Excitation of paramagnetic impurities by a tunneling electron

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The additional current produced in a metal-dielectric-metal system by interaction of the electrons with a disordered system of paramagnetic impurities is calculated. It is shown that the specific constants of this interaction can be determined by investigating the singularities in the dependence of the differential conductivity on the voltage. The self-energy contributions connected with the inelastic tunneling are analyzed.

Study of the interaction of electrons with paramagnetic impurities has led to an explanation of the nature of the zero-point anomalies in tunnel junctions (see, e.g., [1,2]). It is typical that in all the studies devoted to this question they considered the case of an isolated impurity. A very interesting result is that the contribution to the tunnel current from the paramagnetic impurity depends in oscillating fashion on its location in the junction[3]. The fact that the period of the oscillations is close to the atomic period is cause for some suspicion, inasmuch as in the real situation the impurities have a random distribution and this raises the question whether their averaging over the distribution leads to a significant change in the order of magnitude of the quantities. We therefore consider here the case when the impurities are randomly distributed in one of the junctions of the electrode and in the region located in the immediate vicinity of this electrode. In addition, we assume that the impurity concentration is large enough to establish ferro- or antiferromagnetic ordering between the impurities via indirect exchange. This case has not been considered in the past (with the exception of the case of ferromagnetic metals[4]). It appears that the reason is that ordering removes the characteristic temperature logarithm. Nonetheless, as will be shown below, tunneling also makes it possible to obtain sufficiently detailed information in this case on the interaction of the electrons with the impurities and on the specific constants of this interaction.

The action of impurities on a tunneling electron proceeds via two channels: 1) "dressing" of the electrons (the current connected with this channel makes it possible to investigate the dependence of the electron self-energy part on the frequency); 2) inelastic tunneling with excitation of the impurity; this tunneling has a threshold character (it appears at ev $>$ u, where v is the voltage on the junction and u is the internal field).

It is important to emphasize that the impurities inside the metal and in the barrier region play different roles. The impurities inside the metal "prepare" the electronic states, i.e., they lead to the "dressing" of the electrons. The role of impurities inside the barrier, on the other hand, reduces to the possibility of acquiring magnetic moment and energy from the tunneling electrons, so that the total spin moment and energy in the electron-plus-impurity system remain the same before and after the tunneling.

It is interesting to note that the different contributions to the current, connected with the "dressing" and with inelastic tunneling, can be separated by investigating the conductivity components that are even and odd in ev.

GENERAL RELATIONS

We assume that the conduction electrons in a tunnel junction consisting of two bulky metals and an insulating interlayer interact in exchange fashion with the paramagnetic impurities. It is easy to write out the Hamiltonian for such a system in the approximation of Zener's "s–d exchange" model[5]:

$$H=\int d\mathbf{r}\psi_s^+(\mathbf{r})\left[\frac{\mathbf{p}^2}{2m}\delta_{ss'}+U(r)\delta_{ss'}-\frac{J}{n}\sum_j\sigma_{ss'}\mathbf{S}_j\delta(\mathbf{r}-\mathbf{r}_j)\right]\psi_{s'}(r), \quad (1)$$

where $\psi_s^+(\mathbf{r})$ and $\psi_s(\mathbf{r})$ are respectively the operators for the creation and annihilation of a particle with spin s at the point $\mathbf{r}$, $U(\mathbf{r})$ is the potential of the barrier, J is the exchange-interaction constant of the spin S of the impurity and of the electron spin, σ are Pauli matrices, and n is the electron concentration.

Following the method used in[6,7], we break up the Hamiltonian into a Hamiltonian for the left-hand and right-hand electrons and the interaction Hamiltonian. In addition to the usual interaction term $H_{T0} = A_0 + A_0^+$ of[8], there appears here an additional term connected with the tunneling due to the paramagnetic impurities:

$$H_{T1}=A_1+A_1^+=-\frac{J}{n}\sum_j\int d\mathbf{r}\psi_{sl}^+(\mathbf{r})\sigma_{ss'}\mathbf{S}_j\delta(\mathbf{r}-\mathbf{r}_j)\psi_{s'r}(\mathbf{r})+\text{H.c.}$$

The operators ψ_{sl} and ψ_{sr} are those parts of the total operator ψ_s which are responsible for the annihilation of the electrons in the left-hand and right-hand metals.

Just as in[6], we obtain for the tunnel current from the left-hand metal to the right-hand one:

$$I=-2e\,\mathrm{Im}\int_{-\infty}^{\infty}dt\,e^{ievt}i\theta(t)\langle[A_T^+(t),A_T(0)]_-\rangle. \quad (2)$$

here the angle brackets denote averaging over the equilibrium ensemble of the noninteracting subsystems, $A_T^+(t)$ is the operator $A_T^+ = A_0^+ + A_1^+$ in the interaction representation, and $\theta(t)$ is the Heaviside function.

