sorption in the drops or by the cold screen. The position of this spectral region was linked directly to the magnetic induction B.[5,6] Thus, the absorption spectrum could be obtained by simple division of the photoresponse obtained as a result of the excitation of germanium by the photoresponse in the case of complete modulation of the background radiation and conversion of the magnetic induction to the photon energy or wavelength, corresponding to the selective sensitivity region at each value of B in accordance with Ref. 6. The spectral dependence of the absorption in the electron—hole drops calculated in this way is plotted in Fig. 4. This figure includes also the absorption spectrum of drops in germanium taken from the papers of Vavilov *et al.*[1,2] It is clear from the figure that the curves are similar although curve 1 was obtained using a cooled detector tuned by a magnetic field and curve 2 using a grating monochromator. In the former case the absorption could be interpreted as the radiation emitted from the electron—hole drops because of the absence of any source of absorbed radiation, apart from the room-temperature background.

We thus failed to observe submillimeter radiation of the electron—hole drops in germanium although we used highly sensitive photodetectors of two different types. Hence, we concluded that the intensity of the long-wavelength drop radiation emitted from germanium (if it existed at all) was several orders of magnitude weaker than that described by Vavilov *et al.*[1,2] However, the room-temperature background radiation passed through an excited germanium crystal and produced a large detector signal with a maximum in the plasma frequency region of the drops. This signal could be erroneously interpreted[1,2] as the radiation emitted from the drops.

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[1] V. S. Vavilov, V. A. Zayats, and V. N. Murzin, Pis'ma Zh. Eksp. Teor. Fiz. **10**, 304 (1969) [JETP Lett. **10**, 192 (1969)].
[2] V. A. Zayats, Tr. Fiz. Inst. Akad. Nauk SSSR **75**, 74 (1974).
[3] T. M. Bragina, V. A. Kosobukin, and Yu. G. Shreter, Pis'ma Zh. Eksp. Teor. Fiz. **25**, 524 (1977) [JETP Lett. **25**, 492 (1977)].
[4] V. N. Aleksandrov, E. M. Gershenzon, A. P. Mel'nikov, R. I. Rabinovich, and N. A. Serebryakova, Pis'ma Zh. Eksp. Teor. Fiz. **22**, 573 (1975) [JETP Lett. **22**, 282 (1975)].
[5] E. H. Putley, in: Semiconductors and Semimetals (ed. by R. K. Willardson and A. C. Beer), Vol. 1, Physics of III-V Compounds, Academic Press, New York (1966), p. 289.
[6] E. Gornik, W. Müller, and F. Gaderer, Infrared Phys. **16**, 109 (1976).

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Electric resistance of metals with unfilled *f* shells

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The method of linear response in the paramagnetic phase is used to analyze the resistance of metals with an ϵ_f level of localized f electrons that are located near the Fermi surface. The strong intra-atomic Coulomb repulsion of the f electrons and their hybridization with the s electrons leads, at low temperatures, to the relation $R(T)=R_0+AT^2$, where the residual resistance R_0 of the ideal metal and the sign of A depend on the filling of the f level. It is shown that hybridization scattering accounts for the experimentally observed large logarithmic deviation of $R(T)$ from the linearity called for by the phonon scattering mechanism. In the region of strong hybridization ($|\epsilon_f|/g<1$) at large values of R_0 the resistance can have a minimum. A qualitative comparison of the results of the theory with the experimental $R(T)$ dependence is carried out for a large class of f metals (primarily for metals with variable valence).

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1. It is well known that rare-earth metals,[1-3] actinides,[4] a number of their intermetallic compounds,[5-8] as well as some d-metals[9] have in the paramagnetic phase, both at low and high temperatures, an anomalously varying resistance $R(T)$. At high temperatures, $R(T)$ deviates strongly from linearity, and sometimes even decreases with increasing T, while at low temperatures $R(T)$ can vary either quadratically or have a minimum. This behavior of $R(T)$ is connected with the scattering of the conduction s electrons by the f electrons,[4,10-12] which form either a narrow band near the Fermi surface or a deep level.

If the single-electrons ε_f levels of the unfilled localized-electron shells are much farther from the chemical potential μ than the characteristic energies of the interaction of the localized electrons with the conduction electrons, scattering does not change the number of localized electrons on a site. Then the mechanism that leads to nonlinearity of $R(T)$ can be effective s–f exchange interaction. The situation is then analogous to the case of the Kondo effect in scattering by magnetic impurities, except that in a regular metal the concentration of such "impurities" is equal to unity.[12]

We consider in detail in this paper the electric resistance in another case, when one of the ε_f levels is near μ so that it becomes easier for the shell configuration to change via a direct transition of the localized electrons to the conduction band. These transitions are brought about by the hybridization interaction.

