ESR near a metal-insulator transition

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Some conclusions regarding the nature of the metal-insulator transition in uncompensated semiconductors are drawn from the results of recent ESR measurements near the transition in Si:P [S. Ikehata and S. Kobayashi, Solid State Commun. **56**, 607 (1985); M. A. Paalanen *et al.*, Phys. Rev. Lett. **57**, 2061 (1986)].

1. ESR measurements have recently been carried out[1,2] near the metal-insulator transition in uncompensated metallic Si:P. It has been shown (see also Ref. 3) that the spin susceptibility χ increases sharply as the temperature is lowered, not only in the insulating phase[4] but also on the metallic side of the transition, over a fairly broad range of phosphorus concentrations $n \gtrsim n_c$ (n_c corresponds to the transition; in Si:P it has the value $n_c \cong 3.2 \times 10^{18}$ cm^{-3}). Ikehata and Kobayashi[1] observed an anomalous increase in χ even in a sample with $n = 4.5 \times 10^{18}$ cm^{-3}. Paalanen *et al.*[2] carried out measurements on two samples, with $n/n_c = 1.09$ and 1.25. They found the very interesting result that as the temperature is lowered, the width of the resonance line, $\Delta H_{1/2}$, begins to increase in proportion to χ at $T \sim 1$ K.

In this letter we offer an interpretation of the experiments of Refs. 1 and 2. An increase in the spin susceptibility in the metallic phase might result from the presence of singly filled electron states—localized magnetic moments formed as a result of

fluctuations in the distribution of impurity atoms—deep below the Fermi level.[5] On the other hand, an increase in χ might result from an anomalous intensification of the interaction of electrons scattered by impurities.[6–9] The proportionality between χ and $\Delta H_{1/2}$, which was observed in Ref. 2 in Si:P near the transition is, in our opinion, the key to an understanding of the physics of the metal-insulator transition in uncompensated semiconductors.

The analysis below shows the following: a) The assumption that an increase in χ on the metallic side of the transition results from localized moments apparently fails to explain the proportionality of χ and $\Delta H_{1/2}$. b) The corrections to χ and $\Delta H_{1/2}$ for the interaction of diffusing electrons agree only in first order in the amplitude Γ_2, which describes the interaction of spin density fluctuations. The importance of this coincidence was overestimated in Refs. 10 (When the higher orders in Γ_2 are taken into account, it is found that a significant increase can occur only in χ, not in $\Delta H_{1/2}$.) c) In order to achieve a proportionality of χ and $\Delta H_{1/2}$, it is necessary that the spin susceptibility $\chi(r=0)$ be proportional to χ. In other words, an anomalous intensification of the function $\chi(q)$ should occur not exclusively at a zero momentum q but in a certain region of momenta of finite radius.

The following conclusion can be drawn at this point: In uncompensated semiconductors, in contrast with other disordered systems, an analysis of diffusion modes is insufficient for describing the metal-insulator transition. It may be that the reason for the difference between the metal-insulator transition in Si:P and that in compensated semiconductors[11] is that local modes are generated near the transition in Si:P.

2. Let us examine the suggestion that on the metallic side of the transition in Si:P there are both delocalized spins (which we will label by means of a subscript e) and localized spins (subscript s). The physics of the ESR in the presence of two spin subsystems depends on whether the bottleneck regime occurs (a joint resonance of e and s electrons). Since the g-factors of the delocalized and localized electrons must be equal in Si:P ($g_e = g_s$), we should assume that we are dealing with the bottleneck regime. A theory of the ESR of magnetic moments in a metal was put in a systematic form in the review by Barnes.[12] In the case of a bottleneck, the width of a resonance line is[1)]

$$\Delta H_{1/2} \equiv \frac{1}{T_{eff}} \approx \frac{\chi_s / T_{sL} + \chi_e / T_{eL}}{\chi_s + \chi_e}, \qquad (1)$$

where T_{sL} and T_{eL} are the spin-lattice relaxation times in the s and e spin subsystems, respectively. The physical meaning of expression (1) is simply that the fraction of the magnetization corresponding to each of the subsystems is multiplied by the relaxation rate in that subsystem. As the temperature is lowered to 30 mK, the susceptibility $\chi = \chi_s + \chi_e$ increases several fold, so that χ_s— the localized-spin component— should be substantially greater than the Pauli susceptibility of the delocalized electrons, χ_e. It follows that we have $1/T_{\text{eff}} \approx 1/T_{sL}$.

