Physics – Uspekhi **41** (7) 719 – 726 (1998)

CONFERENCES AND SYMPOSIA

PACS numbers: 01.10 Fv

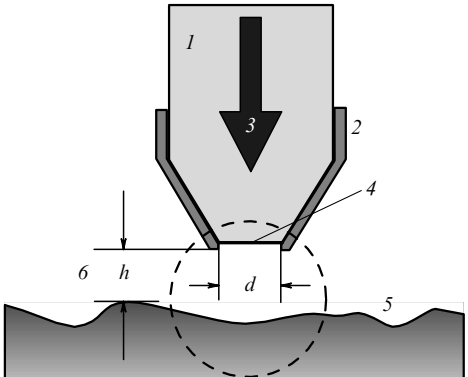
Scientific session of the Division of General Physics and Astronomy of the Russian Academy of Sciences (26 November 1997)

A scientific session of the Division of General Physics and Astronomy of the Russian Academy of Sciences was held on 26 November 1997 at the P L Kapitza Institute for Physical Problems, RAS. The following reports were presented at the session:

(1) **Zhdanov G S, Libenson M N, Martsinovskiĭ G A** (S I Vavilov State Optical Institute, St Petersburg) "Optics in the diffraction limit: principles, results, and problems";

(2) **Zabrodskiĭ A G** (A F Ioffe Physicotechnical Institute, Russian Academy of Sciences, St Petersburg) "Coulomb gap and metal – insulator transitions in doped semiconductors".

Brief presentations of both reports are given below.



which a pattern is imprinted as the surface is scanned by the probe. The required scanning rate is related to the illuminating power, which is limited by the probe's thermal stability. As noted earlier, in typical conditions only one-millionth of the light flux reaches the sample, while the main fraction is absorbed by the metallic coating of the probe and heats it up. Kurpas et al. [12] found that the temperature distribution in the probe strongly depends on the probe's microgeometry and the structure of the field near the probe's tip. Conditions may be such that the most heated region is far from the tip. The calculated ratio of the maximum rise in the probe's temperature, ΔT, to the absorbed power P for ordinary aperture angles of the cone is $\Delta T/P \approx 10^5$ K W^{-1}, which agrees with the results of measurements. At $P \sim 10$ mW or at $P_0 \sim 10$ nW for the radiation that has reached the sample, the probe may disintegrate because of melting of the aluminum coating.

A considerable increase in P_0 can be achieved if the standard quartz probes with an aluminum coating are replaced by all-metal probes. Gurevich and Libenson [13] suggested using metal for the rod, the light being fed to the tip of the rod by exciting a cylindrical surface electromagnetic wave (SEW). This eliminates the difficulties caused by the field cut-off in a sharpened quartz fiber probe and the associated large energy losses. Analysis shows that an SEW field at the probe's tip is concentrated within a region comparable in size to the diameter of the tip.

When examining the interaction of light and matter in the near-field contact region (see Fig. 1), one must bear in mind that the mean free path of the non-equilibrium carrier generated in the process of light absorption and the size of the effective interaction zone may be much larger than the size of the light spot. The zone is formed as a result of a cascade of processes in which the electron and phonon subsystems of the sample participate [14, 15]. In the steady state, the maximum rise in temperature in this zone is a function of the parameter $\zeta = R/\sqrt{D\tau}$, where R is the radius of the light spot, and D and τ are the diffusion coefficient and the lifetime of the non-equilibrium carriers.

The range of applications of NFO is rapidly broadening. A number of new tracks of research are in the stage of idea formulation or in the experimental stage. One of these ideas is related to the possibility of using the NFO method to control the elements of high-power optics [16]. Usually, optical breakdown of the materials and elements of optics is initiated by defects whose nature is not always known. The most natural approach to the detection of such defects consists in analyzing the surface and thin layers by radiation with the same frequency as that of the high-power light. The possibility of visualizing small optical inhomogeneities and doing a spectral analysis of these inhomogeneities in an NSOM suggests that using this device constitutes an effective way of solving the problem.