In the description of the localized electrons it is of fundamental importance to take into account the Coulomb repulsion U between the electrons on one site. It is well known that this interaction cannot be accounted for within the framework of the Hartree-Fock approximation. We assume that the parameter U of the intra-atomic Coulomb interaction of the localized electrons is the largest energy in the system and take it account exactly; the hybridization interaction with parameter g will be regarded as a perturbation and localized shells from different sites will be assumed non-overlapping, so that their direct interaction can be neglected.

Such a model describes primarily the rare earths, the actinides, and their compounds, whose f shells can be regarded as well localized and for which an intermediate valence is observed, e.g., α-Ce, γ-Ce, $YbAl_2$, and $YbAl_3$.[13] These compounds undergo, generally speaking, a phase transition with change of valence.[14] The presence of such a phase transition indicates that the localized level is close to the chemical potential. It appears that this model also describes qualitatively transition metals having a narrow d band that cross the Fermi surface.

We note that the spin-fluctuation has been resorted to recently[11] to describe the resistivity of systems with a narrow band of localized electrons near the Fermi surface. Our analysis differs in principle from this approach, where the correlation interaction U is assumed small.

Another description of $R(T)$ of the systems in question is based on replacing the hybridization interaction g by the effective s–f exchange interaction and taking the crystal field into account.[10] This replacement involves the use of the canonical Schrieffer–Wolff transformation,[15] which takes correct account of only terms of second order in the parameter $g/|\varepsilon_f-\mu|$ and assumes this parameter to be small. For a satisfactory description of the resistance $R(T)$ of, say, $CeAl_2$ or $CeAl_3$ it is necessary to assume this parameter to be larger than or of the order of unity.[10]

It will be shown below that the small parameter in our analysis is $\rho g^2/|\varepsilon_f-\mu|$, where ρ is the state density of the s electrons. At the typical values $\rho\sim 10^{-5}\,K^{-1}$ it is possible to describe correctly not only the case of weak hybridization $g/|\varepsilon_f-\mu|<1$, but also the case of strong hybridization. For example, at $g\sim 5\cdot 10^3\,K$, $g/|\varepsilon_f-\mu|=3$ we have $\rho g^2/|\varepsilon_f-\mu|\sim 0.15$. The expression for the electric resistance will be derived below with account taken of all terms of first order in ρg. It can be seen at the same time that in the higher orders in g each hybridization transition of the electron from the s band to the f level and back leads to a higher order in ρg.

This paper deals with the resistance $R(T)$ of only the paramagnetic phase of the metal. The lower limit of the considered temperatures is imposed by the condition that the system remain paramagnetic. More accurately, we assume not only the absence of spontaneous magnetic ordering, but also the absence of any other coherent state of the system of s and f electrons, a state that arises inevitably at sufficiently low temperatures. The determination of the character of such a coherent state and an estimate of the transition temperature constitute a complex separate problem (see, e.g.,[16]), and in subsequent references to the residual resistance we shall ignore the possibility of the transition of the electron system to such a coherent state.

It is known[17,18] that in the case of the equilibrium situation the presence of the correlation interaction U does not make it possible to take exact account of the s–f hybridization interaction g, and leads, in the hybridization transition of the electron from the s band to the f level and back, to a damping Γ of both the s and f electrons, as well as to a renormalization of the level ε_f. In the problem of the electric conductivity, the s-electron scattering takes place in second order in g from fluctuations of the charge population of the f level of the lattice sites. Since the f electrons have an intrinsic damping that hinders their dragging, a nonzero finite relaxation time of the s electrons appears in the fourth order in g.

In the low-temperature limit this should lead to a residual resistance which will be shown to depend substantially on the average filling of the f level, and should therefore change in transitions in which the valence is changed.

In contrast to the equilibrium situation, the kinetic renormalizations for the electrons situated on the Fermi level turn out in the low-temperature limit to be logarithmically dependent on Γ and T, and not on $|\varepsilon_f-\mu|$. Expansion of the function $R(T)$ at low temperatures ($T\ll\Gamma$) leads to a quadratic dependence of R on T ($R=R_0+AT^2$). The coefficient A of T^2 depends on the residual resistance, with $A>0$ if the shell is completely filled or empty, and $A<0$ in the intermediate case. At high temperatures, when the phonon mechanism of scattering is taken into account, a logarithmic deviation of $R(T)$ linearity is obtained. The sign of the curvature of $R(T)$ in the case of strong hybridization is then determined by the sign of the coefficient A, depending on the filling of the f shell. The phonon scattering mechanism is accounted for within the framework of the relaxation time under the assumption that the characteristic reciprocal relaxation time τ^{-1} of the s electrons on the phonons is much less than $|\varepsilon_f-\mu|$. Substantial deviations from the Matthiessen rule are obtained in this case.

