Repulsion between energy levels and the metal-insulator transition

B. L. Al'tshuler, I. Kh. Zharekeshev, S. A. Kotochigova, and B. I. Shklovskiĭ

B. P. Konstantinov Institute of Nuclear Physics, Academy of Sciences of the USSR, Leningrad
(Submitted 28 July 1987)
Zh. Eksp. Teor. Fiz. **94**, 343–355 (March 1988)

An analysis is made of the statistics of one-electron energy levels in a finite (bounded) system with a statistical disorder. A study is made of the variance $\langle[\delta N(E)]^2\rangle$ of the number of levels $N(E)$ in an energy band of width E due to variation of the realization of the random potential. A scaling theory is used to deduce a qualitative description of the influence of a metal-insulator transition on the value of $\langle[\delta N(E)]^2\rangle$. It is shown that at the transition point the variance is proportional to the average number of levels $\langle N(E)\rangle$ in a band, exactly as for a state well within the insulator range, but the coefficient of proportionality is less than unity. This theory is compared with the results of computer modeling carried out by applying the Anderson model to the case of a simple cubic lattice of $5\times5\times5$ sites with cyclic boundary conditions. The influence of a change in the degree of disorder and of the metal-insulator transition on the statistics of separations between the nearest levels is considered.

1. INTRODUCTION

Fluctuations of the residual conductivity of small metal samples due to variation of the realization of the random impurity potential, known as mesoscopic fluctuations (see, for example, the review in Ref. 1 and the references given there), are currently attracting much attention.

According to Thouless, the conductivity of a cube with a side L at low temperatures $T\ll E_c$, where

$$E_c=\hbar/\tau_D=\hbar D/L^2, \tag{1}$$

is governed by the energy levels of electrons lying within a band of width E_c centered on the Fermi level [D in Eq. (1) is the electron diffusion coefficient and τ_D is the diffusion time of electrons across the whole sample]. The average, over the realizations of a random potential, admittance G (representing the reciprocal of the impedance) of a sample measured in units of $e^2/\hbar$ is simply equal to the average number of these levels:

$$G=(e^2/\hbar)\langle N(E_c)\rangle. \tag{2}$$

Al'tshuler and Shklovskiĭ[2] drew attention to the fact that fluctuations of the admittance of a cube from one realization to another are largely governed by the corresponding fluctuations of $N(E_c)$, which is the number of levels in a band of width E_c. Al'tshuler and Shklovskiĭ[2] investigated the problem of the variance

$$\langle[\delta N(E)]^2\rangle\equiv\langle[N(E)-\langle\delta N(E)\rangle]^2\rangle \tag{3}$$

of the number of levels in a band of arbitrary width E. The angular brackets denote averaging over the realizations of the random potential. These authors considered the case when $\langle N(E)\rangle$ is small compared with the total number of levels in the system. The quantity $\langle[\delta N(E)]^2\rangle$ for a metal sample was determined by the impurity diagram technique in the range of parameters where $L\gg l\gg\lambda$; here, l and λ are, respectively, the mean free path and the wavelength of an electron.

Dyson[3] studied earlier the problem of statistics of energy levels in complex nuclei and dealt with a similar problem of eigenvalues of an ensemble of random matrices (Hamiltonians) in which all the matrix elements are distributed normally near zero and are characterized by the same variance. For the variance $\langle[\delta N(E)]^2\rangle$ in the simplest case of real symmetric matrices (orthogonal ensemble) Dyson found that

$$\langle\delta N^2\rangle=\frac{2}{\pi^2}[\ln\langle N(E)\rangle+B]\equiv\langle\delta N^2\rangle_D \tag{4}$$

[here and later we shall use $\langle\delta N^2\rangle$ for the quantity in Eq. (3)]. The constant B was calculated by Dyson and Mehta[4] and was found to be $B\approx2.18$.

An interesting feature of Eq. (4) is the smallness of the fluctuations $\langle\delta N^2\rangle\ll\langle N(E)\rangle$. This means that the sequence of levels differs considerably from the random Poisson sequence, which should be characterized by $\langle\delta N^2\rangle=\langle N(E)\rangle$. The additional "stiffness" of the system of levels is due to their quantum-mechanical repulsion.

The results of Ref. 2 for $\langle\delta N^2\rangle$ of a metal cube surrounded by an insulator and, therefore, containing unbroadened levels agree with the Dyson formula of Eq. (4) if $E\ll E_c$ (only the value of the constant B cannot be determined by the impurity diagram technique). This agreement is in our opinion due to the fact that in a characteristic time $\hbar/E$ a diffusing electron can travel across the whole sample, so that the matrix elements of the Hamiltonian relating to various states lying within an energy band of width E are of the same order of magnitude.

If the energy levels exhibit decay represented by γ due to, for example, the possibility of escape of a particle from a sample, it follows from Ref. 2 that $\langle N(E)\rangle$ on the right hand side of Eq. (4) should be replaced with E/γ and for $\gamma\sim E$ the variance $\langle\delta N^2\rangle$ is of the order of unity, i.e., it is even smaller than $\langle\delta N^2\rangle_D$.

If $E\gg E_c$, the value of $\langle\delta N^2\rangle$ obtained in Ref. 2 is considerably greater, irrespective of the boundary conditions, than the Dyson variance $\langle\delta N^2\rangle_D$ and depends on E_c:

$$\langle\delta N^2\rangle=\frac{2^{1/2}}{6\pi^3}\left(\frac{E}{E_c}\right)^{3/2}. \tag{5}$$

The reason for the increase in the scale of fluctuations is that in the range $E\gg E_c$ an electron can cross only a small proportion of a sample in the characteristic time $\hbar/E$ and this part

 0038-5646/88/030625-07$04.00

of the sample is roughly speaking a tiny cube of side

$$L_E=(D\hbar/E)^{1/2}.$$

Individual tiny cubes of this kind have practically independent systems of levels. This means that fluctuations of the number of levels in each tiny cube are independent and $\langle\delta N^2\rangle$ is proportional to their number $(L/L_E)^3$:

$$\langle\delta N^2\rangle=\langle\delta n^2\rangle(L/L_E)^3=\frac{2^{1/2}}{6\pi^3}(L/L_E)^3, \qquad (6)$$

where $\langle\delta n^2\rangle$ is the variance of the number of levels in a cube of size L_E when these levels lie within an energy band E. Since such a cube is open, it follows that $\gamma\sim D/L_E^2=E$ and $\langle\delta n^2\rangle\sim 1$.

