{12}$. The third well has practically no effect on these states. It has an eigenstate with wavefunction $\Psi_0(\mathbf{r} - \mathbf{r}_3)$ and with $s = 2x_{23}$. Attention should be drawn to the fact that the level shift in the resonance situation, when the electron is collectivized between two wells, is proportional to the

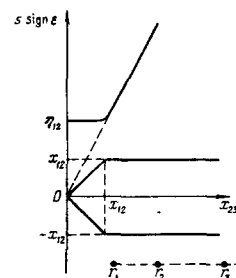


FIG. 5. Energy levels for three potential wells as functions of the distance $r_{23} = x_{23}/\alpha$ (the point η_{12} corresponds to $2x_{12}$).

overlap integral ($s = x_{12}$), while that in the nonresonance situation is proportional to its square ($s = 2x_{23}$).

Entirely analogously, for $r_{23} < r_{12}$ we obtain a doublet collectivized by the wells 2 and 3, with $s = x_{23}$, and a state in the well 1, with $s = 2x_{12}$. The essential point is that if, for example, the wells 1 and 2 are close to each other, then their states are collectivized and the two levels that appear "repel" each other so strongly that they move out of resonance with the third level.

A state belonging in equal measure to all three wells arises only if $r_{12} = r_{23}$. It is important to understand that the maximum permissible deviation from this equality for which the states are still collectivized is equal to the radius α^{-1} of the state. This is the key to an understanding of the situation as a whole. The point is that the average spacing between impurities is much greater than α^{-1} . For this reason, the probability of ordered configurations is negligibly small, and in a system of any number of wells the states will be singlets and doublets with the wavefunctions (4.9) and (4.14). Thus, the possibility of the spreading of a wave packet over a band is completely ruled out.

It is easy to understand what the density of states looks like in the Lifshitz model. It is obvious that the characteristic energy determining the spread of the levels (the width of the impurity band, if the potential wells are associated with impurities) is of the order of

$$\Delta = \lambda N^{1/3} \exp(-\alpha N^{-1/3}). \quad (4.16)$$

This estimate is obtained if we substitute the average spacing between wells in place of r in (4.13) (N is the concentration of wells). We note that the density of states has a minimum at the point $\varepsilon = 0$. In fact, only those states around which there are no other wells within a distance much greater than the average spacing between wells have small level shifts $\varepsilon \ll \Delta$. But the probability of such voids is small. Thus, the density of states is a double-humped curve with a minimum λ at $E = E_0$, each hump having a width of the order of Δ .

Thus, the electron states in the Lifshitz model should be localized. Of course, this conclusion is a consequence of the assumption that the average spacing between wells is large compared with the radius of the wavefunction ($\alpha N^{-1/3} \gg 1$). For values of $\alpha N^{-1/3}$ of order unity, extended states arise even in the Lifshitz model. In the two-dimensional case this transition has been traced by means of a computer,²³ but it was not possible to determine definitely the critical value of $\alpha N^{-1/3}$.

5. EXAMPLES OF ANDERSON TRANSITIONS

The ideas behind the Anderson transition form the basis for a most important concept in the theory of disordered systems—the concept of the mobility edge. This concept plays a fundamental role in the theory of amorphous semiconductors. According to the modern theory, the band structure of an amorphous semiconductor has the form depicted in Fig. 6. The presence of short-range order leads to the result that the concept of forbidden and allowed bands is preserved. However, the numerous structural imperfections create a density-

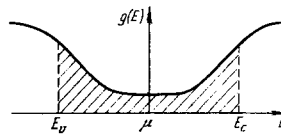


FIG. 6. Density of states in an amorphous semiconductor. The localized states are shaded.

of-states "tail" in the forbidden band, so that the band edges (in the sense of the vanishing of the density of states) are smeared out. The decrease in the density of states leads to the result that states in the gap are found to be localized, and, in a certain sense, the localization thresholds play the role of the band edges. The Fermi level lies in the region of localized states, and so charge transfer is effected by thermal excitation of carriers into the region of extended states or by activated hops between localized states (see the book by Mott and Davis²⁴). Both ways lead at low temperatures to an exponential increase of the resistance with temperature. The statement that there is strict localization of electron states plays a very important role here. If the possibility of spreading of the wave packet existed, activationless motion of electrons in an electric field would be possible. At sufficiently low temperatures this transport mechanism would have undoubted preference, and the electrical conductivity would cease to depend on the temperature.