A spin-lattice relaxation of the magnetization of localized spins occurs in Si:P by virtue of a hyperfine interaction with phosphorus nuclei. In this case we have

$$1/T_{sL} = \frac{1}{2} \frac{<\omega_{hf}^2>/T_{se}}{T_{se}^{-2} + (\Delta\omega)^2} \cong \frac{1}{2} <\omega_{hf}^2> T_{se}, \quad (2)$$

where ω_{hf} is the hyperfine structure constant, $\Delta\omega$ is an analog of the Knight shift for a localized spin, and T_{se} is the time scale of the relaxation of the magnetization of the localized electrons which results from the exchange interaction with delocalized electrons. Expression (2) describes an ordinary precession relaxation mechanism, in which the precision time is controlled by the interaction with conduction electrons. Using the balance equation $T_{se}/T_{es} = \chi_s/\chi_e$, we then find

$$\Delta H_{1/2} \propto T_{es}\chi_s/\chi_e, \quad (3)$$

where T_{es} is the time scale of the relaxation of the conduction electrons, which results from the exchange with localized moments.

It would seem at first glance that we have obtained the expected result, $\Delta H_{1/2}(T) \propto \chi(T)$, since χ_e does not depend on the temperature, while we have $1/T_{es} = 2\pi c\rho J^2$ (ρ is the state density of the Fermi surface, J is the exchange-interaction constant of the s and e electrons, and c is the concentration of localized spins). However, we need to take account of the circumstance that as the temperature is lowered, the susceptibility increases considerably more slowly than would follow from the Curie law: $\chi_s = (g_s\mu_B)^2 c/4T$. This result might have been explained on the basis that there is a gradual freezing of the localized spins into pairs or clusters,[2)] so the effective concentration c is a function of the temperature: $c = c(T)$. In that case, however, the relation $1/T_{es} \propto c$ would mean that the temperature dependences $\Delta H_{1/2}(T)$ and $\chi(T)$ would be different. The model of two species of electrons (at least in its simplest form) thus fails to explain the experimental data.

3. Let us examine the broadening $\Delta H_{1/2}$ as the effect of an interaction of electrons which are scattered by impurities. The correlation function for the spin density takes the following form when k and ω are small:

$$\chi(k, \omega) = \chi_e \gamma_\sigma(0) \frac{D_s k^2 + \frac{<\gamma_\sigma^2>}{\gamma_\sigma(0)} \frac{1}{T_{eL}} + i\omega_0}{D_s k^2 + \frac{<\gamma_\sigma^2>}{\gamma_\sigma(0)} \frac{1}{T_{eL}} - i(\omega - \omega_0)}. \quad (4)$$

Here $\chi_e = \frac{1}{2}(g_e\mu_B)^2\rho$; D_S is the spin diffusion coefficient; ω_0 is the ESR frequency; $\gamma_\sigma(0)$ is the vertex part with a small momentum transfer, which describes the renormalization of the spin susceptibility, $\chi = \chi_e\gamma_\sigma(0)$; and $1/T_{eL}$ is a seed spin relaxation rate. Furthermore, expression (4) incorporates the renormalization of the interactions, which may be a source of a spin-lattice relaxation (this might be a hyperfine interaction or a spin-orbit interaction): $1/T_{eL}$ is multiplied by $\langle\gamma_\sigma^2\rangle$, which is the square of the vertex part, $\gamma_\sigma(q)$, averaged over the momentum transfer[3)] q. Finally, the appearance of $\gamma_\sigma(0)$ along with T_{eL} results from the renormalization of ω and ω_0.