Let us examine in greater detail the kernel of the integrand in (2). We express it as a sum of three terms:

$$i\theta(t)\langle[A_T^+(t),A_T(0)]_-\rangle=K_{00}(t)+[K_{10}(t)+K_{01}(t)]+K_{11}(t). \quad (3)$$

The term with K_{00} leads here to the usual tunnel current I_{00}. The increments containing K_{10} and K_{01} are due to the imposition of different tunneling mechanisms (elastic and inelastic). The contribution made to the current by these terms will be designated I_{10}. Finally, the last term in (3) leads to a purely inelastic contribution to the tunnel current with excitation of the impurity (I_1). The currents I_{10} and I_{11} are due to taking the interaction of the electron spins with the impurity spin system into account. For a direct calculation of all these currents it is useful

to make use of the possibility of constructing the Fourier component of the function K(t) by analytically continuing, into the upper half-plane, the temperature Green's function $K^c(\omega_0)$ (see, e.g., [6]), considered on the imaginary time axis from $i\beta$ to $-i\beta$ (ω_0 runs through a discrete set of values $\omega_0 = i\cdot 2\pi n/\beta$, where β is the reciprocal temperature). With this in mind, we determine the expansion of the Green's function $K^c(t)$ in a Fourier series:

$$K^c(t)=i\beta^{-1}\sum_{\omega_0}e^{-i\omega_0 t}K^c(\omega_0)=\frac{1}{i}\langle TA_T^+(t)A_T(0)\rangle,$$

$$K^c(\omega_0)=\int_0^{-i\beta}dt\,e^{i\omega_0 t}K^c(t).$$

Here T is the operator of ordering along the imaginary axis $-\beta \le it \le \beta$. The current I is now given by $I = -2e\,\mathrm{Im}\,K^c(ev + i\delta)$, where $\delta = +0$.

Calculating $K^c_{00}(\omega_0)$, we obtain

$$K_{00}^c(\omega_0)=\sum_{\mathbf{p},\mathbf{q}}|T_{\mathbf{pq}}|^2\sum_{\omega_{0'}}\mathrm{Sp}\,G_r(\mathbf{q},\omega_0')G_l(\mathbf{p},\omega_0'+\omega_0). \tag{4}$$

Here $G_l(\mathbf{p}, \omega_0)$ and $G_r(\mathbf{q}, \omega_0)$ are the single-particle electron Green's functions of the right-hand and left-hand metals in the absence of tunnel interaction between them; the trace is taken over the spin variables; the frequency ω_0 takes on only the odd values $i(2n + 1)\pi/\beta$; the matrix element is

$$T_{\mathbf{pq}}=\frac{1}{2m}\int d\mathbf{r}_\perp\left(\chi_{\mathbf{p}}^{+*}\frac{\partial\chi_{\mathbf{q}}^-}{\partial z}-\chi_{\mathbf{q}}^-\frac{\partial\chi_{\mathbf{p}}^{+*}}{\partial z}\right)\Big|_{z=0}.$$

The wave functions $\{\chi^{\pm}_{\mathbf{p}}\}$ are the single-particle electronic states with the aid of which the breakdown into left-hand (−) and right-hand (+) electrons is made possible.

We consider below the case of an asymmetrical tunnel junction, which is realized, as a rule, in experiment. The point is that even if the junction consists of identical metals, present-day technology results in considerable asymmetry. It is therefore of interest to consider the extremely asymmetrical case when the impurities are located in only one of the metals (for the sake of argument, in the left-hand metal) and in the insulator region directly adjacent to this metal. The Green's function for the right-hand metal is therefore independent of the spin variables, and the Green's function of the left-hand electrons can be conveniently subdivided into two parts, one spin-dependent and another spin-independent:

$$G_l(\mathbf{p},\omega_0)=G_0(\mathbf{p},\omega_0)+\boldsymbol{\sigma\tau}G_1(\mathbf{p},\omega_0), \tag{5}$$

where $\boldsymbol{\tau}$ is the direction of ordering of the impurities. For the functions $G_0(\mathbf{p}, \omega_0)$ and $G_1(\mathbf{p}, \omega_0)$ there exists a spectral representation [9]

$$G_{0,1}(\mathbf{p},\omega_0)=\int\frac{d\omega}{2\pi}\frac{A_{0,1}(\mathbf{p},\omega)}{\omega_0-\omega}, \tag{6}$$

where the integration is carried out along the real axis and the spectral intensities A_0 and A_1 on the integration contour satisfy the inequalities $A_0 > A_1 > 0$.

Carrying out the summation with respect to ω_0 and with respect to the spin orientations in (4), with the representations (5) and (6) taken into account, we obtain for I_{00} the expression

$$I_{00}=2e\sum_{\mathbf{p},\mathbf{q}}|T_{\mathbf{pq}}|^2\int\frac{d\omega}{2\pi}A_r(\mathbf{q},\omega)A_0(\mathbf{p},\omega+ev)[f(\omega)-f(\omega+ev)]. \tag{7}$$

Here $f(\omega)$ is the Fermi distribution function and $A_r(\mathbf{q}, \omega)$ is the spectral intensity of the Green's function of the right-hand metal. It is important that the self-energy effects are contained in the spectral intensity $A_0(\mathbf{p}, \omega)$.