2. The system considered by us is described by the Hamiltonian

$$H=H_s+H_f+H_{sf}, \tag{1}$$

where

$$H_s=\sum_{\mathbf{k},\sigma}\varepsilon_{\mathbf{k}}a_{\mathbf{k}\sigma}{}^+a_{\mathbf{k}\sigma},\quad H_f=\sum_{\mathbf{m},\sigma}(\varepsilon_\sigma n_{\mathbf{m}\sigma}+{}^1/{}_2Un_{\mathbf{m},\sigma}n_{\mathbf{m},-\sigma})=\sum_{\mathbf{m},\sigma}\varepsilon_\sigma Z_{\mathbf{m}}{}^{\sigma\sigma}+\varepsilon_2\sum_{\mathbf{m}}Z_{\mathbf{m}}{}^{22},$$

$$H_{sf}=gN^{-1/2}\sum_{\mathbf{k},\sigma,\mathbf{m}}(e^{-i\mathbf{k}\mathbf{m}}a_{\mathbf{k}\sigma}{}^+d_{\mathbf{m}\sigma}+\text{h.c.})=gN^{-1/2}\sum_{\mathbf{k},\mathbf{m},\sigma}[e^{-i\mathbf{k}\mathbf{m}}a_{\mathbf{k}\sigma}{}^+(2\sigma Z_{\mathbf{m}}{}^{0\sigma}+Z_{\mathbf{m}}^{-\sigma2})+\text{h.c.}],$$

$$n_{\mathbf{m}\sigma}=d_{\mathbf{m}\sigma}{}^+d_{\mathbf{m}\sigma},\quad \varepsilon_2=2\varepsilon_\sigma+U,\quad \sigma=\pm{}^1/{}_2.$$

Here $a_{k\sigma}$ and $d_{m\sigma}$ are the second-quantization operators of the s and f electrons; m is the coordinate of the lattice site; g is the s–f hybridization constant; U is the parameter of the intra-atomic Coulomb interaction of the f electrons; H_s is the Hamiltonian of the s electrons, which we describe by a single conduction band of width 2D and with a constant state density ρ; H_f is the zero-order Hamiltonian of the localized f electrons with allowance for their strong correlation on one site. We assume that the f electrons pertaining to different sites do not interact with one another, and neglect, for simplicity, their degeneracy in the projections of the orbital angular momentum.

To make the allowance for the strong interaction U, we go over in the zeroth approximation in H_f and H_{sf} to the second-quantization operators of the eigenstates of the f shells[19]:

$$Z_{\mathbf{m}}{}^{\sigma0}=2\sigma d_{\mathbf{m}\sigma}{}^+(1-n_{\mathbf{m},-\sigma}),\quad Z_{\mathbf{m}}^{2-\sigma}=d_{\mathbf{m}\sigma}{}^+n_{\mathbf{m},-\sigma},\quad Z_{\mathbf{m}}{}^{22}=n_{\mathbf{m}\sigma}n_{\mathbf{m},-\sigma},$$

$$Z_{\mathbf{m}}{}^{\sigma\sigma}=n_{\mathbf{m}\sigma}(1-n_{\mathbf{m},-\sigma}),\quad Z_{\mathbf{m}}{}^{00}=(1-n_{\mathbf{m}\sigma})(1-n_{\mathbf{m},-\sigma}),\quad Z_{\mathbf{m}}^{\lambda_1\lambda_2}Z_{\mathbf{m}}^{\lambda_3\lambda_4}=\delta_{\lambda_2\lambda_3}Z_{\mathbf{m}}^{\lambda_1\lambda_4},$$
$$\lambda=0,\quad \sigma,\quad 2. \tag{2}$$

Interest attaches to two cases of the location of the Fermi surface relative to the single-electron levels $\varepsilon_f=\varepsilon_\sigma+U$ and ε_σ (all the levels will be reckoned hereafter from the chemical potential μ), namely, μ is situated either near ε_f or near ε_σ. Then, owing to the large value of U, we can consider in H_{sf}, respectively, either only the transitions $|\sigma\rangle\to|2\rangle$, retaining the terms with $Z_m{}^{\sigma2}$ and $Z_m{}^{2\sigma}$, or the transitions $|0\rangle\to|\sigma\rangle$, retaining the terms with $Z_m{}^{0\sigma}$ and $Z_m{}^{\sigma0}$. We shall consider the first case. The results for the second can be obtained in similar fashion. The Hamiltonian of the system takes the form

$$H=\varepsilon_f\sum_{\mathbf{k}_1}X_1{}^+X_1+\sum_1\varepsilon_1a_1{}^+a_1+N^{-1/2}\sum_1 g(a_1{}^+X_1+X_1{}^+a_1),$$
$$X_{\mathbf{k}\sigma}=N^{-1/2}\sum_{\mathbf{m}}e^{-i\mathbf{k}\mathbf{m}}X_{\mathbf{m}\sigma},\quad X_{\mathbf{m}\sigma}=Z_{\mathbf{m}}^{-\sigma2}. \tag{3}$$

The index 1 denotes here the state $(\mathbf{k}_1, \sigma_1)$.