It therefore follows from Ref. 2 that in the region of high metallic conductivity the variance of the number of levels in a band of given width depends strongly on E_c, i.e., it depends on the admittance G of the sample. Clearly, the statistics of the levels should be sensitive, in contrast to the average number of levels $\langle N(E)\rangle$, to a metal-insulator transition. We shall provide a qualitative description of the dependence of $\langle\delta N^2\rangle$ on E for a transition from a good metal (via a critical region) to an insulating state. In the next section we shall discuss the dependence of the variance of the number of levels outside the metal-insulator critical region, i.e., we shall discuss this dependence for a good metal and an insulator with strongly localized electron states. In Sec. 3 we shall discuss qualitative ideas on the behavior of the dependence of $\langle\delta N^2\rangle$ on E in the critical region, based on the scaling relationship for the metal-insulator transition. The results of a numerical modeling of the problem by the application of the Anderson model to a cube of $5\times5\times5=125$ sites, carried out for a wide range of the scatter of the levels, are presented in Sec. 4. A detailed quantitative comparison of the results of this machine experiment with theoretical predictions for the metallic range is made in Sec. 5. In addition to the dependence of $\langle\delta N^2\rangle$ on E, we shall consider how the distribution functions of spacings between the two nearest levels, which is the problem of major importance in discussing the repulsion of levels, behaves in the region of this transition. The results will be given in Sec. 6.

2. STATISTICS OF ENERGY LEVELS OUTSIDE THE CRITICAL REGION

In the case of a good metal when $l\gg\lambda$ at sufficiently low energies E the value of $\langle\delta N^2\rangle$ is given by Eq. (4) or (5). The dependences given by these equations are valid as long as L_E is greater than the mean free path l, as long as $E\ll\hbar/\tau$, where τ is the mean free time. If $E\gg\hbar/\tau$, then fluctuations $\langle\delta N^2\rangle$ cease to rise on increase in E. The order of magnitude of the fluctuations is given by

$$\langle\delta N^2\rangle\sim(L/l)^3. \qquad (7)$$

This is true because the shifts of the levels under the action of the random potential do not exceed $\hbar/\tau$ and, consequently, the contribution made to δN by a band of width E comes solely from its boundary regions of width $\hbar/\tau$. A graph of the dependence $\langle\delta N^2\rangle/\langle N(E)\rangle$ on E in the case when $l\gg\lambda$ is shown schematically in Fig. 1 (curve 2) together with the graph of the dependence (4) (curve 1). As l decreases and approaches λ, the value of E_c decreases and $\langle\delta N^2\rangle$ rises for bands of width $E>E_c$. If $l\approx\lambda$, at the limit of

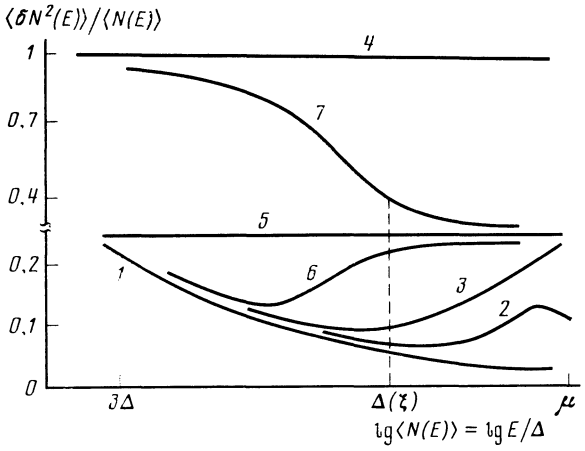

FIG. 1. Schematic representation of the theoretical dependences of $\langle\delta N^2\rangle/\langle N(E)\rangle$ on the average number of levels $\langle N(E)\rangle$: 1) Dyson formula (4); 2) good metal ($l\gg\lambda$); 3) limit of the critical region ($l\approx\lambda$); 4) insulator [Eq. (9)]; 5) transition point [Eq. (14)]; 6) metal in the critical region; 7) insulator in the critical region.

the critical region near the metal-insulator transition, the value of $\hbar/\tau$ is of the order of the maximum energy scale $\hbar^2/m\lambda^2\equiv\mu$, where μ is the Fermi level. Then the range of validity of Eq. (7) vanishes and for $E<\hbar^2/mL^2$ we find that Eq. (4) applies, whereas for $\hbar^2/mL^2<E<\mu$, we have to use Eq. (5). This behavior of $\langle\delta N^2\rangle$ is represented by curve 3 in Fig. 1, which can be called the boundary of the critical region of the metal-insulator transition on the metal side.

On the other hand, it is clear that in the insulator phase far from the metal-insulator transition the distribution of levels on the energy axis should be absolutely random (of the Poisson type). This is easiest to understand using the familiar Anderson model. The Hamiltonian of this model is

$$H=I\Big[\sum_i \varepsilon_i a_i^+ a_i+\sum_{i,j} a_j^+ a_i\Big], \qquad (8)$$

where a_i^+ (a_i) are the creation (annihilation) operators of an electron at a site i in a lattice (for the sake of argument, a simple cubic lattice); j are the numbers of six nearest neighbors of the site i in the lattice; ε_i is the random energy of the site i measured in units of the overlap integral I of the nearest sites and distributed uniformly between $-V$ and V.

