SOVIET PHYSICS JETP VOLUME 34, NUMBER 5 MAY, 1972

HOPPING CONDUCTIVITY OF SEMICONDUCTORS IN STRONG MAGNETIC FIELDS

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Submitted May 13, 1971

Zh. Eksp. Teor. Fiz. 61, 2033–2040 (November, 1971)

A theory of hopping conductivity of semiconductors in strong magnetic fields is developed. As is well known, calculation of hopping conductivity reduces to the problem of the conductivity of a three-dimensional random network each element of which corresponds to a certain impurity pair. The problem was solved by a percolation-theory approach. It is shown that the hopping resistance should grow with the magnetic field strength as $\exp(-H^{1/2}\ln^{1/2}H)$. The longitudinal and transverse magnetoresistances in this case should be close to each other. This conclusion is in satisfactory agreement with the experiment[2].

In a semiconductor having such a low impurity density that the overlap of the impurity wave functions is small, the contribution of the impurities to the conductivity is determined by two mechanisms. At relatively high temperatures, the conductivity is due to electrons thrown from the impurity levels into the conduction band. (For concreteness we shall speak of donors.) With increasing temperature, the number of electrons in the band decreases sharply, and the principal role in the conductivity is assumed by hops of the electron from donor to donor, due to the exponentially small overlap of the wave functions of the two states. (Free donors are usually present as a result of compensation.) This is called hopping conductivity. The random potential produced by the charged donors and acceptors causes the levels of different donors to differ somewhat. Therefore hopping of an electron can occur only with participation of phonons, and the dependence of the hopping resistance on the temperature T has an activation character:

$$\rho = \rho_3 e^{\varepsilon_3/kT} \tag{1}$$

(ρ_3 and ϵ_3 are the standard symbols). The resistance ρ_3 is also exponentially large. This is due to the fact that under the conditions of hopping conductivity the overlap of the impurity wave functions is exponentially small. The strong magnetic field squeezes the wave functions, decreasing still further the overlap of their exponential tails. Therefore the resistance ρ_3 should increase exponentially under the influence of the magnetic field. The present paper is devoted to this phenomenon.

The first to observe the exponential increase of the hopping resistance in a magnetic field was Sladek[1]. In the n-InSb crystals investigated by him, the impurity concentration was so large that in the absence of a magnetic field the impurity band overlapped the conduction band and the conduction was metallic in character. Under the influence of a magnetic field, however, the overlap of the wave functions decreased, the impurity band became separated from the conduction band, and at temperatures below 2°K the conductivity became of the hopping type. Further increase of the magnetic field led to an exponential growth of the hopping resistance, for which an increase of 10^5 times was attained.

As is well known, the transverse dimension of the wave function decreases strongly in a magnetic field, whereas the longitudinal dimension changes little. At first glance, it therefore seems that the transverse hopping magnetoresistance should greatly exceed the longitudinal one. It will be shown below that in fact the longitudinal and transverse magnetoresistances are close in magnitude. Using the percolation ideas, we shall show that in a sufficiently strong magnetic field H the principal dependence of ρ_3 on H and on the donor concentration N is determined by the formula

$$\rho_3 \sim \exp\{q[\lambda^2 a_H N]^{-1/2}\}. \tag{2}$$

Here $\lambda = (c\hbar/eH)^{1/2}$ is the magnetic length, e the absolute value of the electron charge, c the speed of light, $a_H = \hbar/\sqrt{2mE_H}$ the characteristic length of the decrease of the wave function in the direction of the magnetic field, m the effective mass (the electron spectrum is assumed isotropic and quadratic), E_H the donor ionization energy in the magnetic field, and q a numerical coefficient close to 0.9. The result (2) is valid if H satisfies the conditions

$$\lambda < a_H / (Na_H^3)^{1/2}, \quad \lambda < a_H / (Na_H^3)^{1/6}. \tag{3}$$

Such fields are easily realized in experiments with InSb. For example, in[1] the field satisfied these conditions.