We seek the electric conductivity $\mathfrak{S}_{\alpha\beta}$ of our system by the Kubo method of linear response.[20] Since the f electrons are assumed localized, the conductivity $\mathfrak{S}_{\alpha\beta}$ is governed only by the s electrons and is given by [21]

$$\mathfrak{S}_{\alpha\beta}=-\frac{e^2}{V}\sum_0 v_{\mathbf{k}_0}{}^\alpha F_{0\beta}^{(1)}(\omega=0),$$
$$F_{0\beta}(z)=\langle\langle a_0{}^+a_0|B^\beta\rangle\rangle_z,\quad z=\omega+i\xi,\quad \xi\to+0, \tag{4}$$

where $v_{k_0}^\alpha$ is the s-electron velocity; eB^β is the dipole moment of the system; $F_0^{(1)}$ is the two-dimensional temperature Green's function corresponding to the deviation of the distribution function from the equilibrium value under the influence of an external electric field; α and β are Cartesian indices which we shall omit hereafter, assuming the crystal to have cubic symmetry.

To find $F_0^{(1)}$, we obtain a system of coupled equations for the higher-order Green's functions. Prior to the decoupling, the obtained Green's functions are connected with the following operators:

$$A_0^{(1)}=a_0{}^+a_0,\quad A_0^{(2)}=a_0{}^+X_0,\quad \bar A_0^{(2)}=X_0{}^+a_0,\quad A_0^{(3)}=X_0{}^+X_0,$$
$$A_{01}^{(4)}=a_0{}^+R_{01}{}'a_1,\quad A_{01}^{(5)}=a_0{}^+\overline{R_{01}{}'X_1},\quad \bar A_{01}^{(5)}=\overline{X_1{}^+R_{10}{}'}a_0, \tag{5}$$

where

$$R_{01}{}'=R_{01}-\delta_{01}K,$$
$$R_{01}=[X_0,X_1{}^+]_+=N^{-1}\sum_{\mathbf{m}}\exp[i(\mathbf{k}_0-\mathbf{k}_1)\mathbf{m}](\delta_{\sigma_0\sigma_1}Z_{\mathbf{m}}{}^{22}+Z_{\mathbf{m}}^{-\sigma_0,-\sigma_1}), \tag{6}$$
$$\delta_{01}K=\langle R_{01}\rangle=\delta_{01}(\langle Z_{\mathbf{m}}{}^{\sigma\sigma}\rangle+\langle Z_{\mathbf{m}}{}^{22}\rangle),\quad R_{\mathbf{m}\sigma\sigma_1}=[X_{\mathbf{m}\sigma},X_{\mathbf{m}\sigma_1}]_+.$$

In the paramagnetic case K is the average number of f electrons with fixed spin per site and does not depend on the site **m** or on the spin σ (a feature common to all the Green's functions and to the mean values of operators with a single spin). The bar over several f operators in the **k** representation means that in the transition to the site representation the summation is over non-coinciding sites, e.g.,

$$\overline{R_{01}{}'X_1}=N^{-3/2}\sum_{\mathbf{m}_1,\mathbf{m}_2}\exp[i(\mathbf{k}_0-\mathbf{k}_1)\mathbf{m}_1-i\mathbf{k}_1\mathbf{m}_2]R'_{m_1\sigma_0\sigma_1}X_{\mathbf{m}_2\sigma_1}(1-\delta_{\mathbf{m}_1\mathbf{m}_2}).$$

It is easy to obtain for the Green's function of the operators (5) the following exact system of equations:

$$zF_0^{(1)}=-i\lambda_0^{(1)}+g(F_0^{(2)}-\bar F_0^{(2)}), \tag{7}$$

$$(z+\varepsilon_{0f})F_0^{(2)}=-i\lambda_0^{(2)}+gKF_0^{(1)}-gF_0^{(3)}+g\sum_1 F_{01}^{(4)}, \tag{8}$$

$$zF_0^{(3)}=-i\lambda_0^{(3)}-gK(F_0^{(2)}-\bar F_0^{(2)})+g\sum_1(\bar F_{10}^{(5)}-F_{10}^{(5)}). \tag{9}$$