It is known that in the Anderson model an increase in V results in a metal-insulator transition at $V=V_c\approx8$ (Ref. 5). Clearly, if $V\gg V_c$, we can ignore the overlap of the wave functions at the lattice sites and we find that the wave functions are localized at individual sites. In this case the distribution of the energy levels is practically identical with the distribution of the "bare" energies ε_i, i.e., it is absolutely random (Poisson-type). We then have

$$\langle\delta N^2\rangle/\langle N(E)\rangle=1. \qquad (9)$$

The result given by Eq. (9) is represented by a straight line 4 in Fig. 1.

It therefore follows that we now know the dependence of $\langle\delta N^2\rangle$ on E on both sides of the critical region near the metal-insulator transition. We shall therefore determine

how the transition takes place between these sides, i.e., how $\langle \delta N^2 \rangle$ behaves in the critical region near the metal-insulator transition.

3. QUALITATIVE BEHAVIOR OF $\langle [\delta N(E)]^2 \rangle$ IN THE CRITICAL REGION

It is natural to begin an analysis of the critical region from the metal-insulator transition point itself. It follows from the scaling theory that if $T = 0$ then at the transition point the admittance and the diffusion coefficient depend in such a way on the spatial scale L that the admittance of a cube of any size L is G_c, which is independent of L. According to the majority of the modern data,[6] we have

$$G_c \approx 0.03\, e^2/\hbar. \tag{10}$$

It follows from Eq. (10) that

$$D(L) = G_c/ge^2L, \tag{11}$$

where g is the density of states at the Fermi level. Consequently, in the case of a cube of size L, we have

$$E_c = \frac{\hbar D(L)}{L^2} \approx \frac{G_c}{e^2/\hbar}\frac{1}{gL^3}, \tag{12}$$

i.e., $E_c \lesssim \Delta$, where $\Delta \equiv (gL^3)^{-1}$ is the average separation between the levels. Clearly, in this case the range of validity of the Dyson formula, $E \lesssim E_c$, generally vanishes. For all the energies $E > \Delta$ the inequality $E \gg E_c$ is satisfied at the transition point. We can then estimate $\langle \delta N^2 \rangle$ using Eq. (6). In using this equation we need to find first the size $L(E)$ of the tiny cube through which an electron runs in a time $\hbar/E$. The quantity $L(E)$ is described by

$$D(L_E)\hbar/E = L_E^2. \tag{13}$$

Substituting Eq. (11) into Eq. (13), we obtain $L_E^3 = \hbar G_c/gEe^2$ or, from Eqs. (6) and (10),

$$\frac{\langle \delta N^2 \rangle}{\langle N(E) \rangle} = \frac{2^{1/4}}{6\pi^3}\frac{gEL^3e^2/\hbar}{G_c\langle N(E)\rangle} \equiv \varkappa, \tag{14}$$

where $\varkappa \approx 0.25$.

Therefore, at the transition point, as well as deep inside the insulator, we have $\langle \delta N^2 \rangle \propto \langle N(E) \rangle$, but the magnitude of the fluctuations $\langle \delta N^2 \rangle$ is approximately 4 times less. The result given by Eq. (14) is represented by straight line 5 in Fig. 1.

In fact, we do not note the exact value of the coefficient $\varkappa$. This is because Ref. 13 simply gives the order of magnitude since the diffusion coefficient D depends critically not only on the energy, but also on the frequency and wave vector. We were unable to include these dependences within the framework of the one-parameter scaling treatment without additional assumptions. However, in our opinion the most important conclusion is that the ratio $\langle \delta N^2 \rangle / \langle N(E) \rangle$ in the critical region is equal to a constant smaller than unity.

We shall now consider the critical region on the metal side (i.e., the region between curves 3 and 5 in Fig. 1). We shall do this bearing in mind that in this region Eq. (11) is valid only for scales L such that $L < \xi$, where ξ is the correlation length of the metal-insulator transition. In the Anderson model this correlation length can be written in the form

$$\xi = a|V_c/(V - V_c)|^{\nu} \quad (V < V_c), \tag{15}$$

where a is the lattice constant. If $L \gg \xi$, then instead of Eq. (11), we now have

$$D(L) = G_c/ge^2\xi \equiv D(\xi). \tag{16}$$

We shall consider such values of $V_c - V$ that $L \gg \xi \gg a$. It then follows from Eq. (16) that

$$E_c = E_c(\xi) = \hbar D(\xi)/L^2 = \hbar/ge^2\xi L^2 \gg \Delta \tag{17}$$

and if $E_c(\xi) \gg E \gg \Delta$, then the Dyson formula (4) should apply. If $E \gg E_c(\xi)$, then Eq. (6) applies and $L(E)$ can be found from the condition $D(\xi)\hbar/E = L_E^2(\xi)$, i.e.,

$$\langle \delta N^2 \rangle \approx [L/L_E(\xi)]^3 \approx [E/E_c(\xi)]^{3/2}. \tag{18}$$

Equation (18) is meaningful only if $L(\xi) \gg \xi$, i.e., if

$$E \ll \Delta(\xi) \equiv (g\xi^3)^{-1}.$$

In the opposite limiting case of $E > \Delta(\xi)$ or $L_E(\xi) \ll \xi$, the behavior of $\langle \delta N^2 \rangle$ should be indistinguishable from the behavior of the transition point, i.e., it should be identical with Eq. (14). The expected nature of the dependence of $\langle \delta N^2 \rangle / \langle N \rangle$ on E in the critical region is represented by curve 6 in Fig. 1. On increase in ξ the points at both kinks $(gL^2\xi)^{-1}$ and $(g\xi^3)^{-1}$ approach Δ and the dependence becomes practically indistinguishable from Eq. (14) (curve 5) if $\xi \approx L$. Conversely, when ξ is reduced to a, curve 6 is converted to curve 3.

