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INTERACTION OF DIFFUSION MODES AND SPIN FLUCTUATIONS NEAR THE METAL-INSULATOR TRANSITION IN DISORDERED SYSTEMS

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Abstract. – The results of the theory describing the electrons scattering on the impurities via diffusion mode interaction are presented. An application of this theory to describe a critical region of the metal-insulator transition is discussed. The spin-density instability in the system of the interacting disordered electrons is considered and the recent ESR measurements in uncompensated Si:P are discussed. In our opinion the results of these experiments favour the many-particle correlation effects though their interpretation requires going beyond the limits of the diffusion mode theory.

1. Survey of the theory of diffusion modes

1.1 In the past decade attempts have been made to describe the metal-insulator transition in disordered systems by methods of the second order phase transition theory. The strategy of this approach is that starting with short distances (where a substance possesses properties of a metal) one includes consecutively the long wave diffusion modes, which determine properties of a substance in the critical region of the transition. This approach has been put forward in [1].

The experiments made after 1980 have shown that in the metal-insulator transition in disordered systems conductivity vanishes gradually rather than by a jump. Thus, there are indeed grounds to use some scaling theory. For free electrons a mathematical foundation of the idea of the paper [1] was given by Wegner [2], who reduced the initial quantum problem of the electron scattering on impurities to a field-theoretic problem of interaction of diffusion modes described by an effective functional. Regarding a physics of a construction of the effective functional of diffusion modes, it is analogous to a reduction of the initial problem in the theory of magnetism to the Heisenberg functional describing the spin wave interaction: \( \mathcal{L} = f^{-1} (\nabla n)^2 \), \( n^2 = 1 \). Unfortunately, in the problem under study the local parameter of the metallic state – the counterpart of \( n \) – proves to be a rather complicated matrix \( Q \). This matrix has replica (i, j) indices (as usual, when we deal with disordered systems), energy (\( n, m \)) indices, and, besides, elements \( Q_{im}^n \) are \( 4 \times 4 \) matrices (spin quaternions). In terms of \( Q \) effective functional of a free electron in a disordered system is

\[
\mathcal{F}_D = \frac{T\pi\rho}{8} \int \left[ DS\eta (\nabla Q)^2 - 4ZSp (\xi Q) \right] d\mathbf{r} \tag{1}
\]

where the matrix \( Q \) satisfies the following constraints: \( Q = Q^\dagger, \text{Sp} Q = 0, Q^2 = I (I \text{ is a unit matrix}) \). In (1) \( D \) is the electron diffusion coefficient, the constant \( \rho \) is the density of states without diffusion corrections, \( \xi \) is the diagonal matrix formed by the Fermi frequencies \( \varepsilon_n = (2n + 1)\pi T \). The role of the parameter \( Z \) introduced in (1) will be discussed later (for free electrons \( Z \equiv 1 \)).

The frequency term in \( \mathcal{F}_D \) is an analogue of the magnetic field in the Heisenberg model – it violates the symmetry of \( \mathcal{F}_D \) with respect to the rotation of the matrices \( Q \) and fixes the equilibrium position of \( Q \). The transversal deviations of \( Q \) from the equilibrium position correspond to the diffusion modes, which are the counterparts of magnons in ferromagnet. There are two types of diffusion modes: "diffusons" (the momentum transfer \( K \) and the frequency transfer \( \Omega \) are small) and "cooperons" (the total momentum \( K \) and the frequency transfer \( \Omega \) are small). The propagators of these modes are singular and proportional to \( (DK^2 + Z |\Omega|)^{-1} \).

The functional \( \mathcal{F}_D \) is invariant with respect to a homogeneous rotation of quaternions – this is a result of invariance relative to time inversion when a particle is converted into a hole. Besides, there is invariance relative to the rotation in the spin space. A magnetic field violates the time inversion invariance. It does not influence the diffusion modes, until the Zeeman splitting is taken into account, but it suppresses long-wave cooperons – in the singular propagator of these modes a cut-off factor appears. With the Zeeman splitting taken into account the invariance relative to the rotation in the spin space is violated as well, and only the diffusons corresponding to zero spin projection on the magnetic field direction (\( S_H = 0 \)) remain singular. Finally, when there are magnetic impurities, a cut-off factor is present in propagators of all the diffusion modes except one corresponding to a diffusion of the total density of particles (\( S = 0 \)). Continuing the analogy with ferromagnet we can conclude [3] that in the functional of diffusion modes a magnetic field and magnetic impurities play the role of magnetic anisotropies in ferromagnets.
1.2 Due to electron-electron interaction there appear new terms in the functional of diffusion modes $\mathcal{F}$ [4, 5]:

$$\mathcal{F} = \mathcal{F}_D + \mathcal{F}_S + \mathcal{F}_t + \mathcal{F}_C.$$  \hfill (2)