For the Green's functions and for the corresponding mean values of the operator $A^{(i)}$ we introduce the symbols

$$\varepsilon_{0f}=\varepsilon_0-\varepsilon_f,\quad \varepsilon_{01}=\varepsilon_0-\varepsilon_1,\quad \bar\lambda^{(i)}=i\langle[\bar A^{(i)},B]\rangle,\quad \bar F^{(i)}=\langle\langle\bar A^{(i)}|B\rangle\rangle,$$
$$\lambda^{(i)}=i\langle[A^{(i)},B]\rangle,\quad F^{(i)}=\langle\langle A^{(i)}|B\rangle\rangle_z,\quad f^{(i)}=\langle A^{(i)}\rangle,\quad \bar f^{(i)}=\langle\bar A^{(i)}\rangle.$$

In the derivation of (7)–(9) and hereafter we make use of the fact that the Green's functions and $\lambda_1^{(i)}$ are odd in $\mathbf{k}_1$. We also use the fact that for Hermitian-conjugated operators the Green's functions are connected by the relation $\bar F^{(i)}(\omega+i\xi)=[F^{(i)}(-\omega+i\xi)]$, i.e., in the case $\omega=0$ of interest to us they are complex-conjugate. To take into account of the correlation of the f electrons on one site it is necessary, when commuting the operators with H_{sf}, to change over to the site representation of the f-electron operators and to separate the corresponding mean values on one site.

Since we wish to find an expression for the system with account taken of all the terms linear in the small parameter ρg of our problem, the decoupling cannot be carried out in the framework of Eqs. (7)–(9). It is easily seen that the next two chains of equations, e.g., for $F_{01}^{(4)}$ from (8), lead to summation over new indices $\mathbf{k}_2$

and $\mathbf{k}_3$, and in the case of decoupling in the "g^4 approximation" there appears $\sum_{\mathbf{k}_2} \sim \rho$. Starting with Eq. (8), ever two commutations with H_{sf} must, without fail, be carried out after the decoupling to the higher power of ρg in the final expression for $F_0^{(1)}$. It is then necessary, in each stage, to separate from the operators $A^{(i)}$ all the possible mean values in the resultant new Green's functions of order higher than the preceding ones. For the new $F^{(i)}$ that describe the correlation between the fluctuations it is then easy to determine the order (in ρg) of the terms to which they can lead in the final expression for $F_0^{(1)}$. For the Green's function $\sum_{\sigma 1} F_{01}^{(4)}$, for example, we have the following equation:

$$(z+\varepsilon_{01}) \sum_{\sigma_1} F_{01}^{(4)} = -i\lambda_{01}^{(4)} + g \sum_{1} (F_{01}^{(5)} - \bar{F}_{01}^{(5)})$$
$$+ gN^{-1} [\bar{f}_1^{(2)} F_0^{(1)} - (2-K-f_0^{(1)}) \bar{F}_1^{(2)} + (2-K-f_1^{(1)}) F_0^{(2)} - f_0^{(2)} F_1^{(1)}]. \quad (10)$$

We have left out of (10) the Green's functions that describe the correlation between fluctuations with different spins and lead, as can be seen, to terms of order $(\rho g)^2$. Typical functions of this kind are

$$\delta_{-\sigma_2\sigma_0} \delta_{\sigma_1\sigma_2} \langle\langle (a_0^+ a_1 - \delta_{01} f_0^{(1)}) (a_2^+ X_{\mathbf{k}_0-\mathbf{k}_1+\mathbf{k}_2,\sigma_2} - \delta_{01} f_2^{(2)}) | B \rangle\rangle,$$
$$\delta_{\sigma_1\sigma_0} \delta_{-\sigma_2\sigma_0} \langle\langle (a_0^+ X_1 - \delta_{01} f_0^{(2)}) (a_2^+ X_{\mathbf{k}_0-\mathbf{k}_1+\mathbf{k}_2,\sigma_2} - \delta_{01} f_2^{(2)}) | B \rangle\rangle. \quad (11)$$

The equation for the Green's function $F^{(5)}$, the decouplings that lead to a closed system of equations for the functions $F^{(1-5)}$, as well as the main stages of the solution of this system are given in the Appendix. We note only that when Green's functions of the type (11) are separated we use for the mean values a more accurate relation that can be readily obtained from the equations for the equilibrium Green's functions:

$$\varepsilon_{0f} f_0^{(2)} + g f_0^{(3)} - K g f_0^{(1)} - g \sum_1 f_{01}^{(4)} = 0. \quad (12)$$

It is also shown in the Appendix how the field terms $\lambda_{01}^{(4)}$ and $\lambda_{01}^{(5)}$ are expressed in terms of $\lambda^{(2)}$ and $\lambda^{(3)}$ with the aid of the corresponding equilibrium Green's functions, with allowance for the fact that

$$\lambda_{01}^{(i)} = \left(\frac{\partial}{\partial \mathbf{k}_0} + \frac{\partial}{\partial \mathbf{k}_1}\right) f_{01}^{(i)}, \quad \lambda_0^{(i)} = \frac{\partial}{\partial \mathbf{k}_0} f_0^{(i)}. \quad (13)$$