Another important application of the ideas discussed in the preceding sections is to the problem of the metal-insulator transition in doped semiconductors. As is well known, in strongly doped semiconductors the conductivity at low temperatures has a metallic character, in the sense that it depends weakly on the temperature (in order of magnitude, of course, this conductivity is considerably smaller than the conductivity of typical metals). The strong-doping condition (see the reviews of Refs. 25, 26) has the form $N a^3 \gg 1$, where N is the impurity concentration and a is the Bohr radius of the impurity state. When this condition is fulfilled the electron gas is found to be almost ideal. The energies of interaction of the electrons with the impurities and with each other become considerably smaller than the Fermi energy. But at low impurity concentrations the current carriers turn out to be localized. In fact, at low temperatures in an n -type semiconductor the electrons are situated at the donors. The absence of an electron at one of the donors will be an elementary excitation. It is natural to raise the question of the excitation spectrum and the density of states. Here it is necessary to take into account that an excitation can be situated on any of the donors. If we neglect the potential that is created by the neutral donors, we arrive at the Lifshitz model discussed in the preceding section. It follows from this that the states should be localized. This means that at zero temperature a hole appearing on one of the donors cannot migrate to another donor. Thus, the low-temperature conductivity should be activational in character, i.e., it should decrease exponentially with temperature. The potential of the neutral donors produces a spread of the hole levels, which depends in a power-law manner on the impurity concentration. On the other

hand, the width of the impurity band in the Lifshitz model [formula (4.16)] is associated with the overlap and falls off exponentially with the concentration. Therefore, at low concentrations we cannot neglect the potential of the neutral donors. However, as we know from the analysis of the Anderson model, a spread of the levels only facilitates localization of states.

When the impurity concentration is increased a transition from activation to metallic conduction should occur. In practice, it occurs at $Na^3 \approx 0.02$ (see the review of Ref. 27). (In *p*-Ge, e.g., it occurs at a concentration 10^{17} cm^{-3} .) It is customary to call this transition a Mott transition, although it is far from identical with the transition described in Sec. 2. The principal difference is that, in the case under consideration, the states in the dielectric phase turn out to be localized, which is a signal of an Anderson transition. On the other hand, this is not, of course, an Anderson transition, since the electron-electron interaction undoubtedly plays a paramount role near the transition. At the transition point the electron-screening radius is comparable with the Bohr radius, and this leads to the destruction of the bound states at the impurities.

An example of a genuine Anderson transition is, apparently, the metal-insulator transition in strongly doped semiconductors under the influence of compensation. We suppose that in a strongly doped *n*-type semiconductor there is a compensating impurity (acceptors), with concentration N_A very close to the donor concentration N . At low temperatures each of the acceptors takes just one electron from a donor and becomes negatively charged. The remaining electrons, with concentration $n = N - N_A$, lie in the conduction band and are subjected to the action of the potential created by the donors and acceptors. It is usually said that, in a strongly doped semiconductor at low levels of compensation, when $n \approx N$, the potential of the impurities is small compared with the Fermi energy μ . However, if $N_A \rightarrow N$, and n decreases, the Fermi energy falls and the potential increases, since the electron screening is weakened. The theory of strongly compensated semiconductors has been developed in papers by Shklovskii and Éfros.²⁸⁻²⁹ The energy scheme that they obtained is presented in Fig. 7. The curve represents (in coordinate space) the bottom of the conduction band, distorted by the impurity potential. If there is no correlation in the disposition of the impurities, the maximum size and

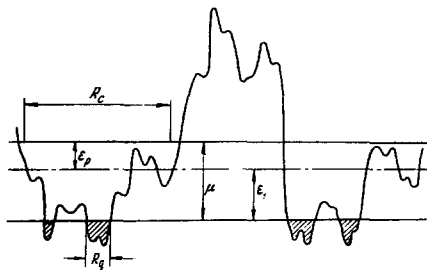


FIG. 7. This, according to Shklovskii and Éfros,²⁸ is how the potential energy of an electron in a compensated semiconductor can appear. The regions occupied by electrons are shaded.

amplitude of the potential fluctuations are determined by the electron screening. It is clear, however, that the screening in this situation is completely unlike Debye screening. It has been found that the role of the screening length is played by the length $R_c = N^{1/3}/n^{2/3}$. The amplitude of the fluctuations of the potential energy of an electron is of the order of $e^2 N^{2/3}/\kappa n^{1/3}$ (κ is the dielectric permittivity). The electrons form metallic drops, isolated from each other and located in the deepest parts of the potential contour. The characteristic size of a drop is

$$R_q = a (Na^3)^{-1/9} \ll R_c.$$

The electrons at the Fermi level are localized in regions of the order of R_q . With increase of the energy the localization length of the electron states increases, and, finally, at an energy equal to the percolation energy ϵ_p , the states become extended. Electrons having energy greater than ϵ_p can move over macroscopic distances while remaining all the time in classically allowed regions. The energy ϵ_p is determined from the solution of the so-called continuum problem of percolation theory.¹⁵ Conduction is effected by thermal excitation of electrons to the percolation level. The activation energy ϵ_i corresponding to this process is depicted in Fig. 7. (At very low temperatures the activation energy decreases as a result of the increase in the role of tunneling, but the conductivity at zero temperature is strictly equal to zero.) With increase of the electron concentration n the Fermi level increases, and when it reaches the percolation energy a metal-insulator transition occurs. In essence, this transition is a quasi-classical variant of the Anderson transition. This variant of the transition was first considered by Ziman.³⁰