Before we calculate the quantities A_0, let us consider the interference and inelastic contributions to the tunnel current. For the calculation it is necessary to use the easily proved relation

$$K_{01}^{c*}(\omega+i\delta)=K_{10}^c(\omega-i\delta), \tag{8}$$

which enables us to consider only the term with K_{10}. It is easy to find that

$$K_{10}(\omega_0)=\beta^{-1}\sum_{\mathbf{p},\mathbf{q},\omega_0'}A_{\mathbf{pq}}\,\mathrm{Sp}\,G_r(\mathbf{q},\omega_0'-\omega_0)\Sigma(\mathbf{p},\omega_0')G_l(\mathbf{p},\omega_0'),$$

where

$$A_{\mathbf{pq}}=T_{\mathbf{pq}}C_{\mathbf{pq}}^*,\qquad C_{\mathbf{pq}}=\int d\mathbf{r}\,\chi_{\mathbf{p}}^{+*}(\mathbf{r})\chi_{\mathbf{q}}^-(\mathbf{r}),$$

The function $\Sigma(\mathbf{p}, \omega_0')$ is the self-energy part of the electrons in the left-hand metal and is determined by the equation

$$-\frac{J}{ni}\left\langle\!\!\left\langle\sum_j\delta(\mathbf{r}-\mathbf{r}_j)\sigma_{s\sigma}\langle T\mathbf{S}_j(t)\psi_\sigma(\mathbf{r},t)\psi_{s'}^+(\mathbf{r}',t')\rangle_l\right\rangle\!\!\right\rangle$$
$$=\int d\bar{\mathbf{r}}\,d\bar{t}\,\Sigma(\mathbf{r},t;\bar{\mathbf{r}},\bar{t})G_l(\bar{\mathbf{r}},\bar{t};\mathbf{r}',t'), \tag{9}$$

where the double angle brackets denote averaging over the impurity disposition.

After summing over the frequencies and spin orientations in the expression for $K^c_{10}(\omega_0)$ and after analytic continuation to real frequencies with allowance for (8), we obtain the following relation for the interference contribution to the tunnel current:

$$I_{10}=-8e\sum_{\mathbf{p},\mathbf{q}}(\mathrm{Re}\,A_{\mathbf{pq}}\int\frac{d\omega_1\,d\omega_2}{(2\pi)^2}[f(\omega_1)-f(\omega_1+ev)]A_r(\mathbf{q},\omega_1)$$
$$\times\left[A_0(\mathbf{p},\omega_2)\,\mathrm{Im}\frac{\Sigma_0(\omega_1+ev+i\delta)}{\omega_1-\omega_2+ev+i\delta}+A_1(\mathbf{p},\omega_2)\,\mathrm{Im}\frac{\Sigma_1(\omega_1+ev+i\delta)}{\omega_1-\omega_2+ev+i\delta}\right]. \tag{10}$$

Here Σ_0 and Σ_1 are connected with Σ by the relation

$$\Sigma=\Sigma_0+\boldsymbol{\sigma\tau}\Sigma_1.$$

To calculate the inelastic contribution I_{11} to the tunnel current, it is necessary to calculate K_1, for which we can obtain the expression

$$K_{11}(t)=\left(\frac{J}{n}\right)^2\frac{1}{i}\left\langle\!\!\left\langle\sum_{j,k}\int d\mathbf{r}_1\,d\mathbf{r}_2\delta(\mathbf{r}_1-\mathbf{r}_j)\delta(\mathbf{r}_2-\mathbf{r}_k)\right.\right.$$
$$\left.\left.\times\mathrm{Sp}\langle T\mathbf{S}_j(t)\boldsymbol{\sigma}S_k^\beta\psi(\mathbf{r}_1,t)\psi^+(\mathbf{r}_2,0)\rangle_l\right\rangle\!\!\right\rangle\sigma^\beta G_r(\mathbf{r}_2,0;\mathbf{r}_1,t).$$

This relation can be greatly simplified by expressing K_{11} in terms of the spectral intensities and the self-energy parts of the electrons. To this end it is necessary to generalize the definition of the Green's function in the following manner:

$$G_l(11',\mathrm{U})=-i\langle TP\psi_s(\mathbf{r},t)\psi_{s'}(\mathbf{r}',t')\rangle/\langle TP\rangle. \tag{11}$$

The operator P is determined by the equation

$$P=\exp\{-i[\mathbf{S}(1)\mathbf{U}(1)]\}, \tag{12}$$

where summation or integration is carried out with respect to the repeated variables (j, $\mathbf{r}$, t) over the entire range of variation of these quantities (from 0 to $-i\beta$ with respect to time), i.e.,

$$S^\alpha(1)=S_j^\alpha(t),\quad U^\alpha(1)=U_j^\alpha(t);$$
$$\mathbf{S}(1)\mathbf{U}(1)=\sum_j\int_0^{-i\beta}dt\,\mathbf{S}_j(t)\mathbf{U}_j(t),$$

$\mathbf{U}_j^\alpha(t)$ is an arbitrary vector function of the time and of the number of the impurity.

Using the definitions (11) and (12), we can easily reduce K_{11} to the form

$$K_{11}(t,t')=-i\,\mathrm{Sp}\,V(1'-2)\Big[\mathbf{M}(2)+i\frac{\delta}{\delta U(2)}\Big]\tilde{\Sigma}(1\bar{1})G_l(\bar{1}1')\sigma G_r(1'1). \quad (13)$$

In this relation it is not necessary to integrate with respect to the times t and t', and the quantity $V(1-2)$ is given by

$$V(1-2)=-\frac{J}{n}\delta(t-t_2)\delta(\mathbf{r}-\mathbf{r}_j);$$

The self-energy part $\tilde{\Sigma}(1\bar{1})$ is taken prior to averaging over the impurity distribution, and $\mathbf{M}(2)$ is determined with the aid of the variation derivative

$$\mathbf{M}(2)=i\frac{\delta}{\delta\mathbf{U}(2)}\ln\langle TP\rangle.$$

The functional $\tilde{\Sigma}$, which enters in (13), satisfies the equation

$$\tilde{\Sigma}(11')=\delta(1-1')V(1-2)\mathbf{M}(2)\sigma+i\frac{\delta\tilde{\Sigma}(1\bar{1})}{\delta\mathbf{U}(2)}G_l(\bar{1}1')\sigma V(2-1').$$

Using this relation and the equation for the Green's function G_l, we obtain the following expression for K_{11} after averaging over the disposition of the impurities:[1)]

$$K_{11}(t,t')=-i\,\mathrm{Sp}\,\Sigma(1\bar{1})G_l(\bar{1}2)G_{0l}^{-1}(21')G_r(1'1). \quad (14)$$

Here, as in (22), the times t and t' are free, G_{0l} is the Green's function of the left-hand metal without allowance for the interaction with the paramagnetic impurities, and Σ is given by (9), i.e., it is taken after averaging over the disposition of the impurities.