The system of equations (7)–(10) and (A.1) leads to the following expression for $F_0^{(1)}$:

$$F_0^{(1)} = -\frac{1}{2\pi\rho g^4 (1-K^2)} \{\lambda_0^{(1)} [\varepsilon_{0f} + Kg^2 - \varepsilon_{0f} \Delta(\varepsilon_0) + 2g^2 \psi(\varepsilon_0)]$$
$$-2g\lambda_0^{(2)} (\varepsilon_{0f} - \Delta(\varepsilon_0) + \delta) - \lambda_0^{(3)} g^2 [1 + 2K^{-1} \psi(\varepsilon_0)]\}. \quad (14)$$

Here

$$\Delta(\varepsilon_0) = g^2 N^{-1} \sum_{\mathbf{k}_1} \frac{2-2K-f_1^{(1)}}{\varepsilon_0 - \varepsilon_1},$$
$$\psi(\varepsilon_0) = gN^{-1} \sum_{\mathbf{k}_1} \frac{f_1^{(2)}}{\varepsilon_0 - \varepsilon_1}, \quad \delta = K^{-1} g N^{-1} \sum_{\mathbf{k}_1} f_1^{(2)}. \quad (15)$$

Expression (14) for $F_0^{(1)}$ describes effectively the renormalizations, connected with the hybridization interaction, of the field terms $\lambda_0^{(1-3)}$, and the relaxation time, which is proportional to $(1-K^2)^{-1}$ and which can be seen to vanish in the case of complete occupation of the level ε_f: $\varepsilon_f \to -\infty, K \to 1$.

3. To determine the temperature dependence of the electric resistance we obtain in explicit form the field terms $\lambda_0^{(1-3)}$ in $F_0^{(1)}$ and the renormalizations Δ and ψ, and take account also of the additional (phonon and impurity) scattering mechanisms.

We present the equilibrium Green's functions, which we need to find the corresponding mean values $f_0^{(1-3)}$ and which are obtained within the framework of the same decouplings that have led to closure of the system (7)–(10), (A.1) and take into account all the first-order terms in the small parameter (ρg) of the problem:

$$\langle\langle X_0 | X_0^+ \rangle\rangle = K(\omega - \varepsilon_0) M^{-1}, \quad \langle\langle a_0 | X_0^+ \rangle\rangle = g(\omega - \varepsilon_0)^{-1} \langle\langle X_0 | X_0^+ \rangle\rangle,$$
$$M = [\omega - \bar{\varepsilon}_f + i\Gamma(\omega)] (\omega - \varepsilon_0) - Kg^2, \; \Gamma(\omega) = g^2 K^{-1} (1-K^2) \,\mathrm{Im}\, N^{-1} \sum_{\mathbf{k}_1} \langle\langle a_1 | a_1^+ \rangle\rangle,$$
$$\langle\langle a_0 | a_0^+ \rangle\rangle = (\omega - \bar{\varepsilon}_f) M^{-1}, \quad \bar{\varepsilon}_f = \varepsilon_f + \delta. \quad (16)$$

The functions (16) describe the hybridization of the s band with the f level, the renormalization δ of this level [see (15)], and the damping $\Gamma(\omega)$. Changing to hybridized bands, it is convenient to reduce the equilibrium Green's functions to the form

$$\langle\langle X_0 | X_0^+ \rangle\rangle = \sum_i t_i (E^{(i)} - \bar{\varepsilon}_f)^{-2} \frac{K^2 g^2}{\omega - E^{(i)} + i\Gamma_i},$$
$$\langle\langle a_0 | X_0^+ \rangle\rangle = \sum_i t_i (E^{(i)} - \bar{\varepsilon}_f)^{-1} \frac{Kg}{\omega - E^{(i)} + i\Gamma_i}, \quad (17)$$
$$\langle\langle a_0 | a_0^+ \rangle\rangle = \sum_i t_i \frac{1}{\omega - E^{(i)} + i\Gamma_i},$$

where

$$t_i = \frac{(E^{(i)} - \bar{\varepsilon}_f)^2}{(E^{(i)} - \bar{\varepsilon}_f)^2 + Kg^2}, \quad \Gamma_i = \frac{\pi\rho g^4 (1-K^2)}{(E^{(i)} - \bar{\varepsilon}_f)^2 + Kg^2},$$
$$E^{(1,2)}(\varepsilon_{\mathbf{k}}) = {}^1/_2 [(\varepsilon_{\mathbf{k}} + \bar{\varepsilon}_f) \mp ((\varepsilon_{\mathbf{k}} - \bar{\varepsilon}_f)^2 + 4Kg^2)^{1/2}], \quad E^{(2)} > E^{(1)}, \quad i = 1, 2.$$

We confine ourselves to the case when the chemical potential is farther than the temperature and the damping from the hybridized gap of width $\sim \rho g^2$, i.e., $|\bar{\varepsilon}_f| > T$, $|\bar{\varepsilon}_f| \gg \rho g^2$. In the calculation of the mean values $f_0^{(1-3)}$ we then neglect the damping in (17) and verify that in the approximation linear in ρg all that is left of $\lambda^{(1-3)}$ in the numerator of (14) are the terms proportional to $\partial f(E^{(i)})/\partial E^{(i)}$, where f is the Fermi function. This means that the electrons contributing to the conductivity are those on the Fermi surface, as should be the case.