The question of Anderson localization in the theory of MIS (metal-insulator-semiconductor) structures has also turned out to be very important. Most often, this structure is a silicon dioxide film (the insulator), situated between a silicon support (the semiconductor) and a planar metallic electrode. A potential applied to the metal bends the bands and redistributes the charge in such a way that a narrow inversion layer, i.e., a layer with current carriers of opposite sign to those in the bulk, is formed on the surface of the semiconductor (Fig. 8). By changing the applied potential it is possible to change the concentration of carriers in the inversion layer, and, consequently, the surface conduc-

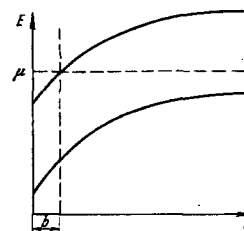


FIG. 8. Band scheme near the surface of the semiconductor in an MIS structure. d is the distance from the surface, and b is the width of the inversion layer. The Fermi level is shown by the dashed line μ .

tivity of the layer, with extremely wide limits. This is the basis of a field-effect transistor, which is such a structure. The inversion layer is occupied by a two-dimensional electron gas, situated in a random potential produced principally by the inhomogeneities of the insulating film. According to the ideas of Mott³¹ and Stern,³² Anderson localization of carriers occurs in this potential. At low carrier concentrations the conductivity of the inversion layer is activation in character, with an activation energy that decreases with temperature at low temperatures. This means that in the vicinity of the Fermi level there are localized states, between which hopping occurs. When the carrier concentration is increased the Fermi level is found in the region of extended states and the conduction has a metallic character (for a detailed discussion of the extensive experimental material, see the review by Mott *et al.*³³). This simple way of varying the concentration by means of an applied voltage makes it possible to investigate the electrical conductivity near the Anderson threshold comparatively easily. There then arises a further interesting theoretical problem, to the discussion of which we now turn.

6. ELECTRICAL CONDUCTIVITY AND ELECTRON WAVE FUNCTIONS IN THE VICINITY OF THE ANDERSON TRANSITION

We shall suppose that the Fermi level approaches the Anderson threshold from above. We ask: does the electrical conductivity at zero temperature vanish discontinuously or continuously (Fig. 9)?

There is no rigorously substantial answer to this question. Below we discuss the point of view of Mott,^{34,36} which is close to ours and evidently occupies a dominant position in the literature, although it has been subjected repeatedly to criticism (see Refs. 37–39).

Let the Fermi level be in the middle of the allowed band. If the disorder is small and the electrons are almost free, the conductivity is expressed by the usual Drude formula

$$\sigma = \frac{e^2 k_F l}{3\pi^2 \hbar}, \quad (6.1)$$

where l is the mean free path and k_F is the wave vector at the Fermi surface. Mott's point of view is based on the assertion (put forward by the pioneers of the physics

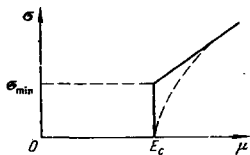


FIG. 9. Electrical conductivity at zero temperature as a function of the position of the Fermi level μ . The electrical conductivity should vanish at the point at which the Fermi level passes through the localization threshold E_c . But does it vanish discontinuously (the solid curve) or smoothly (the dashed curve)?

of disordered systems, A. F. Ioffe and A. R. Regel⁴⁰) that the mean free path, by its actual physical meaning, cannot be shorter than the electron wavelength. In the case of a half-filled band, $k_F \sim a_0^{-1}$, where a_0 is the lattice constant, and the statement that $k_F l = l/a_0 > 1$ is perfectly clear. It follows from it that the electrical conductivity cannot be smaller than the quantity

$$\sigma_{\min} = \frac{C_3 e^2}{\hbar a_0}, \quad (6.2)$$

where C_3 is a constant. Mott's concept is, in essence, that at zero temperature an electron gas cannot possess any conductivity other than that which is described in general physics courses and which is expressed, in order of magnitude, by the formula (6.1). But such a conductivity has a minimum possible value (6.2). From this, Mott concludes that, with increase of the disorder (e.g., with increase of the quantity W in the Anderson model), the conductivity decreases and, after reaching the value (6.2), goes to zero discontinuously (cf. Fig. 9). In the literature, this point of view has been named the "concept of minimum metallic conductivity". Of course, if we are talking microscopically, the reason that the conductivity vanishes is the Anderson localization, and the point at which this occurs corresponds to the Anderson limit.