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PACS number: 71.30.+h

Coulomb gap and metal – insulator transitions in doped semiconductors

A G Zabrodskiĭ

1. Gapless models of localization and hopping transport

Doped semiconductors belong to disordered systems that are widely used in studying problems associated with the metal – insulator transition and low-temperature electron transport. At a certain critical value N_c of the concentration of the primary impurities, 'metallization' of the impurity levels near the Fermi level occurs in such systems. But when $N > N_c$, the reverse metal – insulator transition may be induced by introducing a compensating impurity, which captures the primary charge carrier. The compensation lowers the Fermi level and introduces what is known as 'vertical' disorder into the system in addition to the 'horizontal' disorder due to the random distribution of the impurities.

Since the 1970s, the common approach to describing such a metal – insulator transition is to use the one-electron Anderson model, in which a random field leads to localization of the states near the Fermi level [1] when the level coincides with the mobility edge. This model makes it possible, among other things, to explain why a compensated semiconductor with a partially filled ground-state impurity band does not have metallic conduction at an arbitrarily small impurity concentration N. What is important to the discussion below is that in the Anderson model the density of states $g(E)$ has no singularity and remains finite near the Fermi level. In this sense we call this model 'gapless,' because the insulator state in it corresponds not to a gap near the Fermi level but to what became known as the 'mobility gap' between the Fermi level and the mobility edge.

According to Mott [2], in the insulator state with a finite density of states near the Fermi level E_F, low-temperature electron transport occurs via tunnel hopping near the Fermi level with variable activation energy and range (variable range hopping, or VRH) and is accompanied by emission or absorption of phonons, which in the three-dimensional case yields the well-known $T^{-1/4}$-law for the electrical conductivity,

$$\rho \propto \exp\left(\frac{T_0}{T}\right)^x, \qquad (1)$$

where $x = 1/4$, the parameter $T_0 \propto \left[a^3 g(E_F)\right]^{-1}$, and a is the localization length.

On the other hand, in the 1970s a number of theoretical papers [3–5] appeared whose authors found that allowing for the Coulomb interaction between a hopping electron and the hole forming at the point occupied by the electron before hopping must lead to an enhancement of localization and formation of a gap or quasigap near the Fermi level and, hence, to an increase in the exponent x in Eqn (1) up to unity. Nevertheless, by the mid-1970s it was the validity of the one-electron Anderson model (without the Coulomb interaction) and the corresponding Mott law that were corroborated for many disordered systems.† It seemed that the Mott law could be observed in any 'dirty' object with a fairly high value of $g(E_F)$.

2. The empirical $T^{-1/2}$-law and the quasigap near the Fermi level

At approximately the same time, I wrote a paper [6] in which it was established that the observed low-temperature conductivity with a variable activation energy for various heavily doped compensated semiconductors is described by Eqn (1) with $x = 1/2$ rather than $1/4$. In the same paper it was also established that the empirical $T^{-1/2}$-law can be interpreted as a three-dimensional VRH in a parabolic quasigap near the Fermi level:

$$g = g_0(E - E_F)^2\,, \quad T_0 = \frac{A}{g_0^{1/3}a}\,, \tag{2}$$

where g_0 and A are constants.

Qualitatively this agrees with the prediction of the one-electron Shklovskiĭ–Efros theory [5] for a Coulomb gap. But to do this, one has to find the coefficient g_0 in Eqn (2) from experiments.

3. One-electron Coulomb gap

This coefficient g_0 was found in a series of papers [7] on the basis of the idea that the observed high-temperature limit of the VRH mode is proportional to the gap width Δ. The gap width and the estimated density of states in the impurity band at the band edges were then used to calculate the coefficient g_0. It was found that in the large-compensation limit (far from the metal–insulator transition) and for an N-series of samples of heavily doped compensated germanium with a constant primary-impurity concentration N and different compensation degrees K the value of this coefficient is close to that predicted by the Shklovskiĭ–Efros Coulomb-gap model [8]:

$$(g_0)_{SECG} = \frac{\varkappa^3}{e^6}\,, \tag{3}$$

where $\varkappa$ is the dielectric constant, and e is the electron charge.

