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Electron spin resonance in disordered metals

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A theoretical study of the spin-resonance signal of electrons in a disordered metal with nuclear-spin impurities is performed. It is found that there are singular corrections to the linewidth near two dimensions. These corrections arise both from disorder and from the disorder-enhanced electron-electron interactions. To lowest order in the triplet scattering amplitude, the increase in linewidth is simply related to the enhancement of the spin susceptibility. These results are consistent with a recent experiment.

The study of the static and dynamic properties of electrons in disordered metals has evoked considerable theoretical and experimental interest in the last decade.[1,2] A complete understanding of the complicated interplay of the disorder and electron-electron interactions, however, has not yet emerged. The latest theoretical advances in understanding the effects of disorder-enhanced Coulomb interactions are the theories of Finkelshtein,[3] and Castellani and co-workers.[4,5] These theories have pointed out the special importance of spin fluctuations near the metal-insulator transition. They predict a strong enhancement of the spin susceptibility at low temperatures, and an equivalent suppression of the spin-diffusion constant.

Uncompensated doped semiconductors, and in particular, phosphorus-doped silicon (Si:P) are useful systems for studying the properties of disordered interacting electrons. The linewidth of an electron-spin-resonance (ESR) experiment on Si:P will be sensitive to any spin-flip scattering in the system, and is therefore a useful probe of the electron spin dynamics. In this paper I will develop a theory for the additional linewidth from spin-flip scattering from impurity nuclei. The theory will be particularly relevant for Si:P where the dominant source of the linewidth at very low temperatures is spin-flip scattering from the phosphorus nuclei. However, the formulation of the theory is general enough to be applicable to other disordered systems with nuclear spin-flip scattering. The results of the analysis are consistent with a recent experiment in Si:P.[6]

The Hamiltonian of the system is

$$H = H_0 + C\sum_i \mathbf{I}_i\cdot\mathbf{S}(\mathbf{r}_i) \;, \tag{1}$$

where H_0 is the Hamiltonian for electrons interacting via Coulomb forces moving in a random spin-independent potential, $\mathbf{I}_i$ is the nuclear spin (assumed to be spin $\frac{1}{2}$) at the site $\mathbf{r}_i$, $\mathbf{S}(\mathbf{r})$ is the electron spin-density operator, and C is the coupling constant. At room temperatures, the electrons will pass by the nuclear spin at the Fermi velocity, leading to a motionally narrowed linewidth. In this paper it is shown, to lowest order in disorder and interactions, that accompanying the slowing down of the spin diffusion and the enhancement of the spin susceptibility, there is a decrease in the amount of motional narrowing. This leads to a broadening of the ESR linewidth as the temperature is lowered. The broadening is associated with the enhanced probability of a diffusing electron returning to a given nuclear spin within a single dephasing time. Upon returning to this nuclear spin, the electron will not see a random nuclear-spin direction, leading to a decrease in the amount of motional narrowing. Unusual effects on the ESR experiment have also been reported in *insulating* phosphorus-doped silicon[7] and can be well understood in terms of the slowing down of spin diffusion.[8]

Hikami, Larkin, and Nagaoka[9] and Altshuler and Aronov[10] have pointed out that in considering the effects of the particle-hole ladder (the diffusion propagator), it is necessary to split the various spin combinations of the electron and hole into a singlet and a triplet. At room temperatures the ESR linewidth in a weak magnetic field H ($H \ll T$, where T is the temperature; this will be assumed throughout) is proportional to the "mass" in the triplet diffusion propagator. This may be calculated by summing the diagrams in Fig. 1 for the particle-hole ladder L (the dashed lines represent normal impurity scattering without spin flip, and the dotted lines are Abrikosov's pseudofermion propagators for the impurity spin fluctuations[11]).