The relation for K_{11} can be further simplified by using an approximation customarily employed in tunneling theory, wherein the Green's function of the semi-bounded metal is replaced by the corresponding Green's function of the bulky metal[2)]. This procedure must be carried out after changing over to the $\mathbf{p}$, $\mathbf{q}$ representation with the aid of the states $\chi_{\mathbf{p}}^{+}$ and $\chi_{\mathbf{q}}^{-}$. We actually arrive in this case at the picture of an interaction between two metals that are on different "sheets" of three-dimensional space. This circumstance was first noted by Kulik and Yanson[10]. As a result of this approximation we obtain for K_{11} the relation

$$K_{11}(\omega_0)=\beta^{-1}\sum_{\omega_0',\mathbf{p},\mathbf{q}}|C_{\mathbf{pq}}|^2\,\mathrm{Sp}\,G_r(\mathbf{p},\omega_0')\Sigma(\mathbf{q},\omega_0+\omega_0')\times[1+G_l(\mathbf{q},\omega_0+\omega_0')\Sigma(\mathbf{q},\omega_0+\omega_0')]. \quad (15)$$

Summing over the frequencies in (15) and continuing this expression analytically to the real axis from the upper half of the complex ω_0 plane, we reduce the expression for I_{11} to the form

$$I_{11}=-2e\sum_{\mathbf{p},\mathbf{q}}|C_{\mathbf{pq}}|^2\int\frac{d\omega_1}{2\pi}A_r(\mathbf{p},\omega_1)[f(\omega_1)-f(\omega_1+ev)]\times\mathrm{Sp}\Big\{\mathrm{Im}\Sigma(\mathbf{q},\omega_1+ev+i\delta)\int\frac{d\omega_2}{2\pi}\Big[\frac{\Sigma(\mathbf{q},\omega_1+ev+i\delta)A_l(\mathbf{q},\omega_2)\Sigma(\mathbf{q},\omega_1+ev+i\delta)}{\omega_1+ev-\omega_2+i\delta}-\pi\delta(\omega_1+ev-\omega_2)\,\mathrm{Im}\,\Sigma(\mathbf{q},\omega_2+i\delta)A_l(\mathbf{q},\omega_2)\,\mathrm{Im}\,\Sigma(\mathbf{q},\omega_2+i\delta)\Big]\Big\}. \quad (16)$$

SPECTRAL INTENSITIES AND ELECTRONIC SELF-ENERGY PART

In the calculation of the spectral intensities one should distinguish between two cases: 1) ferromagnetic ordering of the impurity spins, 2) antiferromagnetic ordering. In the first case, the spectral intensities are connected with the self-energy parts by the relations

$$A_{0,1}(\mathbf{q},\omega)=-\frac{\mathrm{Im}\,\Sigma^{+}(\mathbf{q},\omega)}{(\omega-\xi-\mathrm{Re}\,\Sigma_{+}(\mathbf{q},\omega))^2+(\mathrm{Im}\,\Sigma_{+}(\mathbf{q},\omega))^2}\mp\frac{\mathrm{Im}\,\Sigma_{-}(\mathbf{q},\omega)}{(\omega-\xi-\mathrm{Re}\,\Sigma_{-}(\mathbf{q},\omega))^2+(\mathrm{Im}\,\Sigma_{-}(\mathbf{q},\omega))^2}, \quad (17)$$

where $\Sigma_{\pm}=\Sigma_0\pm\Sigma_1$.

The second case can be obtained from the first by putting $\Sigma_1 = 0$ in (17). The reason is that we confine ourselves below to an impurity antiferromagnet model in which the impurities are located, with equal probability, on arbitrary lattice sites of the main metal. It is assumed here that the effective magnetic moment at each impurity site has a definite direction, but there is no correlation between the directions of the magnetic moments at different sites, so that the average value of the macroscopic magnetization without the magnetic field is equal to zero. More complicated models, which take into account the correlation of the directions of the magnetic moments of different impurity sites (and which usually lead to nontrivial structures, for example of the helical or umbrella-shaped type), call for a special investigation. Preliminary results show that the main contribution to the tunnel current is not sensitive to the type of antiferromagnetic ordering.