It is known that so long as $\lambda \gg a$, where $a = \hbar^2\kappa/me^2$ is the Bohr radius of the impurity in the absence of a magnetic field (κ is the dielectric constant), the value of a_H does not depend on the magnetic field and is equal to a. Then (2) yields $\rho_3 \sim \exp(-H^{1/2})$. On the other hand, when $\lambda \ll a$, i.e., as $H \to \infty$, the value of a_H decreases like $a[\ln(a/\lambda)^2]^{-1}$[2,3]. It follows therefore from (2) that in the limit of very strong fields we have $\rho_3 \sim \exp(-H^{1/2}\ln^{1/2}H)$. In the intermediate region of fields, when $\lambda \approx a$, it is necessary to use in (2) the values of E_H obtained by numerical calculation[3,4]. It is also possible to substitute in (2) the experimental values of E_H obtained from the dependence of the Hall constant on the temperature in the temperature region where the Hall effect is determined by electrons activated into the conduction band.[1]

To obtain (2) it is necessary first of all to calculate the probability W_{ij} of a jumpover of an electron between donors numbered i and j and separated by a distance r_{ij}. The hopping conductivity takes place when W_{ij} is exponentially small. According to[5], the exponentially small factor in W_{ij} is expressed in terms of the overlap integral of the wave functions of the ground state of the electron at each of the donors in the magnetic field

$$W_{ij} \sim \left| \int \psi_i(\mathbf{r})\psi_j(\mathbf{r})\,d\mathbf{r} \right|^2. \tag{4}$$

If we introduce a cylindrical coordinate system ρ, φ, z with center at the point $\mathbf{r}_i$ and axis z directed along **H**, and specify the vector potential in the form $\mathbf{A} = \mathbf{H} \times \mathbf{r}/2$, then the wave function $\psi_i(\mathbf{r})$ assumes for $\lambda < a$ the form[2,3,6]

$$\psi_i = B \exp\left\{ -\frac{\rho^2}{4\lambda^2} - \frac{|z|}{a_H} \right\}. \tag{5}$$

If $\lambda > a$, then the magnetic field influences only the behavior of $\psi_i(\mathbf{r})$ at large distances. In this case, to find the argument of the exponential in the wave function as $r \to \infty$ in the Schrödinger equation, we can neglect the potential energy of the electron in the donor field compared with the binding energy of the electron. For an electron in a magnetic field with binding energy E_H it is possible to obtain a general cylindrically-symmetrical solution of the Schrödinger equation, which decreases at infinity, by separating the variables[7]. This solution is given by

$$\psi_i(\mathbf{r}) = \sum_n B_n L_n \left(\frac{\rho^2}{2\lambda^2} \right) \exp\left\{ -\frac{\rho^2}{4\lambda^2} - \frac{|z|}{\hbar} \sqrt{2m(n\hbar\Omega + E_H)} \right\}. \tag{6}$$

Here $L_n(x)$ are Laguerre polynomials and $\Omega = eH/mc = \hbar^2/m\lambda^2$ is the cyclotron frequency.

If $\hbar\Omega < E_H (\lambda > a_H)$, then all that remains in (6) at $z > \lambda^2/a$ is one term with $n = 0$. In what follows, it is precisely such z that will be important when (3) is satisfied. Therefore for all H satisfying (3) we can use a wave function in the form (5). The wave function of the donor j differs from (5), first, in that **r** is replaced by $\mathbf{r} - \mathbf{r}_j$ and, second, by an additional factor

$$\exp\left\{ -\frac{ie}{2\hbar c} [\mathbf{H}\mathbf{r}_{ij}]\mathbf{r} \right\},$$

connected with the fact that the origin of the vector potential is fixed, as before, at the point $\mathbf{r}_i$[8]. Calculation of W_{ij} in accord with formula (4) yields

$$W_{ij} \sim \exp\left\{ -\frac{x_{ij}^2 + y_{ij}^2}{2\lambda^2} - \frac{2|z_{ij}|}{a_H} \right\}. \tag{7}$$

After finding the paired jumpover probability W_{ij}, calculation of the hopping resistance of the entire crystal is equivalent to the problem of determining the resistance of a three-dimensional random network made up of resistance elements proportional to W_{ij}^{-1}[5]. According to (7), the resistance of the element depends not only on the length of the element ($\mathbf{r}_{ij}$) but also on the angle between $\mathbf{r}_{ij}$ and the magnetic field **H**.