$$L_{\alpha\beta\gamma\delta} = \tfrac{1}{4}(L_s + 3L_t)\delta_{\alpha\beta}\delta_{\delta\gamma} + \tfrac{1}{4}(L_s - L_t)\boldsymbol{\sigma}_{\alpha\beta}\cdot\boldsymbol{\sigma}_{\delta\gamma} \,, \tag{2}$$

where $\boldsymbol{\sigma}$ are the Pauli spin matrices. L_s and L_t are the singlet and the triplet diffusion propagators:

$$L_s = \frac{1}{Dq^2 + |\omega_n|}\,, \quad L_t = \frac{1}{(4/\tau_s^0) + Dq^2 + |\omega_n|} \;. \tag{3}$$

Here q and ω_n are the momentum and frequency carried by the diffusion propagator. (We are using the Matsubara finite-temperature formalism.) The mass in L_t, $4/\tau_s^0$ is $2\pi n_i (C/2)^2 N_1$, where n_i is the density of nuclear spins and N_1 is the density of states at the Fermi level.

This paper calculates corrections to $4/\tau_s^0$ from disorder and Coulomb interactions. Analogous effects have been considered earlier for the *noninteracting* problem. Oppermann[12] has analyzed corrections to the magnetic-field dephasing time. Recently Wegner[13] has independently calculated the renormalization of the spin-flip scattering rate from disorder alone. We show here that there are strong temperature-dependent corrections to $4/\tau_s^0$ which arise from the Coulomb interactions. For Si:P, these are the dominant effects and yield useful information on the electron-spin dynamics. The corrections to $4/\tau_s^0$ from the

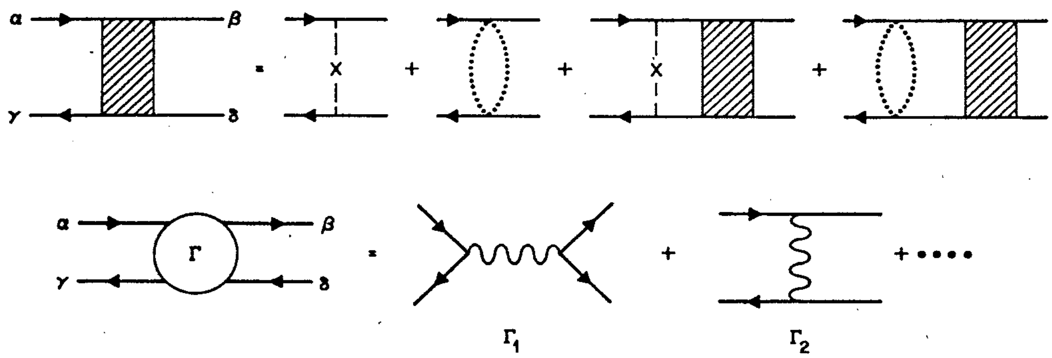

FIG. 1. The particle-hole diffusion ladder (top) and the generalized interaction amplitude between the particle and hole (bottom). The dashed lines represent potential scattering, the dotted lines are impurity spin fluctuations, and the wavy line is the Coulomb interaction.

disorder-enhanced Coulomb interactions yield the expression

$$\frac{4}{\tau_s}=\frac{4}{\tau_s^0 f}[1+G_1(T)] \ . \tag{4}$$

The constant f arises from Fermi-liquid theory and $G_1(T)$ varies rapidly with temperature. In two dimensions $G_1(T)$ behaves like $|\ln(T\tau)|$, where τ is the elastic scattering time, provided $T\tau \ll 1$ and $T\tau_s \gg 1$. We parametrize the corrections to the spin susceptibility in a similar manner:

$$\chi_s=\chi_P[f+G_2(T)] \ , \tag{5}$$

where χ_P is the Pauli susceptibility and $G_2(T)$ is strongly temperature dependent. To all orders in the interaction, $G_1(T)$ and $G_2(T)$ involve only the triplet-scattering amplitude Γ_t and are independent of the singlet interaction Γ_s. (Here, and in the rest of the paper, we will use the notation of Castellani, DiCastro, Lee, and Ma.[4]) To lowest order in Γ_t, $G_1(T)$ and $G_2(T)$ are identical. Since the corrections to the spin-diffusion constant are simply related to the enhancement of the susceptibility,[3,5] this is physically appealing because it relates the broadening of the line to the slowing down of spin diffusion. All of the above conclusions are valid only in the limit $T\tau_s \gg 1$ and to lowest order in the disorder parameter $1/E_F\tau$.