For this reason, the quasigap detected in Ref. [6] was identified in Ref. [7] with the one-electron Coulomb gap, which served as experimental proof that such a one-electron gap exists. Then, in the two papers [8], Zinov'eva and I studied the gap close to the Fermi energy at very low temperatures (the method was also based on studying the sensitivity of the VRH mode to the spectrum of localized states and became known as 'VRH spectroscopy').

The Coulomb gap idea is extremely popular in the physics of disordered systems, although its course to success was not straightforward. At the beginning, Mott published a paper [10] in the same journal in which Shklovskii and Efros had published their paper [5]. In it he objected to their reasoning, thus preparing the ground for a negative attitude toward the results of future experiments in which such a gap would be detected. On the other hand, there were other, objective, difficulties in interpreting the existing experimental data correctly. The primary obstacle was the commonly used crude method of analyzing conduction with a variable activation energy by 'straightening' the conductivity curve on a scale corresponding to a value of the exponent x in Eqn (1) chosen *a priori*. Instead, the problems of determining the possible range of the conductivity for a fixed value of x and this value proper should have been solved directly. To this end, starting with the early papers [6–8], I decided to employ the differential method in studying the temperature dependence of the reduced conduction activation energy:

$$w = \frac{\varepsilon}{kT} = -\frac{d\log\rho}{d\log T}\,. \tag{4}$$

Many troubles stemmed from the macro-inhomogeneities in bulk samples grown from melts, especially in the cases of heavy doping and large compensation. Two basic manifestations of inhomogeneities at low temperatures were constantly detected at low temperatures: the decreases in the effective conducting cross section, and conducting 'shunts,' oriented primarily along dislocations. These shunts are usually capable of reducing the temperature dependence of resistivity very dramatically, e.g. transform a $T^{-1/2}$-law into a $T^{-1/4}$-law or into a power law or even into an anomalously low conductivity of metallic type.‡ To resolve this difficulty, I (later with Zinov'eva) used [7, 9] the method of uniform compensation of an n-Ge sample grown from a melt by neutron doping. Note that neutron doping of Ge amounts to introducing an acceptor germanium impurity (basically) and also donor impurities: As and a small amount of Se. In this way an N-series of samples of compensated n- and p-Ge sample were manufactured with relatively low and high neutron fluences (according to Ref. [7]). In the large-compensation limit these samples made it possible to identify the quasigap detected in 1977 [6] with a one-electron Coulomb gap. Thus it was proved that, for a slightly filled impurity band of a compensated semiconductor, the contribution of Coulomb correlations, which emerge in the hopping transport of a localized electron, to the hopping activation energy in the VRH mode is larger than the contribution of the random field of the charged impurities (the latter would manifest itself in the form of a $T^{-1/4}$-law). However, this was not all: it was found that the Coulomb gap has a simple one-electron nature only in the two limiting cases of an almost empty impurity band or in an almost filled impurity band, while for a moderately filled band the mode of multielectron hopping or multielectron correlations in hopping is realized.

† In 1977 both Philip Warren Anderson and Sir Neville Francis Mott were awarded the Nobel Prize in Physics.

‡ A similar effect takes place in the non-ohmic mode or when the sample is overheated if the applied field or the power dissipated in the sample is not sufficiently low.