Before we solve the problem with the anisotropic W_{ij}, let us recall the idea used in the solution of the simpler isotropic problem of the hopping conductivity without the magnetic field, when $W_{ij} \sim \exp(-2|\mathbf{r}_{ij}|/a)$[9]. We consider all possible chains of donors connecting the two ends of the crystal. In each chain, the resistance elements are connected in series. Therefore the resistance of the chain is determined by the elements with the largest $|\mathbf{r}_{ij}|$. We characterize each chain by a quantity R—the maximum dimension of its element. Chains with small R, if their number is appreciable, determine the resistance of the crystal. It is obvious, however, that in an infinite crystal there is not a single chain with $R \ll N^{-1/3}$. On the other hand, there are many chains with $R \gg N^{-1/3}$. Obviously, there is a certain critical value $R = R_C$, starting with which there appear in the infinite crystal chains that pass through the entire crystal. Moreover, it is clear that R_C is determined from the condition that the volume of a sphere with radius R_C is a quantity on the order of the average volume per donor N^{-1}, i.e., from the condition $(4/3)\pi R_C^3 N = \beta_0$, where β_0 is a coefficient on the order of unity. The quantity β_0 was determined by the Monte Carlo method with a computer in[10]. It turned out that $\beta_0 = 2.32$. In addition, it is shown in[10] that an appreciable fraction of all the donors belong to chains with R exceeding R_C by only 10–20%. In view of the extremely strong dependence of the chain resistance on R, it is clear that the resistance of the entire crystal as a whole is determined by chains having a value R barely larger than R_C, i.e.,

$$\rho_3 \sim \exp\{\alpha / N^{1/3} a\}, \tag{8}$$

where α exceeds by several percent the quantity $2(3\beta_0/4\pi)^{1/3} = 1.64$.

We now generalize the theory developed above to include the case of arbitrary anisotropic jumpover probability $W_{ij}(\mathbf{r}_{ij})$. Just as before, we seek chains with the least possible resistance. To this end, it is convenient to characterize each chain by the maximum value of the logarithm of the resistance of its element, i.e., by the quantity $L = \max \ln W_{ij}^{-1}$. The existence of a chain with a certain L means that there is a sequence of donors, each of which is located inside the surface S_L defined by the equation $-\ln W_{ij}(\mathbf{r}_{ij}) = L$, for which the preceding donor is the center of coordinates.

Obviously, there is not even one infinite chain with L such that the volume V(L) bounded by the surface S_L is small compared with the neighboring volume per donor N^{-1}. In other words, there is no percolation over such small L. It is obvious also that for L such that $V(L)N \gg 1$, percolation does exist. Percolation first arises at a certain critical value $L = L_C$, when bodies with surface S_L and volume V(L) fill an appreciable part of the space. The condition for the determination of L_C is

$$V(L_c)N = \beta_s, \tag{9}$$

where β_S is a quantity on the order of unity and depends, generally speaking, on the shape of the surface S_{L_C}. In the sense of the papers on percolation theory, it is natural to assume that there is an appreciable number of chains with L exceeding L_C by 10–20%. It is just these chains which have the smallest resistance and determine the conductivity of the entire crystal. If the coefficient β_S is obtained by computer calculation, then by starting with L_C from (9), we obtain $\rho_3 \sim \exp(L'_C)$, where L'_C differs from L_C by several percent.