Some details of the derivation of Eqs. (4) and (5) will now be presented. This will be followed by a calculation of the corrections to $4/\tau_s^0$ from disorder alone. For clarity, details of the calculations of the effect of Coulomb interactions will be presented only to lowest order. The Coulomb interactoions are described by a generalized interaction amplitude Γ between the particle and hole:

$$\Gamma_{\alpha\beta\gamma\delta}=\tfrac{1}{4}(\Gamma_s+3\Gamma_t)\delta_{\alpha\beta}\delta_{\delta\gamma}+\tfrac{1}{4}(\Gamma_s-\Gamma_t)\sigma_{\alpha\beta}\cdot\sigma_{\delta\gamma} \ , \tag{6}$$

where Γ_s and Γ_t are the singlet and triplet interaction amplitudes. These are related to the direct and exchange interactions in Fig. 1 by $\Gamma_s=2\Gamma_1-\Gamma_2$ and $\Gamma_t=-\Gamma_2$. (Note that these definitions differ from those of Ref. 4 by a factor of 2.)

The corrections to the diffusion propagator arise from interactions which do not involve an exchange of energy between the particle and the hole.[4] Graphs for the self-energy $\Sigma(q,\omega_n)$ to lowest order in $1/E_F\tau$ are shown in Fig. 2. Representation of the spin-flip scattering by Abrikosov's pseudofermions now emphasizes the fact that the correlations between different scatterings arise from

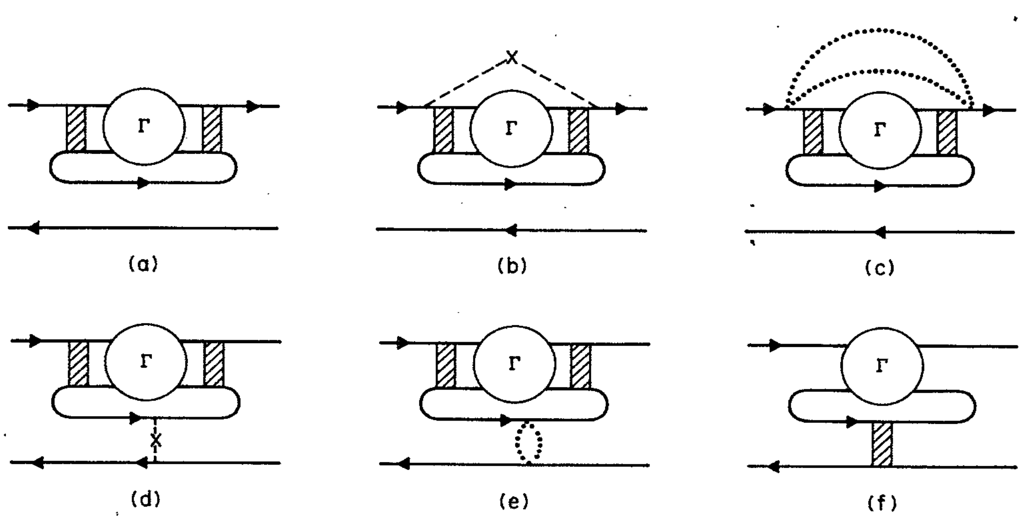

FIG. 2. Diagrams involving electron-electron interactions with a singular contribution to the self-energy of the diffusion propagator.

tracing over the nuclear-spin variables and not from averaging over the positions of the impurities.