It should be noted that, strictly speaking, the concept of a minimum metallic conductivity contradicts the ideas about the Anderson transition that are based on percolation theory (those presented in Sec. 3). Indeed, in the spirit of these ideas we can argue in the following way. We consider a chain of resonance sites, penetrating the whole sample; the wave function of an extended state is nonzero at these sites. It is natural to suppose that an electric current will flow along such chains. In the above discussions concerning the mean free path l that occurs in (6.1) it was tacitly assumed that the system is homogeneous. Near the transition, however, this assumption can scarcely be assumed to be correct. Moreover, it is clear that our chains are chosen in just such a way that the mean free path along them will be relatively large. As a result, the chains play the role of metallic filaments in a dielectric sample. As the transition point is approached the number of filaments penetrating unit area tends gradually to zero. Because of this, the electrical conductivity should vanish continuously, and not discontinuously. This is precisely the situation in two-component systems that are mixtures of a metal with an insulator, if the concentration of the metallic component is close to the percolation limit.¹⁵

Objections of this kind against the concept of a minimum metallic conductivity were put forward in Refs. 37 and 38. The defect of these arguments is, in our opinion, the following. Near the percolation limit the resonance chains become one-dimensional over a considerable length. But, as pointed out in Sec. 3, in a one-dimensional system arbitrarily small fluctuations lead to localization. Thus, the above-described mechanism, by which the electrical conductivity could be arbitrarily small but independent of temperature, evidently does not exist.

These considerations are also evidence that ideas based solely on percolation theory cannot describe the Anderson transition adequately. It is possible, however, to hope that the one-dimensional character of the percolation paths will become important only near the transition itself, and that this will not have a strong influence on the estimates of W_c/I made in Sec. 3.

In the Anderson model, the constant C_2 in (6.2) lies, according to the estimate of Mott *et al.*,³³ in the range 0.025–0.1 (for different lattices). Therefore, σ_{\min} lies in the range 250–1000 ohm⁻¹cm⁻¹.

The concept of a minimum metallic conductivity acquired special interest in the two-dimensional case. In this case,

$$\sigma_{\min} = \frac{C_2 e^2}{h}, \quad (6.3)$$

and the only dimensional quantities that appear in σ_{\min} are universal constants. This gives us grounds to hope that the constant C_2 is also universal and does not depend on the model under consideration. This is confirmed by elegant arguments of the scaling type, adduced by Licciardello and Thouless.⁴¹ The same authors^{18,41} performed a computer calculation by the Monte Carlo method, which confirmed the fact that a minimum metallic conductivity exists. They found that $C_2 = 0.12 \pm 0.03$ (this corresponds to $\sigma_{\min} = 3 \times 10^{-5}$ ohm⁻¹), and that in the framework of the Anderson model C_2 does not depend on the form of the lattice, for the three two-dimensional lattices represented in Table I. Moreover, the quantity C_2 was found to be independent of the ratio I/W , on increase of which the localization limits shifted from the center of the band to its edges (see Fig. 11). It seems to us that it makes sense for anyone who wishes to understand the physics of the Anderson transition to scrutinize the idea of these calculations, and so we shall discuss them in more detail below. However, we note first that, according to Ref. 33, the results of the numerical calculations are in satisfactory agreement with the experimental data on the minimum metallic conductivity that have been obtained for MIS structures.

The basic ideas of the calculation of the electrical conductivity of a two-dimensional system near the localization limit go back to the paper by Edwards and Thouless.¹⁷ We shall consider a square of side L , containing \mathcal{N} lattice sites with unit lattice constant. In accordance with the Anderson model, we assume that the electron energy at each site is a random quantity, uniformly distributed in an interval W . To find the energy levels it is necessary to solve the Schrödinger equation with the Hamiltonian (3.1). Here it is necessary to use particular boundary conditions. We shall assume first that these are periodic ($a_R = a_{R+L}$), and then that they are antiperiodic ($a_R = -a_{R+L}$), and find the level shift ΔE corresponding to the change of the boundary conditions.