Here the term $\mathcal{F}_S$ describes the interaction of density fluctuations (singlet channel), $\mathcal{F}_t$ is the same for spin density fluctuations (triplet channel) and $\mathcal{F}_C$ takes into account the interaction of cooperon modes. The corresponding interaction amplitudes are denoted as $\Gamma_S, \Gamma_t$ and $\Gamma_C$. Singular diffusion propagators will enter the game via el.-el. interaction and will give rise to nonanalytic in temperature corrections in different physical quantities. Such contributions are hardly to be expected from the viewpoint of the conventional fermi-liquid theory. This effect was discovered by Al'tshuler and Aronov [6] (for the review see Ref. [7]). Our task was to construct a renormalization procedure for the functional $\mathcal{F}$, i.e. the consecutive transformation from the relatively short-wave fluctuations to the longer-wave ones. Besides interaction amplitudes $\Gamma_i$ ($i = s, t, c$) and the resistance of a sample measured in units $\hbar/e^2$, in the course of renormalization scheme there appears a new charge $Z$ which is a coefficient in front of the frequency term in the functional $\mathcal{F}$. It has elucidated by the author [4] that the renormalization of the frequency term coefficient ensures the consistency of the particle number conservation condition with the renormalization group (RG) equations. As a result the density correlator $\pi(K, \Omega)$ is of the following form:

$$\pi(K, \Omega) = \frac{\partial n}{\partial \mu} D_s K^2 / (D_s K^2 + |\Omega|).$$  \hfill (3)

Here $D_s = (1 + F_0) D$ is the diffusion coefficient of the interacting electrons, $D$ is the parameter in (1) obtained by renormalization of the functional $\mathcal{F}$; $F_0$ is a standard fermi-liquid constant, $\partial n/\partial \mu = 2\rho/(1 + F_0)$ — diffusion corrections are not essential in $\partial n/\partial \mu$. The Einstein relation follows from (3) and the continuity equation

$$\sigma/e^2 = \frac{\Omega}{K^2} \pi(K, \Omega); \quad \sigma/e^2 = 2\rho D.$$  \hfill (4)

Thus, $\sigma$ can be found directly by renormalization of the coefficient $D$ in the functional $\mathcal{F}$. Further, it was found [5, 8] that the correlator of the spin density is

$$\chi_S(K, \Omega) = \frac{1}{2} (G_{L\mu B})^2 \rho (Z + \Gamma_t) D_s K^2 / (D_s K^2 + |\Omega|),$$  \hfill (5)

where $D_s = D/(Z + \Gamma_t)$ is a spin diffusion coefficient, and a spin susceptibility $\chi_S = \frac{1}{2} (G_{L\mu B})^2 \rho (Z + \Gamma_t)$. Finally, in the paper [9] the frequency renormalization parameter $Z$ has been identified in terms of the specific heat

$$Z = \gamma/\gamma_0, \quad \gamma = C_\nu/T.$$  \hfill (6)

where $C_\nu$ is a specific heat, $\gamma_0 = 2\sigma^2 P/3$. It follows from (3)-(6) that diffusion mode theory has a structure of the conventional fermi-liquid description of disordered electrons but with renormalizable parameters.