The corrections from these graphs to coefficients of q^2 and ω_n are identical to those of Ref. 4 in the limit $\tau/\tau_s \ll 1$. Number conservation constrains Σ to vanish for $q=0$ and $\omega_n=0$.[14] In the presence of spin-flip scattering, however, this only constrains the singlet part to Σ and the triplet part can be nonzero. For $q=0$ and $\omega_n=0$, Figs. 2(a)–2(e) yield

$$\Sigma^{\mathrm{a-e}}_{\alpha\beta\gamma\delta}=-T\sum_{\Omega}\int\frac{d^dp}{(2\pi)^d}\left[\left(Dp^2+\Omega+\frac{3}{\tau_s^0}\right)[\Gamma_s L_s^2(p,\Omega)+3\Gamma_t L_t^2(p,\Omega)]\delta_{\alpha\beta}\delta_{\delta\gamma}-\frac{1}{\tau_s^0}[\Gamma_s L_s^2(p,\Omega)-\Gamma_t L_t^2(p,\Omega)]\sigma_{\alpha\beta}\cdot\sigma_{\delta\gamma}\right]. \tag{7}$$

Figure 2(f) yields in a similar manner

$$\Sigma^{\mathrm{f}}_{\alpha\beta\gamma\delta}=T\sum_{\Omega}\int\frac{d^dp}{(2\pi)^d}\{\tfrac{1}{4}(\Gamma_s+3\Gamma_t)[L_s(p,\Omega)+3L_t(p,\Omega)]\delta_{\alpha\beta}\delta_{\sigma\gamma}+\tfrac{1}{4}[\Gamma_s-\Gamma_t][L_s(p,\Omega)-L_t(p,\Omega)]\sigma_{\alpha\beta}\cdot\sigma_{\delta\gamma}\}. \tag{8}$$

In the limits $T\tau_s \gg 1$ and $\tau \ll \tau_s$, we can expand L_t in terms of L_s and $1/\tau_s$ to obtain the following expression for the total Σ.

$$\Sigma_{\alpha\beta\gamma\delta}=-T\sum_{\Omega}\int\frac{d^dp}{(2\pi)^d}\left[L_s^2(p,\Omega)(\Gamma_s-\Gamma_t)\times\left(\frac{6}{\tau_s}\delta_{\alpha\beta}\delta_{\delta\gamma}-\frac{2}{\tau_s}\sigma_{\alpha\beta}\cdot\sigma_{\delta\gamma}\right)\right]. \tag{9}$$

This is the diffusion propagator self-energy for zero momentum and frequency. It depends upon both the singlet and the triplet scattering amplitudes. Note that the singlet part of Σ vanishes as one would expect from number conservation. Using the known results for $\Sigma(q,\omega_n)$ for small q and ω_n from Ref. 4, the renormalization of the singlet and the triplet diffusion propagators can now be written:

$$L_s=\frac{\xi^2}{D'q^2+z|\omega_n|},\qquad L_t=\frac{\xi^2}{\frac{4}{\tau_s^0}\mu+D'q^2+z|\omega_n|}. \tag{10}$$

The diffusion constant D has been changed to D', z is a renormalization of the frequency scale, and ξ is a diffusion propagator "wave-function" renormalization. The renormalization of the spin-flip scattering time is given by μ which is

$$\mu=1+8T\sum_{\Omega}\int\frac{d^dp}{(2\pi)^d}\Gamma_2L_s^2(p,\Omega)=4t\Gamma_2|\ln(T\tau)|, \tag{11}$$

where the last equality is valid only in two dimensions and $t=1/4\pi^2N_1D$. Note that all the corrections involving the singlet interaction amplitude which appeared in the self-energy have been completely absorbed in the ξ, and μ only involves the triplet interaction amplitude. Using the techniques in Ref. 4, the calculation for μ can be generalized to yield the following expression which is correct to lowest order in t but to all orders in the interactions,