We shall now consider briefly the critical region but on the insulator side of the transition. In this case if $E \gg \Delta(\xi)$, the repulsion between the levels is important in a region of space of dimensions much smaller than ξ and the fluctuations $\langle \delta N^2 \rangle$ are practically the same as at the transition point. If $E \ll \Delta(\xi)$, the average separation between the levels is much greater than ξ, they overlap weakly, and the proximity to the transition has no effect, because the fluctuations $\langle \delta N^2 \rangle$ will be the same as well inside the insulator range. Therefore, the function $\langle \delta N^2 \rangle / \langle N(E) \rangle$ undergoes a one-parameter transition from 1 to $\varkappa$ to at $E \approx \Delta(\xi)$ (see curve 7 in Fig. 1). A reduction of ξ from L to a shifts the "knee" of this curve from $E \approx \Delta$ to $E = \mu$.

4. NUMERICAL EXPERIMENT

The purpose of our modeling experiment was to check the scaling relationship of Fig. 1 in the case of a specific model of a disordered system. We used the Anderson model of Eq. (8) and considered a cube of $5 \times 5 \times 5$ sites with periodic boundary conditions, i.e., we considered an unbounded simple cubic lattice in which the random energies ε_i are periodic and the period amounts to five lattice constants along each coordinate. In this problem the levels are discrete, so that there is no question how to deal with broadened levels.[2] The calculation procedure was as follows. A random number generator created values of ε_i within the interval $[-V, V]$. A 125×125 matrix of the Hamiltonian was diagonalized[1)] and calculations were made of the numbers of levels within a band of energies of width $E_0 = (V + 6)/2$ centered on zero and in narrower bands of width $E_i = E_0/2^{i/2}$, where $i = 1, 2$, and 3. Then each of these bands was divided into 2^k strips of the same width:

$$E_{ik} = E_i/2^k = E_0/2^{k+i/2},$$

where $k = 1, 2, 3, 4$. We calculated the number of levels N in the original bands and in each strip and then we averaged N and N^2 over 2^k strips of each width. The results were then averaged over ≈ 200 realizations of the energy ε_i and finally we found $\langle \delta N^2 \rangle = \langle N^2 \rangle - \langle N \rangle^2$ for each width E_{ik}. The width of the band E_0 was so small that it was not possible to notice significant changes in the density of states from one strip to another within the band. It was therefore natural to assume that all the strips of one width were under the same statistical conditions and represented a single ensemble. This was checked by determining whether the initial width of the energy band E_i had any significant effect $\langle \delta N^2 \rangle$. It was found that in the range $V \geqslant 3$ the points corresponding to all the widths of the strips E_{ik} were located near one curve. There was no systematic dependence on i.

The behavior of $\langle \delta N^2 \rangle / \langle N(E) \rangle$ calculated for different values of V demonstrated by continuous curves in Fig. 2 together with an estimated error. Roughly speaking, we can see that the results of a numerical calculation are in agreement with the theory. Firstly, in the case of a relatively good metal ($V = 3$) the behavior of $\langle [\delta N(E)]^2 \rangle$ is indistinguishable from that predicted by the Dyson formula. Secondly, as V increases, the deviation from the Dyson formula appears first of all at higher energies, as expected theoretically. (In the next section we shall consider in detail the dependence of $\langle \delta N^2 \rangle$ on the energy E in the case of sufficiently small values of V and we shall show that this dependence is in good agreement with the theory and is governed only by the admittance of a sample.) Thirdly, in the region of the transition ($V = 7.5$) we find that $\langle \delta N^2 \rangle / \langle N(E) \rangle$ is indeed not too far from 0.25. Fourthly, if V is large, then $\langle \delta N^2 \rangle / \langle N(E) \rangle$ approaches unity.

There are also some unexpected results. Firstly, at $V = 99$ the variance $\langle \delta N^2 \rangle / \langle N(E) \rangle$ is considerably less than unity at high values of $\langle N(E) \rangle$. This can be understood if we allow for the finite nature of the total number of levels, which is $N_0 = 125$. Clearly, for a random system of N_0 levels, we have

$$\langle \delta N^2 \rangle = \langle N(E) \rangle (1 - \langle N(E) \rangle / N_0) \equiv \tilde{N}.$$

We shall now consider the transition point. We can interpret Eq. (14) so that at the point of the metal-insulator transition in an infinite (unbounded) system the levels cluster (coalesce) in groups of approximately four each, but otherwise their distribution is random. The conclusion that on allowance for the finite nature of N_0 we have $\langle \delta N^2 \rangle = 0.25\tilde{N}$ applies to such a system. Finally, it seems likely that in the range of validity of the Dyson formula the quantity $\langle N(E) \rangle$ of Eq. (4) can be replaced with $\tilde{N}$. We shall therefore assume that in the case of a bounded system when $\langle N(E) \rangle$ is comparable with N_0 and, instead of the dependence of $\langle \delta N^2 \rangle / \langle N(E) \rangle$ on $\langle N(E) \rangle$, we should compare the dependence of $\langle \delta N^2 \rangle / \tilde{N}$ on $\tilde{N}$ with our theory. This modification of the results was carried out in Fig. 3. We can see that the right-hand sides of the graphs for $V = 99$ are no longer bent and agree well with the theoretical law predicting $\langle \delta N^2 \rangle / \tilde{N} = 1$.