The influence of ordering on the self-energy of electrons was considered by Kondo[11]. He has shown that in the case of antiferromagnetic ordering the effective mass of the electron on the Fermi surface is increased by several times (in comparison with the case of free electrons) as a result of interaction with the impurities. As noted by Abrikosov[12] the correction to the electron energy considered by Kondo is the first large term of a certain series containing powers of $JN(0)(\ln u/D)/n$, where N(0) is the state density on the Fermi surface, u is the energy of the impurity in the effective molecular field due to the indirect exchange, and D is a cutoff energy ($D \sim \mu$, where μ is the Fermi energy). We shall therefore present below an expression for Σ in which are summed all the terms containing, in each given order in the constant J, the highest degree of the large logarithm $\ln(u/D)$. It is assumed here that the inequalities $1/\beta \ll u \ll D$ are satisfied. The calculation of Σ can be formally carried out in two stages. In the first stage, account is taken of all the large terms without averaging over the random disposition of the impurities. As a result we get

$$\tilde{\Sigma}(\mathbf{r},\mathbf{r}',\omega_0)=\sum_i U_i(\mathbf{r},\mathbf{r}',\omega_0)=\delta(\mathbf{r}-\mathbf{r}')\sum_i\delta(\mathbf{r}-\mathbf{r}_i)\Sigma_i(\omega_0), \quad (18)$$

with

$$\Sigma_i(\omega_0)=-\frac{J}{2n}M\Big[\frac{1+\sigma\tau_i}{1-\lambda g(u+\omega_0)}+\frac{\sigma\tau_i-1}{1-\lambda g(u-\omega_0)}\Big]. \quad (19)$$

Here $\lambda = 2JN(0)/n = 3J/2\mu$, M is the modulus of the average value of the impurity spin ($\langle\mathbf{S}_i\rangle = \boldsymbol{\tau}_i M$, $\boldsymbol{\tau}_i^2 = 1$), and the function $g(u+\omega_0)$ is given by

$$g(u+\omega_0)=\int_{-\infty}^{\infty}d\omega\frac{f(\omega)+\nu(u)}{\omega-u-\omega_0}, \quad (20)$$

where $\nu(u)$ is the Bose distribution function. Since it is assumed that $\beta u \gg 1$, we can put $\nu(u) = 0$ in (20). The logarithmic divergence in (20) is cut off in the usual manner at $\omega = D$.

During the second stage of the calculations it is necessary to carry out averaging over the random distribution of the impurities. In this case it is assumed for the case of ferromagnetic ordering that the mean

values of the magnetic moments of the impurities are oriented in the same direction, i.e., all the τ_i are equal. A more general case would be, of course, the assumption that they are oriented with predominant probability in a certain direction τ, but such a generalization does not lead to qualitative differences, and the small quantitative differences are immaterial to us. As to the antiferromagnetic ordering, in this case averaging will also be carried out over the directions of the vectors τ_i. When averaging over the impurities, we sum all the diagrams (except the intersecting ones) that make a relative contribution of the order of $(p_0 l)^{-1}$ (p_0 is the Fermi radius and l is the mean free path, see[13]). The result for Σ can then be represented in the form

$$\Sigma(11') = c \int d\tau_i W_i \int d\mathbf{r}_i R_i(11'), \tag{21}$$

where c is the impurity concentration, W_i is the probability of orientation of the magnetic moment of the i-th impurity in a certain direction, and the quantity $R_i(11')$ satisfies the equation

$$R_i(11') = U_i(11') + U_i(1\bar{1}) G(\bar{1}\bar{2}) R_i(2\bar{1}'). \tag{22}$$

Here G(11′) is the averaged Green's function.

Inasmuch as in this case, as seen from (18), U_i contains two δ functions as factors, the equation can be solved relative to R_i. This circumstance is connected essentially with the choice of a local-type Hamiltonian (1) for the s-d interaction model. The solution for R_i is

$$R_i(\mathbf{r}, \mathbf{r}', \omega_0) = \delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{r}-\mathbf{r}_i)\Sigma_i(\omega_0)[1-\Sigma_i(\omega_0)G(0, \omega_0)]^{-1}. \tag{23}$$

Using relations (19), (21), and (23), we obtain after simple transformations an expression for Σ on the real ω axis:

$$\Sigma_0(\omega+i\delta) = F(\omega) - F^*(-\omega), \quad \Sigma_1(\omega+i\delta) = F(\omega) + F^*(-\omega). \tag{24}$$

The function $F(\omega)$ is equal to

$$F(\omega) = -\frac{JLS}{2}[1-\lambda g(u+\omega) - i\pi\lambda(f(u+\omega)+S/2)]^{-1}, \tag{25}$$

where L is the number of impurities per electron (L = c/n). In the derivation of (25) we used the fact that M = S when $\beta u \gg 1$.

It is seen from (25) and (24) that at $\omega < u$ the quantity Re Σ leads to a significant renormalization of the electron spectrum, and the damping is due entirely to the potential scattering by the impurities. When $\omega > u$, the renormalization of the electron energy decreases with increasing ω, and an additional contribution appears in the damping due to the inelastic scattering, inasmuch as in this frequency region the excess energy is already sufficient for the excitation of the impurity.

CONDUCTIVITY OF TUNNEL JUNCTION

The relations for the spectral intensities and for the self-energy make it possible to calculate the dependence of the differential conductivity of the junction ($\sigma = dI/dv$) on the applied voltage. Substituting all the necessary quantities in expression (7), we obtain after simple calculations the correction $\Delta\sigma_{00}$ that must be introduced in the conductivity as a result of the "dressing" of the electrons in the left-hand electrode:

$$\Delta\sigma_{00} = \sigma_0 \frac{\alpha}{\mu} \int dy \frac{\partial f(y)}{\partial y} \operatorname{Re}\Sigma_0(ev+y), \tag{26}$$

where σ_0 is the conductivity without allowance for the influence of the self-energy effects ($\sigma_{00} = \sigma_0 + \Delta\sigma_{00}$).