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*$[\mathbf{H}\mathbf{r}]_{ij}\mathbf{r} = (\mathbf{H} \times \mathbf{r})_{ij} \cdot \mathbf{r}$.

In the foregoing example of isotropic wave functions of the impurities $W_{ij} \sim \exp\{-2|r_{ij}|/a\}$, the surface S_L is a sphere of radius $aL/2$, and starting with L_C from (9) we obtain again (8). In the case of interest to us here, that of a strong magnetic field, the surface S_L is given by

$$(x^2+y^2)/2\lambda^2+2|z|/a_H=L. \tag{10}$$

This surface is made up of two truncated paraboloids of revolution, with axes along **H**, joined together at their bases. The height of each paraboloid is $h = aL/2$, and the radius of the base is $l = \lambda\sqrt{2L}$. The volume of the double paraboloid is equal to

$$V(L)=\pi\lambda^2L^2a. \tag{11}$$

After determining L_C from (9) we obtain (2), where q differs by several percent from the quantity $(\beta_p/\pi)^{1/2}$ (β_p is the coefficient β_S for the double paraboloid).

Let us discuss the question of the quantity β_p. We have said that the quantity β_S, generally speaking, depends on the shape of the surface S_{L_C}. In different magnetic fields at $L = L_C$ we dealt with double paraboloids having different h/l ratios. It could therefore turn out that β_p, remaining on the order of unity, was dependent on H. We shall show, however, that in the case of a random disposition of the impurities there is no such dependence. To this end we restate in a somewhat different manner the problem of percolation in a system of randomly distributed points with concentration N. Assume that a surface S, bounding a volume V, is constructed around each point as an origin. The surfaces S_i and S_j belonging to different i and j differ only by a translation by $\mathbf{r}_{ij}$. We shall say that there is percolation in the system if there exist chains of points penetrating through all of space, in which each succeeding point lies inside the surface belonging to the preceding point. At a fixed shape of S, it is required to find the volume V at which percolation sets in first. The answer to this question is given by the formula $VN = \beta_S$, where β_S depends on the shape of S.

We now prove the following theorem[1]. The coefficient β_S is the same for all the surfaces S obtained from one another by a linear transformation.

To prove this, we consider surfaces S and S′ such that S goes over into S′ after a linear transformation of the surface coordinates $x_i' = A_{ik}x_k$. It is obvious that $V_{S'} = V_S \det A$. We imagine a system of randomly distributed points with concentration N and with surfaces S constructed around each point. We transform simultaneously the coordinates of the points and of the surfaces by the linear transformation $x_i' = A_{ik}x_k$. Here the random Poisson distribution of the points also remains uniform in space and of the Poisson type, but with a different concentration $N' = N(\det A)^{-1}$. Indeed, a Poisson distribution is characterized by the fact that the probability of finding a point in a volume dV is NdV. After transformation, the probability of finding the point in the volume dV′ obtained from dV is $NdV = NdV'(\det A)^{-1} = N'dV'$, i.e., it is again given by a Poisson expression. Thus, it is possible to consider in the transformed system percolation over the surfaces S′. If there was no percolation in the initial system, there is obviously none after the transformation. Conversely, if there was percolation, it will not vanish after transformation either. In the initial system, the condition for the onset of percolation is $NV_S = \beta_S$. Then the percolation sets in simultaneously also for the transformed system, i.e., $N'V_{S'} = \beta_{S'}$. Since $NV_S = N'V_{S'}$, we have $\beta_S = \beta_{S'}$.

Since any two double paraboloids can be transformed into each other by a linear transformation, it follows from the proven theorem that for all double paraboloids β_S is a universal quantity β_p. Consequently, the coefficient q determined from the condition (9) is independent of the magnetic field. To find β_p it suffices to carry out a calculation analogous to that in [10] by the Monte Carlo method for any double paraboloid. The value of β_p, of course, differs from β_0, since a linear transformation does not transform a double paraboloid into a sphere. It seems to us that the degree of proximity of these coefficients can be estimated in the following manner. Let us imagine a double paraboloid and a sphere, having the same centers and equal volumes. It is easy to show that by choosing the ratio h/l it is possible to find a double paraboloid such that is contains more than 90% of the volume of the sphere. In view of the closeness of such a double paraboloid to a sphere, we can assume that the critical percolation concentration for these bodies is also close. Since the volumes are equal, this means that β_p is close to β_0. Thus, it is quite probable that β_p differs from 2.3 by less than 10%. Using this value of β_p, we find that q in (2) is close to 0.9.