1.3 RG analysis of disordered systems deals with logarithmic corrections, essential in the two-dimensional case ($d = 2$) [7]. We have studied the behaviour of different systems at $d = 2 + \varepsilon$, bearing in mind the metal-insulator transition problem. It follows from the structure of the effective functional $\mathcal{F}$ and the dimensional analysis that RG equation should have the following structure

$$d\sigma/dx = \beta (g; \Gamma_i/Z); \quad \frac{d (\Gamma_i/Z)}{dX} = \beta_i (g; \Gamma_i/Z)$$  \hfill (7)

$$dZ/dX = Z \zeta (g; \Gamma_i/Z),$$  \hfill (8)

where $g = \lambda d^{d-2}/(2\pi)^d \rho D$ ($g$ is proportional to the resistance of a sample measured in units $\hbar/e^2$); $\lambda$ is a cut-off momentum decreasing in the course of renormalization $X = \ln \lambda_0/\lambda$ ($\lambda_0 = 2\pi/\nu \nu T$). A critical region of the metal-insulator transition is described by the unstable fixed point of this system. It follows from the form of diffusion propagators that at a finite frequency $\omega$ of the external field the process of renormalization in the critical region stops at the length $L_\omega \sim (D/Z\omega)^{1/2}$. Therefore, in the vicinity of the transition when the correlation length $\xi \gg L_\omega$, the conductivity $\sigma \propto e^2 L_\omega^{2-d}$. Hence, by virtue of equation (4) it follows that $\sigma \propto e^2 (Z\omega)^{(d-2)/d}$. For free electrons $Z$ is not renormalized ($Z \equiv 1$), and, thus, $\sigma (w) \propto \omega^{(d-2)/d}$ [10]. As a result of el.-el. interaction $Z$ is renormalized and in the critical region its behaviour is described by the exponent $\zeta$:

$$Z \sim (\lambda/\lambda_0) \zeta.$$  \hfill (9)

The value of $\zeta$ is determined from equation (8) in the vicinity of the fixed point. At a scale $L_\omega$ one has $Z \sim (\nu / L_\omega)^{\zeta}$ and as a result we get [11]:

$$\sigma \propto \omega^{(d-2)/(d-\zeta)}.$$  \hfill (10)

The $\omega$-dependence of $\sigma$ has been discussed above for $\omega \gg T$. If $\omega < T$ the renormalization procedure is cut off at a temperature length $L_T \sim (D/ZT)^{1/2}$ and therefore in the critical region of the transition

$$\sigma \propto T^{(d-2)/(d-\zeta)}.$$  \hfill (11)

In [11] RG equations for the transition in the presence of a magnetic field or when magnetic impurities are present have been derived. For this purpose the matrices $Q$ in the functional $\mathcal{F}$ have been reduced in
a proper way, so that modes with diffusion propagators containing a cut-off factor and thus inessential at large scales were eliminated altogether. It has turned out that in these both cases the system (7)-(8) derived in the lowest order in $\varepsilon = d - 2$, has a fixed point, corresponding to a transition. Omitting details we resume that the following behaviour of $Z$ is possible in the critical region:

a) $Z \to 0$, $\zeta > 0$. According to the equations derived in the first order in $\varepsilon = d - 2$, this case is realized in a presence of spin scattering: $\zeta = \varepsilon/2$;

b) $Z \to \text{const}$, $\zeta = 0$. This situation is realized when the transition occurs in the magnetic field and the Zeeman splitting is essential;

c) $Z \to \infty$. So far we have no obvious example of such a transition. It is possible, that the transition when the scattering by impurities is purely potential, falls to this category. The corresponding system is Si:P which properties are discussed below.

Despite considerable efforts to study a region of the transition, the dependence of physical quantities on temperature in the vicinity of the transition is not understood enough yet. We shall refer to two rather recent papers. For the transition in the magnetic field in n-GaAs and n-InSb it was found [12] that in the critical region $\sigma (T) \propto T^{1/3}$. In the paper [13] it has been shown that in a persistent photoconductor Al$_{0.3}$Ga$_{0.7}$As : Si where the carrier concentration can be controlled very neatly, $\sigma (T) \propto T^{1/2}$.