We consider now the quantity $\mathcal{N} \Delta \bar{E} g(E)$, where $\Delta \bar{E}$ is the geometric average shift of the levels in a certain energy interval, and $g(E)$ is the density of states in this same interval. What is the value of this quantity in the

limit $\mathcal{N} \rightarrow \infty$? It is easy to understand that if the energy interval under consideration is in the region of localized states, this quantity will vanish exponentially. Indeed, if the wave function of the states considered vanished like $e^{-x/a}$, the shift of the levels with change of the boundary conditions should also be exponentially small: $\Delta E \sim \exp(-L/a)$. The density of states $g(E)$ is a finite quantity, and so

$$\lim_{\mathcal{N} \rightarrow \infty} \mathcal{N} \Delta \bar{E} g(E) = 0. \quad (6.4)$$

The nontrivial statement is that, in the region of extended states,

$$\lim_{\mathcal{N} \rightarrow \infty} \mathcal{N} \Delta \bar{E} g(E) = \frac{2\sigma h}{e^2 f}, \quad (6.5)$$

where σ is the two-dimensional specific electrical conductivity that arises when the Fermi level has the value E , e is the electron charge, and f is a coefficient that depends on the form of the lattice. For a square lattice $f=1$, for a hexagonal lattice $f=\sqrt{3}$, and for a triangular lattice $f=\sqrt{3}/2$.

An elegant proof of the formula (6.5), based on the Kubo–Greenwood formula, is given in Refs. 17 and 18. We confine ourselves here to just a qualitative interpretation. If the mean free path is much shorter than the distance L to a boundary, the level shift ΔE for the nonlocalized electrons is of the order of \hbar/τ , where τ is the time needed for an electron to diffuse to the boundary. According to the diffusion equation, $L^2 = D\tau$, where D is the diffusion coefficient. On the other hand, the electrical conductivity is connected with the diffusion coefficient by the usual relation $e^2 D g(E) = \sigma$. Combining these formulas and taking into account that, for a lattice with unit period, $L^2 = \mathcal{N}$, it is easy to obtain an order-of-magnitude relation of the type of formula (6.5).

Thus, in the two-dimensional case the criterion for localization is that we go over from the formula (6.5) to the formula (6.4). The results of Licciardello and Thouless¹⁸ for the triangular lattice are presented in Fig. 10. The authors assume that the states are localized in a given energy interval if $\mathcal{N} \Delta \bar{E} g(E)$ decreases

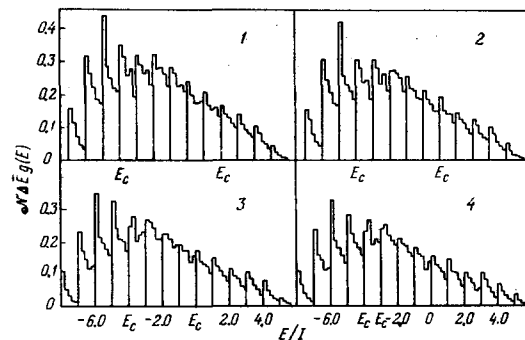


FIG. 10. Dependence of $\mathcal{N} \Delta \bar{E} g(E)$ on the energy for the triangular lattice. The values of W/I are 8.0 (1), 8.5 (2), 9.0 (3), and 9.5 (4). In each energy interval we show the values of $\mathcal{N} \Delta \bar{E} g(E)$ for $\mathcal{N} = 36, 64, 100, 144,$ and 196 , arranged in this order from left to right. The upper and lower boundaries of the extended states are denoted by E_c .

monotonically with increase of \mathcal{N} from $\mathcal{N}=36$ to $\mathcal{N}=196$. But if, in this energy interval, the monotonic behavior is violated, the authors assume that the states there are extended. Figure 11, which is also borrowed from Ref. 18, shows the localization thresholds obtained in this way, the electrical conductivity in the region of extended states, and the density of states, calculated in the usual way. Attention is drawn to the fact that this Figure is not like Fig. 3, in which the same things are depicted schematically. According to Ref. 18, the region of extended states appears neither at the center of the band nor at the maximum of the density of states. It is difficult to comment on this fact. It is possible that the accuracy of the determination of the threshold was insufficient, and it is possible that we still do not understand some important features of this undoubtedly very complicated phenomenon (cf. Ref. 60).

With regard to the concept of a minimum metallic conductivity, one should also bear the following in mind. All the arguments and calculations described above were made in the one-electron approximation. A very important aspect of these arguments is that the density of states at the Fermi level was assumed to be a nonzero constant quantity. As shown in Refs. 42 and 43, the electron-electron interaction leads to the vanishing of the density of states at the Fermi level. In view of this circumstance, the question of a minimum metallic conductivity requires further discussion.

We turn now to another important aspect of the theory of the Anderson transition, namely, to the question of the behavior of the wave functions at energies close to the critical energy E_c that separates the localized and extended states. It follows from general principles of quantum mechanics that the behavior of the wave functions cannot change discontinuously for a small change in the energy. The localized states that are separated from the extended ones by a very small energy should have a large localization length, as it is precisely the

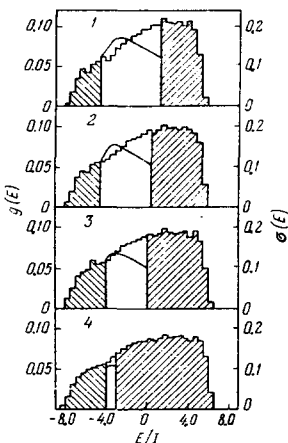


FIG. 11. Histogram of the density of states for 100 samples consisting of 100 sites of a triangular lattice. The values of W/I are the same as in Fig. 10. The regions of localized states are shaded. The electrical conductivity (in units of e^2/\hbar) is shown by the solid curves in the regions of extended states.

energy $E_c - E$ that determines the attenuation of the localized states in the classically forbidden regions.