4. Multielectron Coulomb gap

The idea that multielectron hopping of electrons may dominate over single-electron was developed most thoroughly in the work of Pollak et al. (e.g. see Ref. [11]). It is illustrated by Fig. 1 for a half-filled impurity band (2 electrons for 4 positions), where the ground state of the system is depicted schematically. Suppose that the $1 \to 2$ transition belongs to an infinite cluster and determines conduction, while the activation energy of one-electron hopping is $E_{1e} = E_{2,3} - E_{1,3}$. In the case of two-electron hopping, also including the 'assisting' hopping $3 \to 4$, the activation energy may be lower: $E_{2e} = E_{2,4} - E_{1,3} < E_{1e}$. The example shows that the participation of several electrons is capable of lowering the Coulomb barrier for hopping and making such hopping more probable than single-electron. Recent computer-simulation results [12] yield a $T^{-1/2}$-law for the corresponding resistivity, but with the parameter T_0 approximately ten times smaller than in the case of a one-electron Coulomb gap. Note, however, that the existence of a gap does not follow from Ref. [12]. On the other hand, Andreev and I [13, 14] noticed that if multielectron correlations lower the energy barrier for hopping (a Coulomb barrier), this must narrow the Coulomb gap in comparison to a one-electron. We then suggested a model of an anomalously narrow multielectron Coulomb gap, and this model was supposed to be verified by experiments. Since the divergence of the dielectric constant $\varkappa$ at the metal – insulator transition always narrows a Coulomb gap, the experiments must be done on the insulator side far from the transition. It was also believed that moderate filling of the impurity band (compensation) is the optimum mode to observe multielectron correlations, while the cases $1 - K \gg 1$ and $K \ll 1$ are unfavorable for such observations. For the experiments discussed in Refs [13, 14] we selected a homogeneous $K = 0.35$-series of Ge:Ga samples prepared via neutron doping of pure germanium.† Analysis of the low-temperature curves of the electrical resistivity of the samples showed that the $T^{-1/2}$-law is realized at a temperature considerably lower than in the case of large compensation (Section 3), which is a qualitative indication that the gap narrows. Unfortunately, the high-temperature limit of the $T^{-1/2}$-law for neutron-doped Ge:Ga is not known with an accuracy that would allow using it to estimate, as in Refs [7, 8], the width of the quasigap and, hence, the coefficient g_0 in Eqn (2).

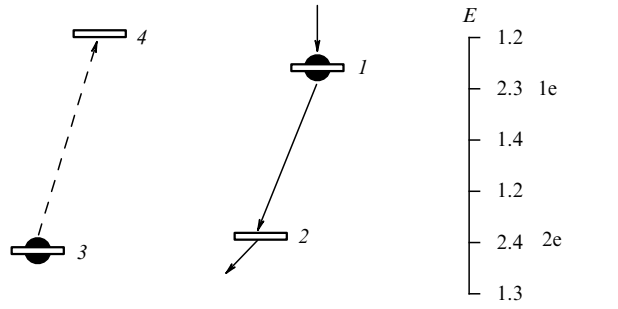

Figure 1.

† At the same time, experiments were carried out to exactly characterize the electrophysical parameters of the material [15]. These experiments showed, in particular, that the compensation of neutron-doped Ge:Ga depends on the 'hardness' of the neutron spectrum.

For this reason I used another variant of the VRH spectroscopy of the density of states in the quasigap, a variant based on Shklovskii's idea about the need to first find the localization length of holes near the Fermi level from studies of the positive magnetoresistance in the VRH mode. (This magnetoresistance stems from the narrowing of the hole wave function in the plane perpendicular to the field.) The localization radius a found by this method (see Refs 13, 14]) is divergent at the transition point N_c. But if the concentration of Ge is reduced, the localization radius reaches the 'insulator' limit $a = 90$ A equal to the Bohr radius of a light hole in Ge. This fact agrees with the idea that the large-distance asymptotic behavior of the hole wave function is determined by the light-hole mass and with the results of studies of nearest-neighbor hopping conduction in neutron-doped Ge:Ga [16]. On the other hand, the observable VRH parameter T_0 increases in value as one moves farther away from the metal – insulator transition, reaching its maximum $(T_0)_{max} = 7.5$ meV. This makes it possible to use the expression for T_0 in Eqn (1) and the asymptotic value of a to arrive at an estimate for the parameter g_0 and, hence, for the quasigap width Δ in the 'insulator' limit:

$$(g_0)_{exper} \cong M(g_0)_{SECG}\,, \quad \Delta_{exper} \cong \frac{\Delta_{SECG}}{M^{1/2}}\,, \quad M \cong 60\,. \quad (5)$$

In Figure 2 the Coulomb gaps of one- and multielectron nature (the data was taken from [9] and [13]) observed in doped Ge in the cases of large and moderate compensation are compared with the predictions of the one-electron Shklovskiĭ – Efros model [8] (curves *1*, *2*, and *3*, respectively). For a complete check on the validity of the above model of anomalous narrowing of a Coulomb gap with multielectron correlations it is advisable to verify that there is no narrowing at small compensations. The relevant data have been published recently by the Haller group [17] and refer to the $K = 0$-series of neutron-doped Ge enriched with the ^{70}Ge isotope (as a result of transmutation this isotope is transformed into Ga). Unfortunately, the researchers only