Using the mean values $f_0^{(1)}$ and $f_0^{(2)}$ defined by the Green's function (17) it is easy to obtain in the same approximation that the renormalizations $\Delta(x)$, $\psi(x)$, and δ are of the form

$$\Delta(\varepsilon_{\mathbf{k}}) = \rho g^2 \sum_i t_i \ln \frac{D}{\{T, E^{(i)}(\varepsilon_{\mathbf{k}})\}}, \quad \delta = -\rho g^2 \ln \frac{D}{|\bar{\varepsilon}_f|},$$
$$\psi(\varepsilon_{\mathbf{k}}) = \frac{K\rho g^2 t_1}{\bar{\varepsilon}_f - E^{(1)}(\varepsilon_{\mathbf{k}})} \ln \frac{\{T, E^{(1)}(\varepsilon_{\mathbf{k}})\}}{\{T, E^{(2)}(\varepsilon_{\mathbf{k}})\}} \quad \{a, b\} \equiv (a^2 + b^2)^{1/2}. \quad (18)$$

Since of the poles of $E^{(i)}(\varepsilon_k)$ is close to zero for the electrons that determine the conductivity, the corresponding logarithm in the kinetic normalizations Δ and ψ in (18) has a strong temperature dependence and allowance for the damping of the Green's functions (17) becomes essential. A self-consistent account of the damping adds an additional damping Γ_i in the curly brackets in (18) for the vanishing $E^{(i)}(\varepsilon_k)$. We call attention to the fact that in our approximation ($|\tilde{\varepsilon}_f| > T$, $|\varepsilon_f| \gg \rho g^2$) no temperature-dependent normalizations arise for the equilibrium Green's functions of the electrons on the Fermi surface.

After changing to hybridized bands and substituting the expressions determined from the Green's functions (17) for $\lambda^{(1-3)}$, Δ, ψ, and δ, we obtain from (4) and (14) for the hybridized resistance $R_g(T)$ the following expression:

$$R_g = \frac{3\Omega_0}{2e^2\hbar v^2\rho}\frac{a}{1+c}, \tag{19}$$

where

$$a = 2\pi\rho g^2 K^{-1}(1-K^2)x,$$

$$c = \frac{\rho g^2}{\tilde{\varepsilon}_f}\left[\frac{2x+1}{x+1}\ln\frac{(T^2+\Gamma^2)^{1/2}}{2\rho\tilde{\varepsilon}_f^2} - \frac{x}{x+1}\ln\frac{1+x}{2\rho|\tilde{\varepsilon}_f|}\right],$$

$$x = \frac{Kg^2}{\tilde{\varepsilon}_f^2}, \quad \Gamma = \frac{\pi\rho g^4(1-K^2)}{\tilde{\varepsilon}_f^2+Kg^2}, \quad \Omega_0 = \frac{V}{N}.$$

We assume now that the s electrons have other scattering mechanisms, phonon and impurity, which can be described in the approximation of the relaxation time τ^{-1}. This relaxation can be formally accounted for by introducing into the equations for the nonequilibrium Green's functions the width in the initial s states, i.e., by replacing ε_k by $\varepsilon_k + i/2\tau$. In (7), for example, this will lead to addition of a term $(-i\tau^{-1}F_0^{(1)})$ in the right-hand side, while in (8) it will lead to replacement of $(z+\varepsilon_{0f})F_0^{(2)}$ by $[z+\varepsilon_{0f}+i(2\tau)^{-1}]F_0^{(2)}$. We assume that the distance from the localized level $\tilde{\varepsilon}_f$ to the Fermi surface is larger than τ^{-1}, whose maximum is reached at high temperatures, and is smaller than or of the order of the Debye temperature. For the electrons on the Fermi surface we shall therefore omit τ^{-1} together with ε_{0f}. This means that Eqs. (7) and (A.1) remain the same as before.

The allowance for τ^{-1} in Eq. (10) for $F_{01}^{(4)}$ is made by replacing the denominators ε_{01} by $\varepsilon_{01} + i\tau^{-1}$ in the renormalizations (15) for Δ and ψ. For the real part of Δ or ψ, which leads to a logarithmic temperature dependence, this reduces effectively to replacing the argument of the logarithm in (18) by the expression $\{T, \Gamma, \tau^{-1}\} \equiv (T^2+\Gamma^2+\tau^{-2})^{1/2}$. Since the phonon part of τ^{-1} increases with increasing T while the part of τ^{-1} due to impurity scattering can be regarded as smaller than the hybridization damping Γ ($\Gamma \sim 100$ K), the logarithmic temperature dependence becomes only stronger. For simplicity, however, we shall disregard this enhancement.