We shall consider, for example, a potential well, and suppose that, as a result of a decrease of its depth, a certain bound state is "expelled" into the continuum. In this case, inevitably, the localization length of this state becomes infinite like $E^{-1/2}$ where E is the energy measured from the boundary of the continuum. We must assume, therefore, that the radius $a(E)$ of the localized states behaves near threshold in accordance with the law

$$a(E) = \frac{a_0}{|E_c - E|^s}, \quad (6.6)$$

where s is an unknown critical index. It should be borne in mind that the corresponding wave functions oscillate on a scale of the order of the lattice constant, and only their envelope behaves like $e^{-r/a(E)}$ (Fig. 12).

The problem of the value of the critical index s is not yet finally solved. If we were talking about a simple potential well, where it can be assumed that the potential at a sufficiently large distance from the well is a constant, the natural answer would be that $s = \frac{1}{2}$. This is just what was assumed, in the first place, by Mott and Davis (see Ref. 24, p. 22). However, there are no serious grounds for such an assumption. In 1972, Anderson,⁴⁴ using results from the theory of self-avoiding walks, showed that the most probable Green's function falls off with distance like $e^{-R/a(E)}$, where $a(E)$ is expressed by the formula (6.6) with $s = 0.6$. It should be noted, however, that the arguments used by Anderson to reduce the problem of the asymptotic form of the most probable Green's function to the problem of self-avoiding walks contain a number of far-from-obvious assumptions. It is interesting, nevertheless, that Abram and Edwards⁴⁵ obtained the same result from entirely different considerations. Freed⁴⁶⁻⁴⁷ obtained the similar, but not identical, result $s = \frac{2}{3}$. A similar result was also obtained by Sadvskii,⁴⁸ who, using Anderson's argumentation and the theory of self-avoiding walks developed by de Gennes,⁴⁹ found that the index s coincides with the correlation-length index of the usual theory of critical phenomena.

It is entirely natural to assume that the index s does not depend on the specific model of the disordered system but does depend on the number of dimensions of space. The index values given above pertain to the three-dimensional case. Abram⁵⁰ showed that in the two-dimensional case $s = 0.75$. Finally, Last and Thouless assumed that, in the three-dimensional case, in the immediate vicinity of the energy E_c there exists an energy region in which the wave functions decrease with distance by a power law.⁵¹ In the same work, a numerical experiment providing evidence in favor of this assumption was performed.

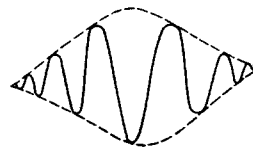


FIG. 12. Wave function near the Anderson transition.

7. SOME ASPECTS OF THE THEORY OF THE ANDERSON TRANSITION. CONVERSATION WITH A THEORIST ABOUT THE THEORY

Theorist. I have read the manuscript of your review. Perhaps it will be good for some, but I didn't like it very much. All you have here is words, and I don't understand words very well. Can we really not see at least something from formulas? I grant, as you say, that there is no satisfactory theory, but surely there is *something* definite? You report a large number of different results. If they are well known, they must have been obtained somehow. And the very fact of the existence of the Anderson transition? Where does that come from? Certainly not from your resonance bands. Incidentally, I have seen papers on this subject. True, I haven't analyzed them myself, but they appeared to be perfectly solid. But you haven't written anything about them.

Author. Your reproach is fair. In my defense I can only say that I have tried to make the review as simple and clear as possible. However, as is clear from what you have said, these concepts are highly subjective. Besides, it seems to me that the analytic methods in the theory of the Anderson transition are still not adequately developed. Nevertheless, I ought, of course, to have talked about the steps made in this direction, especially as everything started from these. The founding paper by Anderson¹ did, in fact, contain the method that has been used in almost all the papers you mentioned.

Theorist. Well, what was in it?

Author. Just what you want, probably. The Green's function in the site representation, a perturbation-theory expansion, a re-expansion taking into account multiple scattering at one site ...

Theorist. Of course, of course! I am convinced that if anything is really happening, this fact should be clear from perturbation theory! In some order, something should necessarily go to zero or to infinity. I wanted to look at this myself before talking with you, but I didn't have time. However, it should be very simple. Surely, what you are stating is... you say that a transition between states belonging to different sites is impossible. Then the states will be strictly localized. Excellent—this means that at a certain energy value, lying on the real axis, the imaginary part of the self-energy of the single-particle Green's function should vanish. This energy will be the threshold of the Anderson transition. Is that correct?