2. Spin fluctuation and the metal-insulator transition

2.1 Let us discuss the behaviour of the system of dimension $d = 2 + \varepsilon$ when the scattering by impurities is purely potential. In the lowest order in $\varepsilon = d - 2$ the RG equations are [14]:

$$
\frac{dg}{dX} = -\varepsilon g + 2g^2 \left[ 5 - 3 \frac{1 + \frac{w}{2}}{w} \ln (1 + w) \right];
$$

$$
\frac{dw}{dX} = g (1 + w)^2
$$

$$
\frac{dZ}{dw} = Z (-1 + 3w) / (1 + w)^2,
$$

(12)

(13)

where $w = \Gamma_1/Z$. In [15] these equations have been successfully applied to explain some data on Ge:Sb. It follows from (13) that at small initial values of $g$, which will be called as $g_0$, the trajectories $g(w)$ reach $g = 0$ at finite values of $w$. However, for $g_0$ exceeding a certain $g_{0\text{c}}$ the character of trajectories changes. For these trajectories $w \to \infty$ whereas $g$ remains finite. It is important that this divergence of $w$ occurs at a finite value $X = X_0$ depending on $g_0$ and an initial value of $\Gamma_1$. The length scale corresponding to the development of the divergence we shall call $\xi_0$. It follows from (13) that when $w \gg 1$ then $Z \propto w^4$ and correspondingly

$$
\chi_S \propto w^4; \quad D_S \propto w^{-4}.
$$

(14)

Thus, if the bare conductivity is small enough, i.e. $g_0 > g_{0\text{c}}$, then there appears a tendency for spin density rearrangement when the length scale $\xi_0$ is approached: $\chi_S \to \infty$ and $D_S \to 0$.

What can be said about further renormalization when the distances $\xi > \xi_0$ are involved?

If there is a magnetic field in the system, then while approaching $\xi_0$ the Zeeman splitting increases due to enhancement of $\chi_S$. Finally, it results in suppression of the corresponding diffusion modes and, hence there occurs a crossover: at $\xi > \xi_0$ the behaviour of the system is described by RG equations derived when the matrix $Q$ is reduced in a proper way. Approximately the same mechanism works when there are localized moments in a sample or due to fluctuations in the distribution of impurity atoms there are regions in a sample where the instability under consideration will occur earlier and as a result islands of localized spin density will be formed. These localized moments will magnetize the remaining electrons. Thus, localized moments in combination with correlation effects cause formation of a random spin density wave on which background the transition takes place. A slow decay of magnetization leads to suppression of the long-wave spin-diffusion modes and cooperons due to splitting of the Fermi surface of electrons with different spin projections and development of the instability ceases.

A system in which a problem of influence of the above discussed spin instability on the metal-insulator transition pattern must be solved by some other way, is uncompensated Si:P, since in the latter the sources of spin relaxation are practically absent. We suspect that this correlates somehow with the fact, that a transition in uncompensated Si:P occurs more abruptly than in other materials: in Si:P the exponent $\nu$ describing $\sigma \propto |n - n_e|^{\nu}$ is close to 0.5 [16], while as a rule it is $\approx 1$ ($n$ is the impurity concentration, $n_e$ corresponds to the transition point). The behaviour of Si:P in the critical region [17] does not allow one to judge unambiguously about the nature of the transition [18]. However, there are indications that in this system correlation effects are essential. Indeed, the measurement of the specific heat $C_v$ of the metallic sample with the concentration $n/n_e = 1.6$ has shown [20] that the coefficient $\gamma = C_v/T$ increases more than twice when the temperature decreases from 1 K up to 0.1 K. This result together with the results of the ESR measurements [21, 22] discussed below demonstrate that in Si:P on the metallic side of the transition there is a rather wide region of concentrations $(n/n_e - 1) \sim 1$ where the electron liquid exhibits strong correlations. We relate this region to $g_M \lesssim g_0 < g_{0\text{c}}$, and attribute its existence to
the discussed instability. An alternative variant of this theory has been suggested in [23], where a transition point $g_c$ is assigned to $g_M$ (see, however, [24]).