In the derivation of (26) we used the approximation proposed by Herman and Schmid[14] for the matrix element T_{pq}:

$$|T_{pq}|^2 = |T|^2\left(1+\alpha\frac{\xi_p+\xi_q}{\mu}\right),$$

where $\alpha = dp_0\sqrt{\mu/4w}$; d is the width of the barrier; w is the energy height; $|T|^2$ is the square of the matrix element $|T_{pq}|^2$ averaged over the angles of the vectors p and q taken on the Fermi surface, and ξ is the electron energy reckoned from the Fermi surface. The integral in (26) can be determined by an interpolation procedure that takes into account the smooth variation of the logarithm. The result for $\Delta\sigma_{00}$ can be then expressed in the form

$$\frac{\Delta\sigma_{00}(ev)}{\sigma_0} = \frac{\alpha L\lambda S}{3}[\Psi_1(ev) - \Psi_1(-ev)],$$

$$\Psi_1(ev) = \left[1 - \frac{\lambda}{2}\ln\frac{(ev+u)^2+\gamma^2\Theta^2}{D^2}\right] \tag{27}$$

$$\times\left\{\left[1-\frac{\lambda}{2}\ln\frac{(ev+u)^2+\gamma^2\Theta^2}{D^2}\right]^2 + \pi^2\lambda^2\left[f(ev+u)+\frac{S}{2}\right]^2\right\}^{-1},$$

where Θ is the temperature and γ is a constant ($\gamma \sim 1$).

The interference contribution to the conductivity can be calculated by using relation (10). Without going into details of this calculation, we note only that the result, from the point of view of the dependence of $\Delta\sigma_0$ on ev, coincides with expression (27) accurate to terms of order u/D. The contribution $\Delta\sigma_{10}$ turns out to be of the same order as $\Delta\sigma_{00}$. However, $\Delta\sigma_{10}$ is of opposite sign, so that the interference contribution cancels out the self-energy effects. This equality of form and the cancellation of $\Delta\sigma_{00}$ and $\Delta\sigma_{10}$ always occurs when the momentum dependence can be neglected in the electronic self-energy part, i.e., when this dependence is very weak in the vicinity of the Fermi surface. The cancellation is only partial, so that the order of magnitude remains the same as in (27), but a case of overcompensation is possible, and then the resultant sign is the opposite of that of $\Delta\sigma_{00}$. The result depends essentially on a comparison of two quantities of the same order, α/μ and $A_{pq}/|T_{pq}|^2$ (A_{pq} and $|T_{pq}|^2$ are averaged over the angles on the Fermi surface). This phenomenon seems to explain the poor reproducibility of the antisymmetrical part of the conductivity $\Delta\sigma_a(ev)$ with respect to voltage in different samples made from the same experimental batch. As seen from the foregoing, slight changes in the shape of the barrier can lead to noticeable changes of $\Delta\sigma_a(ev)$. We emphasize that the antisymmetrical part of the conductivity $\Delta\sigma_a$ is the same, accurate to terms of order u/D, for ferromagnetic and antiferromagnetic ordering.

Figure 1 shows a plot of $\Delta\sigma_a$ against the relative variable x = ev/u at the different Θ for $u/D = 10^{-2}$, $\lambda = \pm 0.2$, S = 1, and S = 5. As seen from the figure, $\Delta\sigma_a$ has a rather sharp anomaly in its behavior in the vicinity of the point x = 1. In addition, the anomaly has a rather complicated variation with changing S. At small S, as seen from (27), the anomaly is proportional to S. On the other hand, if $S \gg \ln(D/\Theta)$, it decreases in proportion to S^{-1}. The curves plotted in Fig. 1 for S = 1 satisfy the condition that S be small, but S = 5 falls in a region intermediate between the two limiting cases. It is also important to note that the sign of $\Delta\sigma_a$ changes with the sign of the interaction constant, and it is typical that the effect becomes more strongly pronounced (other conditions being equal) for the antiferromagnetic constant of

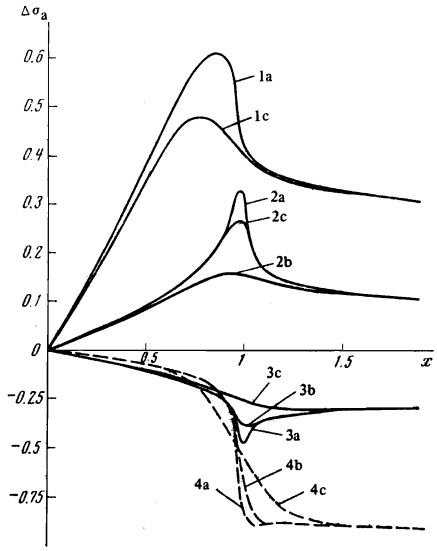

FIG. 1. Dependence of $\Delta\sigma_a$ (in relative units) on x: curves: 1) $\lambda = -0.2$, S = 1; 2) $\lambda = -0.2$, S = 5; 3) $\lambda = 0.2$, S = 1; 4) $\lambda = 0.2$, S = 5. The symbols a, b, and c on this and all other figures correspond to Θ/D of 10^{-5}, 10^{-4}, and 10^{-3}, respectively.