Author. In general yes. But...

Theorist. You want to say that the Green's function G_{in} in the site representation is, in general, off-diagonal in the site index i . So it is not clear precisely what function I am talking about?

Author. Well, no, the point is that...

Theorist. I am talking, of course, of the site-diagonal Green's function. Let's call it G_{00} .

Author. You think that the choice of this site is not important here?

Theorist. Of course it isn't. After averaging, all the sites will be come equivalent. It is strange to hear such a question from a specialist in disordered systems. (Puase) In practice we simply need to write the series for the probability of a transition away from the given site to any other site. At the transition point, if you are right and such a point does indeed exist, this series should vanish. That's all. We start by analyzing the first term of the series. In second order of perturbation theory... Wait, wait... There's a funny thing! This probability will never vanish. No, I no longer understand you at all—I disagree with you completely.

Author. Why?

Theorist. Listen to me for five minutes, and you will understand everything without explanations. In second order of perturbation theory, we have

$$V = \frac{2\pi}{\hbar} \left\langle \sum_m |I(m)|^2 \delta(\epsilon_0 - \epsilon_m) \right\rangle; \quad (7.1)$$

here, V is the transition probability. The sum is taken over the nearest neighbors of the site 0, and $\langle \dots \rangle$ denotes averaging over all values of the energy ϵ_m . Now what form did your energy distribution function have? Aha, formula (3.2) Excellent! We carry out the averaging in (7.1):

$$V = \frac{2\pi}{\hbar} \int_m P(\epsilon) |I(m)|^2 \delta(\epsilon_0 - \epsilon) d\epsilon. \quad (7.2)$$

We make use of (3.2) and obtain

$$V = \frac{2\pi}{\hbar} \frac{\sum_m |I(m)|^2}{W}. \quad (7.3)$$

So, in contradiction to what you said, this quantity does not vanish for any finite values of I/W . Moreover, I see clearly that the same is also true in all orders of perturbation theory. What do you say to that?

Author. You are probably right.

Theorist. But this means that there is no transition at all!

Author. Look carefully at the formula (7.1) that you have written. In it is a summation over the sites that are nearest neighbors of the site 0. What do you think is the probability that amongst these neighbors there will be a site with energy $\epsilon_m = \epsilon_0$?

Theorist. The probability of exact equality is, of course, zero, but we can't argue in this way if there is a δ -function in the expression. Represent it in the form $\pi^{-1} s / [s^2 + (\epsilon_0 - \epsilon_m)^2]$, where s is a very small quantity. After this it is easy to see that the result does not depend on s .

Author. Very good, let's interpret your result assuming that all the levels have a finite width s .

In the system there are a certain number of sites having at least one nearest neighbor with an energy differing from their own energy by an amount not greater than s . For $s \rightarrow 0$ the number of such sites tends to zero, but they give a finite contribution to (7.1) because

they are assigned a very large weight, of the order of $1/s$, in the averaging. This is the way you obtained the expression (7.3), which, as we now see, bears no relation to the matter.

Theorist. I don't see that.

Author. Imagine all this in space. There are pairs within which a transition between the sites is possible. In the Anderson model the distance between the sites of one pair is equal to the lattice constant, and the fraction of sites belonging to such pairs is of the order of s/W . Thus, for small values of s the pairs are isolated from each other and no transitions are possible between them. Can such pairs really ensure spreading of a wave packet over a macroscopic distance?

Theorist. Perhaps you are right. It appears that it is meaningless to average the transition probability. But what then must we calculate?

Author. Anderson represented the probability of a transition from a site (or, more precisely, the imaginary part of the self-energy of the Green's function G_{00}) in the form $W = \lim_{s \rightarrow 0} sX(s)$. In second order of perturbation theory,

$$X(s) = \frac{2}{h} \sum_m \frac{|I_m|^2}{s^2 + (\epsilon_0 - \epsilon_m)^2}. \quad (7.4)$$

This coincides, of course, with what you wrote, but without the averaging over the energies ϵ_m .

Theorist. How can we work with such a quantity? It depends, surely, on which site we take as our starting point.

Author. Do you think that this probability does not in fact depend on the site? Yes, $X(s)$ is a random quantity, and Anderson calculated its distribution function using the second-order expression (7.4). This is very simple to do. It turned out that the distribution function $F(X)$ has a completely well-defined limit as $s \rightarrow 0$. The most probable value of X turns out to be a finite quantity. Because of this, the quantity V is equal to zero with probability unity.

Theorist. But how does this tie in with formula (7.3)?