2.2 In papers [21, 22] by ESR studies it has been shown that in uncompensated Si:P in the metallic regime a spin susceptibility $\chi_S$ increases sharply over a fairly broad range of phosphorus concentrations $n > n_c$ (in Si:P $n_c \simeq 3.2 \times 10^{18}/cm^3$). In [21] the anomalous increase in $\chi_S$ has been discovered even in the sample with $n = 4.5 \times 10^{18}/cm^3$. In [22] measurements have been carried out on two samples with $n/n_c = 1.09$ and 1.25. Here a very interesting result has been found: the width of the resonance line $\Delta H_{1/2}$ broadened in proportion to $\chi_S$ when the temperature was lowered below 1 K. The enhancement of a spin susceptibility in the metallic phase can be explained by assumption that deeply below the Fermi level there are singly occupied electronic states – localized magnetic moments formed as a result of fluctuations of the impurity atom location. On the other hand, the growth of $\chi_S$ can result from the discussed enhancement of the strength of el.-el. interaction. In our opinion, the proportionality between $\chi_S$ and $\Delta H_{1/2}$ observed in Si:P near the transition should be the key to an understanding the physics of the metal-insulator transition in the uncompensated semiconductors [25].

Let us discuss an assumption that in Si:P on the metallic side of the transition there are both delocalized (the corresponding subscript will be “d” ) and localized spins (the subscript “l” ). The ESR physics when the two spin subsystems are present are summarized in reference [26]. Since in Si:P $G$-factors of the delocalized and localized electrons must be equal, $G_e = G_l$, one should suppose that we deal with a “bottlenecked” regime (a joint resonance of “d” and “l” electrons). In this case the width of the resonance line is

$$\Delta H_{1/2} \equiv 1/T_{eff} \approx \frac{\chi_l T_{1l}^{-1} + \chi_c T_{1c}^{-1}}{\chi_l + \chi_c}$$  \hspace{1cm} (15)$$

where $T_{1l}$ and $T_{1c}$ are spin-lattice relaxation times in “d” and “l” spin subsystems, respectively. A physical meaning of equation (15) is just that a part of a magnetization corresponding to each subsystem is multiplied by a relaxation rate in this subsystem. When the temperature decreases down to 30 mK the susceptibility $\chi_S = \chi_l + \chi_c$ increases several times and, consequently, $\chi_l$ – the localized spin contribution – must exceed considerably the Pauli susceptibility of delocalized electrons $\chi_c$. Hence, it follows that $T_{1l}^{-1} \approx T_{1c}^{-1}$.

A spin-lattice relaxation of localized magnetic moments is determined by the precession mechanism of relaxation. If, for example, the precession of localized moments in Si:P proceeds due to the hyperfine interaction with the phosphorus nuclei, then we get:

$$T_{1l}^{-1} = \frac{1}{2} T_{1c}^{-1} + (\Delta \omega)^2 \approx \frac{1}{2} \omega_{hf}^2 T_{1c},$$  \hspace{1cm} (16)$$

where $\omega_{hf}$ is a hyperfine splitting and $\Delta \omega$ is an analogue of the Knight shift for a localized spin. The time of precession is controlled by $T_{1c}$, a relaxation time of a magnetic moment of localized electrons due to an exchange interaction with delocalized electrons. Using the balance equation $\chi_c T_{1c}^{-1} = \chi_l T_{1l}^{-1}$ we find from (16):

$$\Delta H_{1/2} \propto T_{1c} \chi_l/\chi_c$$  \hspace{1cm} (17)$$

where $T_{1c}$ is a spin relaxation time of conduction electrons due to the exchange with localized moments.

At first sight, we have arrived at the desired result $\Delta H_{1/2} (T) \propto \chi_S (T)$, since $\chi_c$ does not depend on temperature and $T_{1c}^{-1} = 2 \pi C \rho_2 \rho^2 (\rho$ is the density of states at the Fermi level), $T$ is a constant of the exchange interaction of “d” and “l” electrons, $C$ is a concentration of the localized spins). However, one should take into account the fact, that as temperature is lowered the susceptibility rises considerably less steeply compared with the Curie law: $\chi_l = \frac{(G_\nu \mu_B)^2 C}{4T}$ ($S = 1/2$). This fact could be explained by gradual freezing of localized spins into pairs or clusters [27] and, hence, the effective concentration $C$ would be a function of the temperature: $C = C (T)$. Then, since $T_{1c}^{-1} \propto C$, the dependence on temperature in $\Delta H_{1/2} (T)$ and $\chi_S (T)$ would prove to be different. Thus, a model of two species of electrons does not describe the experimental data, at least in its simplest form.