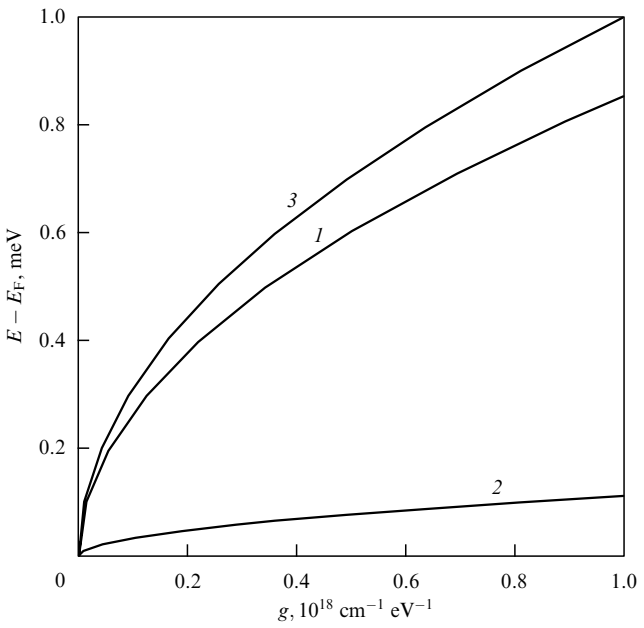

Figure 2.

state the $T^{-1/2}$-law and its connection to the Coulomb gap, without determining the gap parameters. Nevertheless, Andreev, Egorov and I [18] were able to arrive at the right conclusions by comparing the behavior of the parameter T_0 [17] in the 'insulator' limit (□ in Fig. 3) and the data taken from Refs [13, 14] for a multielectron gap (• in Fig. 3). Clearly, the latter are roughly four times smaller. Since in both cases far from the metal–insulator transition the values of the localization radius for p-Ge are the same (and equal to the Bohr radius of a light hole), all the difference must be attributed, according to Eqn (2), to the coefficient g_0: for the data of Ref. [17] it proves to be $4^3 \cong M$ times smaller, which corresponds exactly to the difference between one- and multielectron Coulomb-gap widths [see Eqn (5)]. Thus, it is obvious that the data of the Haller group [17] refer, as expected, to a one-electron Coulomb gap. Note that the difference in the values of the parameter $(T_0)^{1/2}$ in Fig. 3 corresponds to the difference between the observed activation-energy values‡ and within the VRH model can be interpreted as being caused by the difference in the values of g_0.

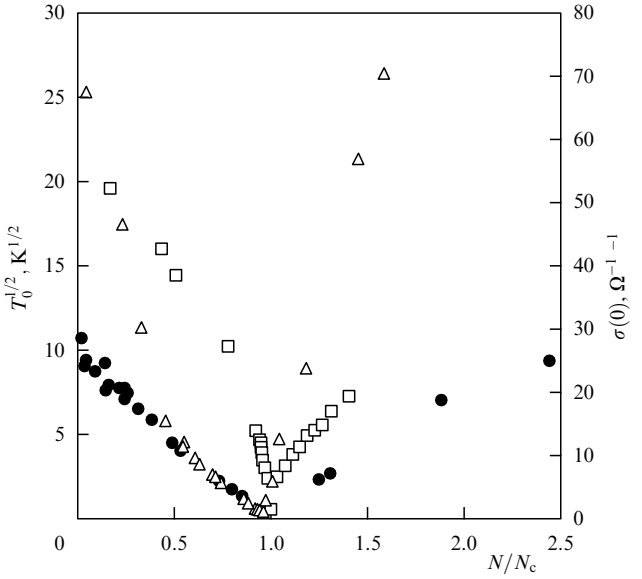

Figure 3.