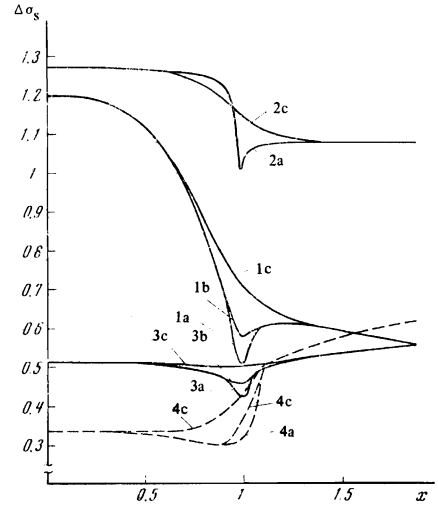

FIG. 2. Dependence of $\Delta\sigma_S$ (relative units) on x ($D \gg JLS$); curves: $1-\lambda = -0.2$, S = 1; $2-\lambda = -0.2$, S = 5; $3-\lambda = 0.2$, S = 5; $4-\lambda = 0.2$, S = 1 (the values of this function are magnified 10 times).

the interaction between the impurities and the electrons[3].

Let us estimate now the contribution made to the conductivity by the term I_{11}. This term produces a conductivity increment $\Delta\sigma_S$ which is symmetrical in the voltage. It is convenient to carry out the analysis in two limiting cases, weak localization of the d electrons, such that the quantity D, which has the meaning of the width of the d-band, satisfies the inequality $D \gg LSJ$. We can then neglect in (16) the term containing the double integration with respect to the frequencies, and the result for $\Delta\sigma_S$ takes the form

$$\frac{\Delta\sigma_s(ev)}{\sigma_0} \approx \frac{4D\alpha^2}{\pi\mu^2}\int dy \frac{\partial f(y)}{\partial y} \operatorname{Im}\Sigma_0(ev+y). \qquad (28)$$

Since the quantity $\Delta\sigma_S$ is connected only with Σ_0, which is the same for any type of ordering, $\Delta\sigma_S$ is insensitive to the character of the ordering in this limiting case, as is also $\Delta\sigma_a$. The integral in (28) can be evaluated with the same accuracy with which formula (27) was derived, i.e.,

$$\frac{\Delta\sigma_s(ev)}{\sigma_0} \approx \frac{4D\alpha^2}{3\pi\mu} LS\lambda[\Psi_2(ev)+\Psi_2(-ev)],$$

where

$$\Psi_2(ev) = \pi\lambda\left[f(ev+u)+\frac{S}{2}\right]\left\{\left[1-\frac{\lambda}{2}\ln\frac{(ev+u)^2+\gamma^2\Theta^2}{D^2}\right]^2 + \pi^2\lambda^2\left[f(ev+u)+\frac{S}{2}\right]^2\right\}^{-1}.$$

We note that the existence of known dispersion relations between the imaginary and real parts of Σ leads in this case to an integral relation of the same type between the symmetrical and antisymmetrical parts of the conductivity. From (28) and (26) we easily obtain

$$\Delta\sigma_a(ev) = \chi\int\frac{d\Omega\Delta\sigma_s(\Omega)}{\Omega-ev},$$

where $|\chi| \sim \mu/4\alpha D$. As to the sign of the coefficient χ, it depends on whether the interference term overcompensates for the self-energy term or not. If not, then $\chi > 0$.

Figure 2 shows a plot of $\Delta\sigma_S$ against the relative variable x at different temperatures, for $u/D = 10^{-2}$, $\lambda = \pm 0.2$, S = 1 and S = 5. As seen from this figure, the region where $\Delta\sigma_S$ changes substantially is located near the same values of the voltage at which an essential nonmonotonicity appears also in $\Delta\sigma_a$. However, since $\Delta\sigma_a$ has different signs at opposite current directions, it will add up with $\Delta\sigma_S$ in one case and be subtracted from it in the other, and consequently one of the quantities can be readily distinguished from the other in experiment. Another characteristic feature of this case is that the effect is much weaker for the ferromagnetic coupling constant.

We consider now the case of strong localization of the d electrons, when the inequality $D \ll LSJ$ is satisfied. In this limit, the principal term is the one containing the double integration with respect to the frequencies. After a number of transformations, we obtain

$$\frac{\Delta\sigma_s(ev)}{\sigma_0} \approx 2\frac{\alpha^2}{\mu^2}\int dy\left(-\frac{\partial f(y)}{\partial y}\right)\{[\operatorname{Re}\Sigma_+(y+ev)]^2+[\operatorname{Re}\Sigma_-(y-ev)]^2\}. \qquad (29)$$

It is easily seen that in this limit the function $\Delta\sigma_S(ev)$ is sensitive to the type of ordering. For ferromagnetic ordering, after an approximate calculation of the integral in (29), we get the expression

$$\Delta\sigma_s(ev)/\sigma_0 \approx (\alpha LS\lambda)^2[\Psi_1^2(ev)+\Psi_1^2(-ev)]. \qquad (30)$$

For antiferromagnetic ordering we have

$$\Delta\sigma_s(ev)/\sigma_0 \approx 1/2(\alpha LS\lambda)^2[\Psi_1(ev)-\Psi_1(-ev)]^2. \qquad (31)$$

Figure 3 shows, for comparison, plots of (30) and (31) for $\lambda = -0.2$. Similar plots are shown in Fig. 4 for $\lambda = +0.2$.