Now, consider broadening of the linewidth as an effect of interaction of electrons which are scattered by impurities. Spin density correlation function in the presence of magnetic field and some source of spin relaxation has the following form:

$$\chi_S (K, \omega) = \chi_0 \gamma \sigma (0) \frac{D_s K^2 + \gamma^{-1}_s (0) (\gamma_s^2) T_{1c}^{-1} + i \omega_0}{D_s K^2 + \gamma^{-1}_s (0) (\gamma_s^2) T_{1c}^{-1} - i (\omega - \omega_0)},$$  \hspace{1cm} (18)$$

Here $\chi_0 = \frac{1}{2} (G_\nu \mu_B)^2 \rho$; $\omega_0$ is the ESR frequency: $\gamma_\sigma (0) = (Z + \Gamma_s)$ is a vertex part with small momentum transfer describing renormalization of spin susceptibility $\chi_S = \chi_0 \gamma_\sigma (0)$; $D_s$ is the spin diffusion coefficient; $T_{1c}^{-1}$ is unrenormalized spin relaxation rate. Besides, (18) includes the renormalization of interactions which can be a source of the spin lattice relaxation: $T_{1c}^{-1}$ is multiplied by $(\gamma_s^2)$ – a square of the vertex part $\gamma_\sigma (q)$, averaged over a momentum transfer $q$ (this av-
eraging must take into account the dependence of $T_{cl}^{-1}$ on $q$ as well. Finally, the appearance of $\gamma_\sigma^{-1}(0)$ results from the renormalization of $\omega$ and $\omega_0$.

We are interested in how $\Delta H_{1/2}$ and $\chi_8$ are related to each other. The width of the resonance line $\Delta H_{1/2} = \gamma_\sigma^{-1}(0) \langle \gamma_\sigma^2 \rangle T_{cl}^{-1}$ and hence, $\Delta H_{1/2}$ will be proportional to $\chi_8$ when

$$\gamma_\sigma(0) \propto \langle \gamma_\sigma^2 \rangle^{1/2}. \quad (19)$$

Since interactions causing the spin-lattice relaxation are local (they can be hyperfine or spin-orbit interactions), then (19) means that in some finite range of momenta $q$ the dependence $\gamma_\sigma(q)$ on temperature must be the same as at $q \approx 0$.

Far from the transition point when $g_M < g_0$, the diffusion corrections to $\langle \gamma_\sigma^2 \rangle^{1/2}$ can be treated by perturbation theory. In the first order in $w$ the corrections to $\gamma_\sigma(0)$ and $\langle \gamma_\sigma^2 \rangle^{1/2}$ prove to be equal [28]. A significance of that was overestimated in [28]. In higher orders in $w$ this equality is broken: $\gamma_\sigma(0)$ increases considerably faster than $\langle \gamma_\sigma^2 \rangle^{1/2}$, when $w \to \infty$.

Closer to the transition when $g_M \lesssim g_0 < g_c$ the internal consistency of the diffusion mode theory breaks down: while reaching the scale $\xi_0$, as has been shown above, $\chi_8$ diverges and $D_8 \to 0$ (besides, $Z \to \infty$ and quasiparticle diffusion coefficient $D_{ap} = D/Z \to 0$). We suppose that as a result local modes are formed. It is assumed at that large scales when the wave vector $q << \xi_0^{-1}$, spin diffusion coefficient $D_8$, and probably $D_{ap}$, vanishes. As a result, in this region of the momenta $\gamma_\sigma(q) = \gamma_\sigma(0)$ and the relation (19) holds.

2.3 An example of the theory where the relation $\chi_8(q = 0) \propto \chi_8(r = 0)$ is fulfilled is a highly correlated electron gas [29], which is realized just in the case of the half-filled conduction band. The highly correlated gas is distinct from the state close to the ferromagnetic instability by a uniform enhancement of $\chi_8(q)$ in the momentum space in the former case. The above allows to conclude that in the uncompensated semiconductors unlike the other disordered systems, the diffusion mode theory is not the whole story. Presumably the metal-insulator transition in Si:P is distinct from that in compensated semiconductors by generation of the local modes near the transition in Si:P. Apparently, the theory of the transition in uncompensated semiconductors should be as different from the diffusion modes theory as the highly correlated electron gas differs from the theory of paramagnons [30]. The diffusion mode theory may still be relevant as the driving term in the formation of the local modes [31].