$$\mu=1+4t\ln\left(\frac{z+\Gamma_2}{z}\right)|\ln(T\tau)|. \tag{12}$$

In perturbation theory, an expression for μ to lowest order in t can be obtained simply by replacing z by 1 in Eq. (12). A renormalization-group equation for μ can also be developed from Eq. (12). Such an analysis suffers from the same difficulties as in Ref. 5: The parameters flow to a strong-coupling regime where the renormalization-group equations are no longer valid, making quantitative predictions difficult. However, if the temperature is large enough, these strong-coupling effects will not have appeared and the renormalization of the spin-flip time will be well described by the perturbation-theory expression in Eq. (12). Using the diffusion propagators in Eq. (9), the wave-vector- and frequency-dependent susceptibility χ_s can be calculated (the renormalization of all quantities is to the lowest nontrivial order in τ/τ_s):

$$\chi_s(q,\omega_n)=\chi_P(z+\Gamma_2^R)\frac{D'/(z+\Gamma_2^R)q^2+\mu/(z+\Gamma_2^R)(4/\tau_s^0)}{D'/(z+\Gamma_2^R)q^2+|\omega_n|+\mu/(z+\Gamma_2^R)(4/\tau_s^0)}. \tag{13}$$

The quantity Γ_2^R is the renormalized value of Γ_2, including a wave-function renormalization. The enhancement of the susceptibility is $z+\Gamma_2^R$. The measured linewidth is $4/\tau_s^0[\mu/(z+\Gamma_2)]$ and yields

$$G_1(T)=2t[2\ln(1+\Gamma_2)-\Gamma_2]|\ln(T\tau)| \tag{14}$$

in perturbation theory to lowest order in t and all orders in Γ_2 after using the known results for $(z+\Gamma_2^R)$.[3–5] This will predict an enhancement of the spin-flip relaxation rate provided the bare Γ_2 is not too large. To lowest order in Γ_2 we also find that $G_2(T)=G_1(T)$, as claimed earlier.

Lastly, the small corrections from the disorder alone are considered. The graphs in Fig. 3 yield logarithmic contributions to $\Sigma(q=0,\omega_n=0)$ near two dimensions, leading to the following corrections to the spin-flip rate:

$$\frac{4}{\tau_s}=\frac{4}{\tau_s^0}\left(1+\frac{1}{\pi N_1}\int\frac{d^dp}{(2\pi)^d}\frac{1}{Dp^2+1/\tau_{e\text{-}e}}\right). \tag{15}$$

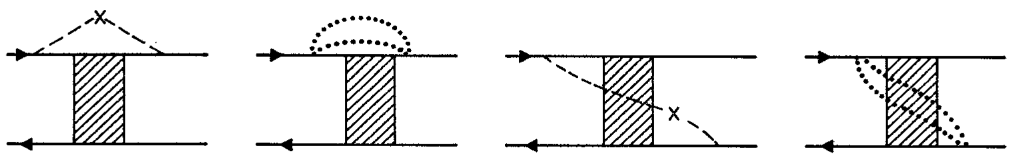

FIG. 3. The self-energy of the diffusion propagator in the absence of Coulomb interactions.

The quantity $1/\tau_{e\text{-}e}$ is the inelastic scattering time and we have assumed $\tau_{e\text{-}e}^{-1} \gg \tau_s^{-1}$. The contributions from these graphs to $\Sigma(q \neq 0, \omega_n)$ cancel among each other to lowest order in q^2 and do not effect the well-known weak localization corrections to the diffusivity. To lowest order in $1/E_F\tau$, the correction to the spin-flip rate in Eq. (15) is just the inverse of the weak localization correction to the diffusivity.[15] Thus, as we found for the interaction corrections, the ESR line broadening and the slowing down of diffusion are closely related.

To conclude, we have shown that associated with the slowing down of the spin diffusion, there is an enhancement of the ESR linewidth and its magnitude has been calculated. Unlike the experiments on *nuclear*-spin relaxation,[16] it is possible to perform ESR in a very weak magnetic field and not perturb significantly the physics of the disordered interacting electron system. In addition to the recent experiment in Si:P (Ref. 6), ESR experiments on other systems will be of great interest.

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