The second, more serious and not catered for by the transition from Fig. 2 to Fig. 3, unexpected feature is the absence of critical behavior of curves, i.e., their approach at high energies to a curve corresponding to the metal-insulator transition, which is manifested clearly in the theoretical results in Fig. 1. In general, the picture in Figs. 2 and 3 is smeared out compared with Fig. 1 to such an extent that we cannot say whether the transition takes place. As mentioned earlier, in the case of large systems we have $V_c \approx 8$. However, we are speaking here of a tiny cube with periodic boundary conditions. These conditions might shift V_c toward higher values, for example, to $V_c \approx 9$–10. The region near these values of V_c was not investigated in small steps of V, as one would have to do it in investigating the critical behavior, because—on the one hand—the error of the results was too large for this procedure to be meaningful. On the other hand, the unexpectedly small values of $\langle \delta N^2 \rangle / \langle N \rangle$ for $V = 30$ and 15 and larger values for $V = 7.5$ limited so much the potential critical region that we could not see how the "knees" corresponding to Fig. 1 could develop here.

We can postulate two possible reasons for such a behavior of $\langle \delta N^2 \rangle / \tilde{N}$. The first is that the investigated system is simply too small to exhibit critical behavior. Unfortunately, because of the limited capacity of the computer (BÉSM-6) we were unable to check this hypothesis. Secondly, we could assume that smoothing out of all the singularities in Figs. 2

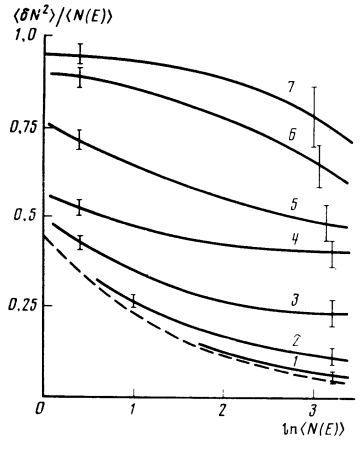

FIG. 2. Dependences of $\langle \delta N^2 \rangle / \langle N(E) \rangle$ on $\langle N(E) \rangle$ calculated on a computer for different degrees of disorder V: 1) 3; 2) 5; 3) 7.5; 4) 10; 5) 15; 6) 30; 7) 99; the dashed curve represents the Dyson formula (4).

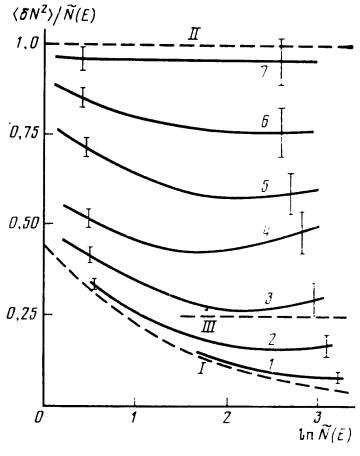

FIG. 3. Same as in Fig. 2, but after conversion from $\langle N(E) \rangle$ to $\tilde{N} = \langle N(E) \rangle [1 - \langle N(E) \rangle / N_0]$ allowing for the finite total number of levels N_0. The dashed curves correspond to: I) Dyson formula (4); II) Eq. (9); III) Eq. (14).

and 3 is a consequence of the invalidity of the proposed scaling relationships in the case of the metal-insulator transition. Very roughly speaking we could imagine that for a given value of V the fluctuations of the characteristic parameter ξ from sample to sample near the transition could become so large that the whole pattern in Fig. 1 is essentially smeared out. It is possible that both factors are important in our case.

5. CORRECTION TO THE DYSON FORMULA IN THE WEAK LOCALIZATION REGION

It is clear from Fig. 3 that at low values $V = 3$–5 the difference between $\langle \delta N^2 \rangle$ and the value predicted by the Dyson formula (4) is small. However, this difference is significant and it increases with both V and E. In the present section we shall consider the correction to the Dyson formula (4) for a good metal, which is obtained using the impurity diagram technique, and we shall compare this correction with the results of computer calculations.

The problem of fluctuations of the density of states and of the number of levels in a band of given width of a metal with impurities was solved in Ref. 2. It was shown there that fluctuations of the density of states are described by diagrams containing two diffusion or two Cooper poles (see Fig. 3 in Ref. 2). These diagrams lead to the following expression for the mean square of the fluctuations of the number of states in a band of width E:

$$\langle [\delta N(E)]^2 \rangle = \frac{1}{\pi^2} \sum_{\mathbf{q}} \ln \left[1 + \left(\frac{E}{Dq^2 + \gamma} \right)^2 \right], \tag{19}$$

where γ is the width of a level and $\mathbf{q} = (q_x, q_y, q_z)$ is the momentum of a diffuson, which assumes values discrete and dependent on the boundary conditions. In a cube of side L in the case of periodic boundary conditions, which are used in the calculation on a computer, we have

$$q_\alpha = \frac{2\pi}{L} n_\alpha, \quad \alpha = (x, y, z), \quad n_\alpha = 0, \pm 1, \pm 2, \ldots . \tag{20}$$

As shown in Ref. 2, inclusion of only the term with $\mathbf{q} = 0$ in Eq. (19) yields an expression analogous to the Dyson formula, or more exactly, differing from this formula only by a constant and by replacement of $N(E)$ with E/γ. In fact, the perturbation theory formula (19) is valid only if $\gamma \gg \Delta$, where Δ is the average spacing between the levels. If this condition is not satisfied, then in a study of the statistics of energy levels we have to go beyond the perturbation theory framework (see, for example, Ref. 7).