Thus, Andreev and I [13, 14] were able to corroborate the model of anomalous narrowing of a Coulomb gap due to multielectron correlations in the hopping of the electrons or, in other words, to prove that a multielectron Coulomb gap does indeed exist.§ The corresponding experiment was conducted in such a way that the narrowing caused by the increases in the dielectric constant due to the proximity of the metal–insulator transition could be ignored. The latter effect is responsible for a narrowing of another sort: the collapse of Coulomb gap at the metal–insulator transition point.

‡ The Δ in Fig. 3 designate the data for the N-series of Ge:As [9], where far from the metal–insulator transition the Coulomb gap is one-electron.

§ The literature contains corroborative evidence, obtained by disparate methods, that such a Coulomb gap exists in other objects.

5. The Coulomb gap and the metal–insulator transition

Figure 4, which depicts the data obtained by Andreev, Zabrodskii, and me [18], illustrates the collapse of a Coulomb gap in neutron-doped Ge:Ga as the metal–insulator transition point is approached. Note that the parameter g_0 vanishes at the point N_{cI} (Fig. 3) and that this is due to the collapse of the gap ($T_0^{1/2}$ becomes infinite) and the divergence of the localization radius a. This point practically coincides with the critical point N_{cM} of the metal–insulator transition, which is commonly associated with the vanishing of the temperature-independent term $\sigma(0)$ in the expression for the metallic conductivity: $\sigma(T) = \sigma(0) + \Delta\sigma(T)$. This means that in addition to Anderson's definition of the critical point of the metal–insulator transition, which uses the vanishing of the metallic state, one can also use the definition based on the vanishing of the insulator state at the point where the Coulomb gap collapses. It is also believed that as the transition point is approached, the manifestation of the multielectron correlations becomes more vivid.

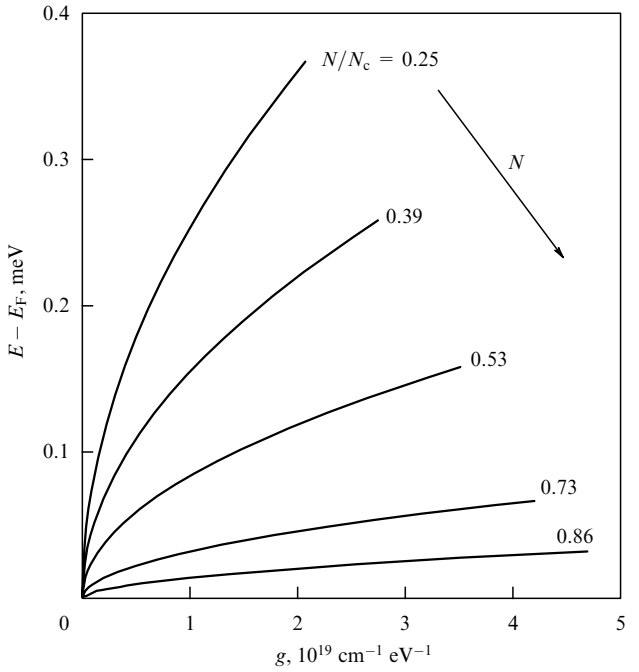

Figure 4.

As for the nature of the transition in neutron-doped Ge:Ga [18] in particular and in doped semiconductors in general, it must be noted that the transition is continuous (in contrast to Mott's idea, which persisted for a long time, that the transition is first-order), is characterized by a certain symmetry on both sides, and can be considered a second-order phase transition. Figure 3 shows that the transition becomes more sudden (the correlation-length index decreases) as the compensation $K \to 0$ tends to zero.

6. Conclusion

Experiments have shown that at low temperatures the insulator state of doped semiconductors is formed via one- and multielectron Coulomb interactions, which results in a

(respective) Coulomb gap appearing near the Fermi level. In such systems the phase transition from the insulator state into the metallic state can be interpreted as a collapse of the Coulomb gap. Thus, it appears that the Coulomb interaction and multielectron correlations play no less a role in the low-temperature properties of the insulator state of doped semiconductors than disorder.

I am grateful to my colleagues who participated in the various studies and to the Russian Fund for Basic Research and INTAS for support.

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