Let us discuss the limits of applicability of (2). It is clear from the foregoing that in the chains that determine the resistance of the crystal the electron executes most frequently hops for which the characteristic values of the components $\mathbf{r}_{ij}$ coincide with the dimensions of the double paraboloid corresponding to $L = L_C$. Thus, for significant hops we have

$$\begin{gathered}|z_{ij}|\approx h(L_c)\approx a_H^{1/2}N^{-1/2}\lambda^{-1},\\ |x_{ij}|\approx|y_{ij}|\approx l(L_c)\approx a_H^{-1/4}N^{-1/4}\lambda^{1/2}.\end{gathered} \tag{12}$$

The asymptotic form of the wave function employed by us is valid for $|z_{ij}| \gg \lambda^2/a_H$. It follows therefore from (12) that our result is valid only for $\lambda < a_H/(Na_H^3)^{1/6}$. In addition, formula (2) is valid only when the argument of the exponential is large, i.e., $\lambda < a_H/(Na_H^3)^{1/2}$. Only in this case is the average volume per particle N^{-1} larger than the "volume" of the wave function $\lambda^2 a_H$ and only then does the conductivity have a hopping character. We have thus arrived at the inequalities (3).

Nowhere in the derivation of (2) did we specify whether we are dealing with longitudinal or transverse resistance. Both resistances are determined by chains with L close to L_C. The difference between the chains used for the longitudinal and transverse conductivities becomes noticeable if attention is focused on the fact that the significant hops occur mainly at an angle on the order of

$$l(L_c)/h(L_c)\approx(\lambda/a_H)^{3/2}(Na_H^{3})^{1/4}$$

to the z axis. In the region of applicability of our theory (see (3)) this angle is small. The appreciable values of $|z_{ij}|$ turned out to be much larger than

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[1] The main idea of the proof belongs to Ya. Sinai.

$N^{-1/3}$, and $|x_{ij}|$ and $|y_{ij}|$ are much less than $N^{-1/3}$. Thus, in order for the electrons to negotiate a unit length in the direction of the magnetic field (z axis) it is necessary to complete fewer hops than in the perpendicular direction. This leads to somewhat different preexponential factors in (2). On the other hand, the arguments of the exponentials are of course the same for the longitudinal and transverse resistances.

Let us dwell briefly on why the result (2) could not be obtained by Sladek in[1]. First, Sladek calculated W_{ij} with the aid of a variational wave function[4]. The asymptotic behavior of this function at large distances from the donor obviously differs from the correct asymptotic form (5). Second, to calculate ρ Sladek averaged W_{ij} directly over all pairs (i, j) with fixed $|r_{ij}|$. Such a mean value, naturally, is determined by pairs with r_{ij} directed directly along z. It is obvious, however, that it is impossible to traverse the entire crystal over such pairs. Therefore the averaging must be carried out not for one isolated pair of donors but for chains penetrating through the entire crystal. To this end it is necessary to use the percolation idea, as was done in the present paper.