We shall be interested in the case when $\gamma = 0$ when the term with $\mathbf{q} = 0$ in Eq. (19) generally becomes infinite. In fact, if the calculations are correct, we should obtain the Dyson formula. The difference between $\langle \delta N^2 \rangle$ and the Dyson value $\langle \delta N^2 \rangle_D$ is described by the sum of Eq. (19) without the term with $\mathbf{q} = 0$. Using Eq. (20), we now obtain

$$\langle \delta N^2 \rangle - \langle \delta N^2 \rangle_D = \frac{1}{\pi^2} \sum_{\mathbf{n} \neq 0} \ln \left[1 + \left(\frac{E}{4\pi^2 E_c} \right)^2 (n_x^2 + n_y^2 + n_z^2)^{-2} \right]. \tag{21}$$

If $E \gg 4\pi^2 E_c$, Eq. (21) reduces to Eq. (5) obtained in Ref. 2 and the latter is insensitive to the boundary conditions. However, if $E \lesssim 4\pi^2 E_c$, then Eq. (21) describes the correction to the Dyson formula valid in the weak localization region. In particular, if $E \ll 4\pi^2 E_c$, then

$$\langle \delta N^2 \rangle - \langle \delta N_D^2 \rangle = C^2 (E/E_c)^2 = C^2 [\langle N(E) \rangle / \langle N(E_c) \rangle]^2 = C^2 (e^2/\hbar G)^2 \langle N(E) \rangle^2, \tag{22}$$

where G is the admittance of the sample associated with $\langle N(E_c) \rangle$ in accordance with Eq. (2) and

$$C = \frac{1}{4\pi^3} \left[\sum_{\mathbf{n} \neq 0} (n_x^2 + n_y^2 + n_z^2)^{-2} \right]^{1/2} \approx 0.033. \tag{23}$$

It follows from Eq. (22) that in the case of a good metal the admittance can be found quite readily by investigating $\langle \delta N^2 \rangle$ corresponding to low values of $\langle N(E) \rangle$.

On the other hand, the admittance of a cube in the case of weak disorder (at low values V) can be calculated analytically if we allow for the scattering of an electron by each site in the Anderson model using the Born approximation. In this approximation the reciprocal of the free time is

$$\frac{1}{\tau} = \frac{2\pi}{\hbar} \langle \varepsilon_i^2 \rangle a^3 g = \frac{2\pi}{\hbar} \frac{V^2}{3} a^3 g. \tag{24}$$

At the center of a zone of a simple cubic lattice with a period a the density of states is

$$g \approx 0.143 (Ia^3)^{-1}. \tag{25}$$

In calculation of the diffusion coefficient, admittance, and mean free path we need the average of the square of the velocity on a constant-energy surface $E = 0$. A calculation performed on a computer gives

$$\overline{v^2} \approx (2.71\, Ia/\hbar)^2. \tag{26}$$

Using Eqs. (24)–(26), we now obtain

$$D = \frac{1}{3} \overline{v^2} \tau = \frac{8.14}{V^2} \frac{a^2 I}{\hbar}, \tag{27}$$

$$G = Dge^2 L = \frac{e^2}{\hbar} \frac{1.17}{V^2} \frac{L}{a}, \tag{28}$$

and

$$l \equiv (\overline{v^2})^{1/2} \tau = 9.06 a/V^2. \tag{29}$$

Substituting Eq. (28) into Eq. (22), we find that for $E \ll 4\pi^2 E_c$ and a cube of side $L = 5a$, we have

$$(\langle \delta N^2 \rangle - \langle \delta N^2 \rangle_D)^{1/2} = \frac{C}{1.17} \frac{a}{L} \langle N(E) \rangle V^2 = 0.0057 \langle N \rangle V^2. \tag{30}$$

Equation (21) can also yield the dependence of $(\langle \delta N^2 \rangle - \langle \delta N^2 \rangle_D)^{1/2}$ on $\tilde{N} V^2$ outside the linear range. A graph of this dependence obtained on a computer is represented by the continuous curve in Fig. 4. The dashed curve in this figure represents the asymptotic dependence (5).

Figure 4 shows the dependences of $\langle \delta N^2 \rangle - \langle \delta N^2 \rangle_D)^{1/2}$ on $\tilde{N} V^2$ plotted using the same data as in Fig. 3. We shall first consider the results obtained for $V \leqslant 5$. We can see that at low values of $\tilde{N} V^2$ the dependences are linear, in agreement with Eq. (30), and their general form is in agreement with the theory. However, the slope at low values NV^2 is somewhat less than 0.0057, which is not surprising because—according to Eq. (20)—we have $l \approx a$ already for $V = 3$, i.e., the scattering is not weak. The Born approximation can be improved by introducing in Eq. (24) a numerical factor $A^{-1}(V^2)$ $[A(0) = 1]$. Then in Eqs. (27)–(29) the

quantities D, G, and l have an additional factor $A(V^2)$. Selecting this factor with the aid of Eq. (21), we can then describe satisfactorily the experimental results obtained for all values in the range $V \leqslant 5.5$. By way of example, we show in Fig. 4 how the curve with $A(V^2) = 1.5$ describes the experimental results for $V = 5.5$. The inset in Fig. 4 gives the values of $A(V^2)$ found in this way and the corresponding dependence $l(V^2)$. It is clear that the dependence $A(V^2)$ is described by $A(V^2) = A(0) + \theta V^2$ with $A(0) = 1.1 \pm 0.15$, which is in agreement with the theoretical value $A(0) = 1$. Therefore, we can see that the numerical experiment in the metallic region is in good agreement with the theoretical predictions based on Eqs. (21) and (28).

We shall consider now the data of Fig. 4 for $V \geqslant 7.5$. Clearly, the deviation from the curve corresponding to a good metal rises rapidly in the range $V \geqslant 7.5$. In particular, it seems that for $V = 10$ and 15 the difference $(\langle \delta N^2 \rangle - \langle \delta N^2 \rangle_D)$ does not tend at all to zero on reduction in $\tilde{N}V^2$. However, this is an indication of the occurrence of the metal-insulator transition.