What is the relation between $\Delta H_{1/2}$ and χ? The width of the resonance line is

$\Delta H_{1/2} = [\langle \gamma_\sigma^2 \rangle / \gamma_\sigma(0)] \frac{1}{T_{eL}}$, so $\Delta H_{1/2}$ is proportional to χ if

$$\gamma_\sigma(0) \propto \langle \gamma_\sigma^2 \rangle^{1/2} . \quad (5)$$

Since the interactions which cause the spin-lattice relaxation are local, relation (5) means that in a finite region of momenta q the functional dependence $\gamma_\sigma(q)$ must be the same as in the limit $q \to 0$.

The metal-insulator transition was discussed in Ref. 9 (see also Ref. 14) on the basis of an analysis of the interaction of "diffusions" in first order straight in $\epsilon = d - 2$. In that approach, progressively longer-wavelength diffusion modes are taken into account starting at short distances, where the substance exhibits good metallic properties. Far from the transition, where the seed value of the conductance G, which characterizes the degree of disorder, is greater than some G_M, a temperature decrease is accompanied by a finite increase in χ. In this regime the diffusion corrections to $\gamma_\sigma(0)$ and $\langle \gamma_\sigma^2 \rangle^{1/2}$ are equal[10] in first order in the amplitude Γ_2. However, it is easy to see that among all the diagrams that determine the growth of $\gamma_\sigma(0)$ (see Fig. 5 in Ref. 7) only one contributes substantially to $\langle \gamma_\sigma^2 \rangle^{1/2}$. Consequently, the equality breaks down in higher orders in Γ_2: $\gamma_\sigma(0)$ increases more rapidly than $\langle \gamma_\sigma^2 \rangle^{1/2}$.

Closer to the transition, with $G_M > G > G_C$ (G_C corresponds to the critical concentration n_c), the theory of diffusion modes becomes internally inconsistent: When a certain scale ξ_G, which depends on G, is reached, the susceptibility χ diverges, and we have $D_S \to 0$ (Ref. 9). We suggest that local modes form here. It is assumed that over a large scale, where the wave vector satisfies $q < \xi_G^{-1}$, the spin diffusion coefficient vanishes ($D_S = 0$), so that in this momentum region we have $\gamma_\sigma(q) = \gamma_\sigma(0)$, so (5) holds. In Ref. 1, the increase in $\chi(T)$ in a sample with $n = 4.5 \times 10^{18}$ cm^{-3} was not accompanied by the broadening of the resonance line. That result confirms the existence of different regimes and may mean that this concentration corresponds to a value of G close to G_M.

A well-known example in which the relation $\chi(q = 0) \propto \chi(r = 0)$ holds is the so-called highly correlated electron gas,[15] which occurs specifically in the case of a half-filled conduction band. A highly correlated gas differs from a state which is close to a ferromagnetic instability and which is described by paramagnons[16] in that that the amplification of $\chi(q)$ in it occurs in a uniform fashion in momentum space. It can be suggested on the basis of the arguments above that the theory of the transition in uncompensated semiconductors should differ from the existing theory for the interaction of diffusion modes to the extent to which the theory of a highly correlated electron gas differs from the theory of paramagnons. The interaction of diffusions may play the important role of the mechanism which triggers the formation of local modes.

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[1)] Strictly speaking, we should replace χ_s and χ_e in the numerator of (1) by χ_s^0 and χ_e^0, which correspond to the respective quantities in the absence of an exchange interaction between e and s electrons. We will not draw a distinction between these quantities here.

[2)] Pairs and clusters of spins lead to a good description of the magnetic properties of Si:P under the condition[13] $n \lesssim 0.7 n_c$.

[3)] This averaging should also incorporate the dependence of $1/T_{eL}$ on q.

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