Author. The point is that for large X the function $F(X)$ falls off only like $X^{-3/2}$, so that the average value of X diverges. Your result is due to just this. As you see, it has no direct bearing on the question of localization.

Theorist. But, permit me, it has now turned out that V is always zero, and, consequently, the states are always localized!

Author. Yes, that is precisely what happens in second order of perturbation theory. But Anderson showed that the perturbation-theory series for the quantity X diverges with probability unity for large values of I/W . The point where it begins to diverge is the localization threshold. Anderson showed that such a point does indeed exist, but he came up against considerable difficulties in estimating the critical value of W_c/I . Nevertheless, he did give an estimate for W_c/I . From the

standpoint of the subsequent computer calculations, this estimate was much too high. The estimate is analyzed comparatively simply in a paper by Ziman.⁵²

Theorist. One is analyzing here the probability of convergence of a series for a random quantity. How is this done?

Author. This is a complicated mathematical problem, and I was not prepared to discuss it in this review. You can form your own opinion with the aid of the articles by Thouless¹⁴ and Licciardello and Economou.⁵³ I should say, incidentally, that the values of W_c/I obtained in Ref. 53 are in good agreement with the computer calculations.

Theorist. Are you saying that the averaged single-particle Green's function, which contains complete information about the density of states, "knows nothing at all" about the Anderson transition, in that the transition point is in no way special for it?

Author. No, I am not prepared to defend so general a statement, but I shall give you a few well known arguments in favor of it. You remarked, correctly, that the Anderson transition corresponds to the vanishing of the imaginary part of the self-energy. But here we must be talking only about the unaveraged quantity. The averaged Green's function always contains an imaginary part, at all energies. To see this, take the free Green's function $G_{ii} = (\epsilon - \epsilon_i + i\delta)^{-1}$ and integrate it with weight $P(\epsilon_i)$. Moreover, there exists a model for which the averaged single-particle Green's function is known exactly. This is Lloyd's model.⁵⁴ It differs from the Anderson model only in the fact that the function $P(\epsilon)$ is expressed not by formula (3.2) but by the formula

$$P(\epsilon) = \frac{\gamma}{\pi(\epsilon^2 + \gamma^2)}. \quad (7.5)$$

All the qualitative arguments given in Sec. 3 apply in equal measure to Lloyd's model. We need only replace W by γ everywhere (with the sole exception, perhaps, of quantitative estimates). Therefore, there is every reason to suppose that an Anderson transition also occurs in Lloyd's model, when γ and I have a certain ratio. Nevertheless, the Green's function found by Lloyd, when averaged over all realizations of the energy, has the form

$$G_k(\epsilon) = (\epsilon - E(k) + i\gamma)^{-1} \quad (\text{Im } \epsilon > 0), \quad (7.6)$$

where $E(k)$ is expressed by formula (2.6).

It is impossible to imagine anything simpler than this function. Its self-energy part not only has no singularities but is also completely independent of the energy. This fact seems to me to be a strong argument that the averaged Green's function in the general case, as you expressed it, "knows nothing" about the Anderson transition (see also Ref. 55).

Theorist. Do you know of any solved model in which the transition can be seen?

Author. Yes, the Anderson model on a Bethe lattice, which is an infinitely branching tree. The method employed to solve it has been used as the basis of approximate calculations for ordinary lattices.^{56,57}

8. CONCLUSION

We have given an account of modern ideas about the localization of quantum states in disordered systems. For definiteness, we have been concerned with electrons, although, to a considerable extent, these ideas can also be extended to vibrational levels in lattices with substituted atoms. Two important concepts, formulated by Anderson and Mott, form the basis of these ideas. One of them is that there exists a narrow boundary between the localized and extended states, and the other asserts that the electrical conductivity vanishes discontinuously when the Fermi level passes through this boundary. It is probable that neither of these concepts is strictly justified. However, as we have seen, the first of them is so firmly ensconced in modern physics that it seems inconceivable that we could explain the enormous volume of experimental material concerning amorphous and doped crystalline semiconductors without using this concept as a basis.

It would be an exaggeration to say the same about the concept of a minimum metallic conductivity, although the recently published experimental data on MIS structures constitute ever more evidence in its favor.^{33,58,59}

We have left aside a large number of extremely interesting papers in which analytic methods for the calculation of the localization thresholds are developed (see the bibliography in Refs. 53 and 54), although the basic ideas of these papers are described in Sec. 7.

It seems to us that the problem of the Anderson transition is similar to the problem of second-order phase transitions, and its solution should be constructed in the spirit of scaling ideas. Probably, this should be preceded by a phenomenological theory, introducing an order parameter and critical indices and similar to the one that has been created in percolation theory. Clearly, the correlation-length index is the index s in (6.6). However, so far as we know, there has not yet been any work of this kind.

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Translated by P. J. Shepherd