6. DISTRIBUTION FUNCTION OF THE SPACINGS BETWEEN THE NEAREST LEVELS

The distribution of spacings between the nearest eigenvalues of random matrices has been investigated on many occasions.[8] In the matrices such that all the elements are distributed near zero and are characterized by the same variance, we find that the probability density $P(s)$ is described well by the Wigner formula

$$P(s) = \frac{\pi}{2}\frac{s}{\Delta^2}\exp\left[-\frac{\pi}{4}\left(\frac{s}{\Delta}\right)^2\right], \qquad (31)$$

where $\Delta \equiv \langle s \rangle$. On the other hand, it is clear that if the diagonal matrix elements are distributed at random between $-V$ and V, the off-diagonal elements vanish and we obtain the Poisson distribution

$$P(s) = (1/\Delta)\exp(-s/\Delta). \qquad (32)$$

The distributions described by Eqs. (31) and (32) are represented in Fig. 5 by continuous and dashed curves, respectively.

Our aim was to investigate whether the transition from Eq. (31) to Eq. (32) occurs in the Anderson model on increase in V, i.e., on transition from a good metal to an insulator far from the transition. With this in mind we followed the diagonalization of the Anderson Hamiltonian by calculations of the spacing between the nearest levels in a band centered around $E = 0$ and of width $E_0 = (V + 6)/2$, where the density of states was assumed to be practically constant. The region $0 < s < 2\Delta$ was divided into 20 segments and sorting of the values in these segments was carried out. The values in the range $s > 2\Delta$ were not sorted, but $P(s)$ was normalized within the interval $[0, \infty]$.

Figure 5 shows the functions found in this way for $V = 7.5$, 15, and 30. If $V = 3$, the experimental curve for $P(s)$ is practically indistinguishable from the Wigner distribution of Eq. (31). A similar result for a good metal was obtained recently in Ref. 9 for the Anderson model with a Gaussian distribution of the energies ε_i. At $V = 5$ in the region of $s \approx 1.2\Delta$ there is a small reduction in $P(s)$ compared with Eq. (31). At $V = 7.5$ this effect is much stronger (Fig. 5). There is a simultaneous increase in $P(s)$ in the region of the tail of the function $(s > 2\Delta)$, which is noticeable on increase of its contribution to the normalization. However, it must be stressed that right up to $V = 7.5$ there is no change in $P(s)$ in the region of the rise, i.e., in the region where $s/\Delta < 0.7$. Beginning from $V = 10$ the nature of the evolution of $P(s)$ on increase in V changes. These curves show a rapid rise of $P(s)$ at low values of s and the maximum shifts toward small values of s. The curves approach Eq. (32), with the exception of the range of very small values of s. In our opinion, this behavior is evidence of a transition to the insulator phase. In the case of an insulator cube of infinite dimensions the function $P(s)$ should tend to unity for $s \to 0$. This occurs because the wave functions of levels adjacent on the

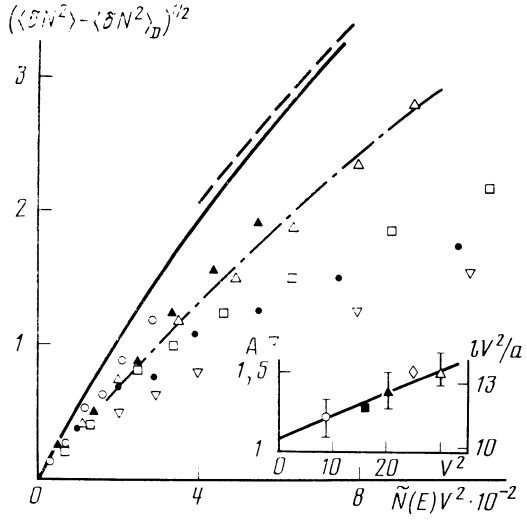

FIG. 4. Dependences of $[\langle \delta N^2 \rangle - \langle \delta N^2 \rangle_D]^{1/2}$ on $\tilde{N}V^2$, where $\langle \delta N^2 \rangle_D$ is found from Eq. (4) for different values of V: ○) 3; ▲) 4.5; △) 5.5; □) 7.5; ●) 10; ▽) 15; ■) 4; ◇) 5. The continuous curve is calculated using Eq. (21) for G corresponding to the theoretical formula (28); the dashed curve represents Eq. (5), which is valid in the case of asymptotically large E. The dash-dot curve is plotted on the basis of Eq. (21) for a value of G which is 1.5 times greater than Eq. (28). The inset shows the dependence of the correction factor $A(V^2)$ and of the expression lV^2/a on V^2.

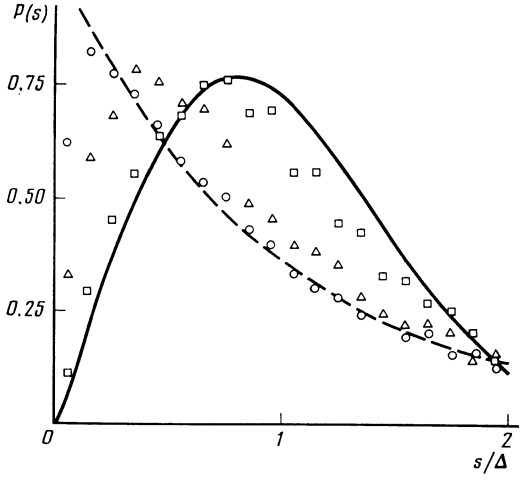

FIG. 5. Distribution function representing the difference between the energies of two adjacent levels $P(s)$ calculated for different values of V: □) 7.5; △) 15; ○) 30. The continuous curve corresponds to the Wigner formula of Eq. (31) and the dashed curve corresponds to Eq. (32).

energy scale are usually localized in different parts of space. The exponential tails of these functions overlap so little that the repulsion of the levels can be ignored. On the other hand, in a small cube there is a minimum splitting of initially very closely spaced levels and this limitation is imposed by the size of the cube. This is responsible vanishing of $P(s)$ in the limit $s \to 0$. If $V = 30$, we can investigate how the dip of $P(s)$ in the limit $s \to 0$ increases on reduction in the cube side from 5 to 4 and then to 3, and we can thus demonstrate that the dip is related to a boundary effect.