In conclusion, we estimate the orders of magnitude of the obtained quantities. For typical tunnel junctions, α reaches 30. The limiting impurity concentration at which ordering usually sets in is on the order of several percent, so that the product αL reaches values on the order of unity, and consequently the corresponding contributions to the conductivity can reach several percent. With modern techniques for the study of tunnel conductivity, one can register junction-conductivity changes on the order of $\sim 10^{-3}$—10^{-4} of the main conductivity. Thus, observation of the considered effects entails no noticeable difficulty. Much more important is a clear-cut discrimination between the even and odd parts of the conductivity. The point is that the derived expressions also

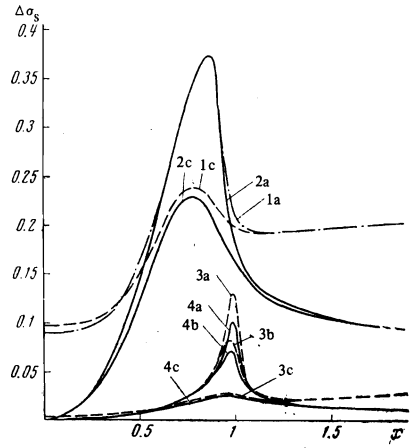

FIG. 3. Plot of $\Delta\sigma_s$ (relative units) against x ($D \ll JLS$) at $\lambda = -0.2$: 1, 2—at S = 1; 3, 4—at S = 5. Curves 1 and 3 are for ferromagnetic ordering and curves 2 and 4 for antiferromagnetic ordering.

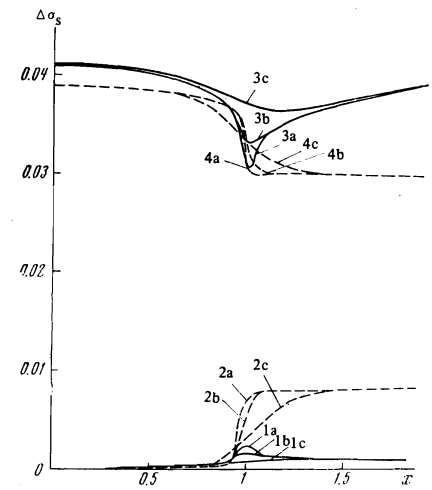

FIG. 4. Dependence of $\Delta\sigma_s$ (relative units) on x ($D \ll JLS$) at $\lambda = 0.2$; 1; 3—at S = 1, 2, 4—at S = 5. Curves 3, 4 are for ferromagnetic ordering and curves 1, 2 are for antiferromagnetic ordering. The values of the function 4 are decreased by a factor 10.

contain admixtures of a certain independence of the conductivity on the voltage, owing to the change in the transparency of the barrier with changing voltage. In all the calculations presented we have disregarded this dependence in view of its monotonic character and very smooth variation. A characteristic scale for this dependence is a voltage on the order of μ/e.

As seen from the derived expressions, the investigation of $\Delta\sigma_a$ and $\Delta\sigma_s$ enables us to measure the exchange-interaction constant, the impurity spin, the energy connected with the internal field, and the character of the ordering.

The authors are grateful to V. G. Bar'yakhtar for useful discussions and interesting remarks.

[1)]It is necessary to put U = 0 in (14), inasmuch as all the intermediate transformations have already been carried out, and U does not enter in the initial relation for K_{11}.

[2)]This approximation was also used to obtain the corresponding expressions for I_{00} and I_{10}.

[3)]The character of the ordering of the impurities in the metal is not determined uniquely by the sign of the constant J, i.e., either ferromagnetic or antiferromagnetic ordering is possible at either sign. The type of ordering is connected with more profound causes (for details see [12]).

[1] J. A. Appelbaum, Phys. Rev. **154**, 633, 1967.
[2] J. Sólyom and A. Zawadowski, Phys. Kondensierten Materie, **7**, 325, 342, 1968.
[3] J. A. Appelbaum and W. F. Brinkman, Phys. Rev. **2B**, 907, 1970.
[4] J. A. Appelbaum and W. F. Brinkman, Phys. Rev. **183**, 553, 1969.
[5] C. Zener, Phys. Rev. **81**, 440, 1951.
[6] Yu. M. Ivanchenko and Yu. V. Medvedev, Zh. Eksp. Teor. Fiz. **64**, 1023 (1973) [Sov. Phys.-JETP **37**, 520 (1973)].
[7] Yu. M. Ivanchenko, E. V. Kochergin, and Yu. V. Medvedev, Fiz. Tverd. Tela **15**, 1734 (1973) [Sov. Phys.-Solid State **15**, 1161 (1973)].
[8] M. H. Cohen, L. M. Falicov and J. C. Phillips, Phys. Rev. **8**, 316, 1962.
[9] L. Kadanoff and G. Baym, Quantum Statistical Mechanics, Benjamin, 1962.
[10] I. O. Kulik and I. K. Yanson, Éffekt Dzhozefsona v sverkhprovodyashchikh tunnel'nykh strukturakh (The Josephson Effect in Superconductive Tunnel Structures), Nauka, 1970.
[11] J. Kondo, Progr. Theor. Phys. **33**, 575, 1965.
[12] A. A. Abrikosov, Usp. Fiz. Nauk **97**, 403 (1969) [Sov. Phys.-Uspekhi **12**, 168 (1969)].
[13] A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskiĭ, Metody kvantovoĭ teorii polya v statisticheskoĭ fizike (Quantum Field Theoretical Methods in Statistical Physics), Fizmatgiz, 1962 [Pergamon, 1965].
[14] H. Herman and A. Schmid, Zs. Phys. **211**, 313, 1968.

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