Let us describe now the change of the low-temperature conductivity of a semiconductor with increasing magnetic field in two cases: 1) $Na^3 \gtrsim 1$ and 2) $Na^3 \ll 1$. In the first case, at H = 0, the impurity band overlaps the conduction band, and the conductivity has a metallic character. The impurity band splits off when the "volume" of the wave function $\lambda^2 a_H$ becomes of the order of N^{-1}, i.e., at $\lambda \approx a_H/(Na_H^3)^{1/2}$. In such a field, the second condition of (3) is satisfied $(Na_H^3 > 1)$. Therefore the resistance should follow (2) with further increase of H. In the second case $Na^3 \ll 1$ the conductivity has a hopping character even without the magnetic field, and ρ_3 is determined by formula (8). So long as the magnetic field is weak, it leads to the occurrence of a small term in the exponent of (8), of the order of $a/\lambda^4 N$[11]. This term increases and becomes comparable with the main term at $\lambda \approx a/(Na^3)^{1/6}$. Starting with such fields, our theory becomes valid, the magnetic term becomes the principal one, and formula (2) can be used. We see that at $\lambda \approx a/(Na^3)^{1/6}$, formula (2) "joins" with (8). At $Na^3 \ll 1$ we write throughout a in place of a_H, since all the characteristic fields satisfy the condition $\lambda \gg a$.

So far we have assumed that the donor distribution in space is absolutely random, i.e., it is an instantaneous snapshot of the distribution in an ideal gas. Such a situation undoubtedly obtains when the doping is with the aid of nuclear reactions brought about by neutron bombardment of the pure semiconductor at low temperatures, when there is practically no impurity diffusion. More frequently the doped semiconductors are grown from the melt in which the impurities are dissolved. In this case the Coulomb repulsion between donors gives rise to a correlation in their arrangement. This correlation, however, is very strongly suppressed by the screening action of a large number of intrinsic electrons and holes. With decreasing temperature, the rate of impurity diffusion decreases exponentially and at a certain temperature T_0, usually close to the melting temperature, the diffusion becomes quenched. The impurity arrangement retained at low temperatures corresponds to the equilibrium at T_0. Since T_0 is quite large, in most cases the impurity distribution is close to random (at any rate there is undoubtedly no long-range order). Let us discuss, nonetheless, how the presence of a repulsion-connected correlation in the arrangement of the impurities is reflected in our result (2). In this case formula (9) remains valid as before, with β_S having a value on the order of unity. As $H \to \infty$, i.e., as $h/l \to \infty$, the value of β_S, remaining of the order of unity, should tend to a certain constant limit $\tilde{\beta}_P$. But we are interested precisely, in the case $h/l \gg 1$, i.e., under the conditions of our problem we can assume that β_S is close to its limiting value $\tilde{\beta}_P$ (the corrections are apparently proportional to l/h raised to a certain power). In the case of appreciable correlation β_S differs from β_P. Therefore for strong correlation the estimate obtained by us for q in (2) is incorrect, but q remains a constant quantity of the order of unity as before.

In conclusion let us discuss the possibility of comparing formula (2) with experiment. The semiconductor most suitable for this purpose is n-InSb, in which the effective mass is so small that λ becomes of the order a already in a field H = 2 kOe. The resistance of InSb crystals with impurity densities in the range 10^{14}–10^{15} cm^{-3} was measured in[1]. In such samples we have $Na^3 \approx 1$, and according to the foregoing, as soon as the resistance becomes of the hopping type, it should follow formula (2), Our qualitative conclusion that the transverse and longitudinal magnetoresistances are close in value is verified by experiment. In[1], the transverse resistance exceeds the longitudinal one by only 2–3 times, even in the strongest magnetic field, H = 28 Oe. A quantitative comparison of formula (2) with the data of[1] is difficult, since it is impossible to determine the exact value of ρ_3. Indeed, as seen from (1), in order to determine ρ_3 it is necessary to have the dependence of ρ on 1/P in a sufficient temperature interval to be able to extrapolate it to $T \to \infty$. In[1], however, even at the lowest temperature T = 1.6°, we deal only with the start of the hopping-conductivity region. Thus, to compare formula (2) with experiment it is necessary to perform experiments at temperatures lower than in[1].

I am grateful to Ya. Sinaĭ for useful discussion on the percolation problem and to A. L. Éfros for a discussion of the results.

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Translated by J. G. Adashko
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