We shall now consider the asymptotic behavior of $P(s)$ at high values of s. It is natural to consider how a transition takes place between two very different types of asymptotic behavior described by Eqs. (31) and (32). We shall show now that this transition is related to the gradual change in the nature of the dependence of $\langle \delta N^2 \rangle$ on $\langle N \rangle$ on increase in V investigated above. In fact, the probability of the absence of any level in a band of width s, where on the average there are $\langle N \rangle$ levels, can be estimated in the range of relatively small Gaussian fluctuations:

$$P(s) \propto \exp\left[-\langle N(s)\rangle^2/\langle \delta N^2(s)\rangle\right] = \exp\left[-s^2/\Delta^2 \langle \delta N^2(s)\rangle\right]. \tag{33}$$

In the case of an insulator, when Eq. (9) applies, we can readily deduce Eq. (32) from Eq. (33). A reduction in V reduces $\langle \delta N^2 \rangle$ and, consequently, increases the rate of fall of $P(s)$. At the insulator-metal transition we obtain from Eqs. (33) and (14) the following probability:

$$P(s) \propto \exp(-\langle N(s)\rangle/\varkappa) = \exp(-s/\varkappa\Delta). \tag{34}$$

The fall in accordance with Eq. (34), although it is faster than that predicted by Eq. (32), is still slower than that described by Eq. (31). In the critical region on the insulator side an increase in s results in a change from the intermediate asymptote of Eq. (32) through a distant asymptote of Eq. (34).

On the metal side the situation is even more complex. For example, even in the case of a good metal as s increases, the law describing the fall of $P(s)$ changes twice. In the intervals 1) $\Delta < s < E_c$, 2) $E_c < s < \hbar/\tau$, and 3) $\hbar/\tau < s < \mu$, we find that instead of $\langle \delta N^2(s) \rangle$, we should substitute in Eq. (34) the formulas (4), (5), and (7). In the third interval ($\hbar/\tau < s < \mu$), we find that

$$P(s) \propto \exp(-\text{const}\,[s/\Delta]^2[l/L]^3) \tag{35}$$

is a law similar to Eq. (31), but the dependence is weaker because of the small numerical coefficient. In the second interval ($E_c < s < \hbar/\tau$) the behavior of $P(s)$ is quite unusual:

$$P(s) \propto \exp\{-\text{const}(s/\Delta)^{1/2}(E_c/\Delta)^{3/2}\}. \tag{36}$$

Finally, in the interval $\Delta < s < E_c$, we find from Eqs. (4) and (33) that

$$P(s) \propto \exp\{-s^2/\Delta^2 \ln(s/\Delta)\}, \tag{37}$$

which differs from the familiar expression (31) only by a logarithmic factor in the argument of the exponential function. We shall now show why in fact this logarithmic factor may be absent and in the range of validity of the Dyson formula (4) we can substitute for $\langle \delta N^2 \rangle$ in Eq. (33) a quantity of the order of unity, which leads directly to Eq. (31). This is because the Dyson formula (4) was obtained by summing the mean squares of fluctuations of the number of levels of different scales,[2] and the smaller the scale, the greater amplitude of the fluctuations of the level number density, so that the contribution to $\langle \delta N^2 \rangle$ from all the scales separately is the same and is of the order of unity. In the case of a very improbable fluctuation of interest to us the density of levels vanishes in a certain segment of width s and, therefore, the amplitude of the fluctuations of the density of all scales is the same and is given by $\langle N(s) \rangle / s$. In this situation only the largest scale of s is important and instead of $\langle \delta N^2 \rangle$ in Eq. (33) we have to substitute a value of the order of unity. We shall limit ourselves to qualitative ideas, because the behavior of $P(s)$ at large values of s was not investigated by us on a computer. Those changes in the contribution of the tail of $P(s)$ to the normalization which can be seen in Fig. 5 are not in conflict with the above ideas.

Note added in proof (February 10, 1988). Additional calculations yielded the function $P(s)$ in the range $2 < s < 4$. The results are in good agreement with Eq. (33). They will be published later [I. Kh. Zharekeshev, Fiz. Tverd. Tela (Leningrad) (in press)].

The authors are grateful to F. M. Izrailev who stimulated the work reported above.

[1)]Programs for inputting the matrix (8) into a computer were checked by diagonalization and sorting of levels in the case when $V = 0$, i.e., when there was no scatter of ε_i. The energy and degree of degeneracy of the levels in a $5 \times 5 \times 5$ cube at $V = 0$ were readily found analytically using the tight-binding method. The computer calculations agreed with these analytic results.

[1]S. Washburn and R. A. Webb, Adv. Phys. **38**, 375 (1986).
[2]B. L. Al'tshuler and B. I. Shklovskiĭ, Zh. Eksp. Teor. Fiz. **91**, 220 (1986) [Sov. Phys. JETP **64**, 127 (1986)].
[3]F. J. Dyson, J. Math. Phys. (N.Y.) **3**, 157 (1962).
[4]F. J. Dyson and L. L. Mehta, J. Math. Phys. (N.Y.) **4**, 701 (1963).
[5]A. MacKinnon and B. Kramer, Phys. Rev. Lett. **47**, 1546 (1981).
[6]M. Kaveh and N. F. Mott, Philos. Mag. **55**, 9 (1987).
[7]K. B. Efetov, Zh. Eksp. Teor. Fiz. **83**, 833 (1982) [Sov. Phys. JETP **56**, 467 (1982)].
[8]C. E. Porter (ed.), *Statistical Theories of Spectra: Fluctuations*, Academic Press, New York (1965).
[9]U. Sivan and Y. Imry, Phys. Rev. B **35**, 6074 (1987).

Translated by A. Tybulewicz