Thus, allowance for the additional scattering mechanism actually reduces in our approximation to a change of only Eq. (7). We thus arrive at the following final expression for R [see (19)]:

$$R(T) = R_g(T) + R_\tau(T), \tag{20}$$

where

$$R_\tau = \frac{3\Omega_0}{2e^2\hbar v^2\rho}\frac{b\tau^{-1}}{1+c},$$

$$b = 1 - x + x^2 + \frac{\rho g^2}{\tilde{\varepsilon}_f}\left[\ln\frac{(T^2+\Gamma^2)^{1/2}}{2\rho\tilde{\varepsilon}_f^2} - x\ln\frac{1+x}{2\rho|\tilde{\varepsilon}_f|}\right].$$

We now analyze expression (20). We note first that at $T=0$, provided that the system remains in the paramagnetic phase, an appreciable residual resistance $R_g(0)$ is observed in an ideal (impurity-free) crystal. $R_g(0)$ is proportional to $x = Kg^2/\tilde{\varepsilon}_f^2$, and $(1-K^2)$ can reach values on the order of 10^2 μΩ-cm in the strong-hybridization region ($x \gg 1$). In transitions with change of valence, the value of K changes strongly and this can lead to a change of the residual resistance ($R_g(0) \to 0$ as $K \to 1$). In the general case the residual resistance consists of two parts, impurity and hybridization.

Next, as seen from (20), the hybridization temperature dependence manifests itself effectively in the impurity and phonon parts of the resistance. This means that a deviation from the Matthiessen rule is observed, such that the temperature part of the resistance $[R(t) - R(0)]$ does not depend on the impurity concentration. This result is due to the fact that the problem is solved in a region beyond the Born approximation (g^4).

At sufficiently large x the logarithmic temperature dependence manifests itself primarily in the denominator $(1+c)$. We note that at small values of the parameter $\rho g \sim 0.05$ the choice $x \sim 10$ does not contradict our approximation $|\tilde{\varepsilon}_f| \gg \rho g^2$. As to the damping Γ, we note also that in the presence of orbital degeneracy of the level and its hybridization with several overlapping conduction bands the state density ρ that enters in expression (20) for Γ can be several times smaller than the true value.[18] We shall bear this in mind in the numerical estimates that follow. Finally, for a situation wherein the chemical potential lies near the level $\tilde{\varepsilon}_\sigma$ and transitions $|0\rangle \leftarrow |\sigma\rangle$ are realized, expression (20) remains fully valid except that $\tilde{\varepsilon}_f$ is replaced by $-\tilde{\varepsilon}_\sigma$ and K from (6) is replaced by $K = \langle Z_m^{\sigma\sigma}\rangle + \langle Z_m^{00}\rangle$. We shall hereafter take ε_f and ε_σ to mean the already renormalized values.

4. Let us see what temperature dependences of $R(T)$ result from (20). We consider first the case of low temperatures $T \ll \Gamma$ and assume that τ^{-1} describes the T-independent impurity scattering. At large values $x \sim 10$ the single-electron level is near the chemical potential, K lies between 1 and 0.5, and this situation corresponds either to a rare-earth compound with non-integer valence or to a d-metal. In this case we have a residual resistance $R_0 \equiv R(0) = R_{0g} + R_{0\tau}$ which is due both to hybridization scattering by fluctuations of the occupation numbers of the localized electrons (R_{0g}) and to scattering of the s electrons by impurities ($R_0 \sim \tau^{-1}$). With decreasing x, say under pressure, R_{0g} should decrease, as follows from (20), and particularly steeply if $K \to 1$ as the level moves, and the f shell becomes either completely empty or filled. This situation is observed in α-Ce under increasesed pressure.[2,3] From the parameters $\rho g = 0.04$, $g = 4 \cdot 10^3$ K, $\varepsilon_\sigma = 1.3 \cdot 10^3$ K, $\Gamma = 50$ K, $K = 0.95$ we get for α-Ce a residual hybridization resistance $R_{0g} = 5 \times 10^{-6}$ Ω-cm, which is close to the total experimentally observed value.[3]

At low temperatures, the expansion of (20) in powers of T/Γ leads to the quadratic law $R = R_0 + AT^2$, with $A > 0$ if the f shell is nonmagnetic, i.e., $\varepsilon_f < 0$ (or $\varepsilon_\sigma > 0$), and $A < 0$ if $\varepsilon_f > 0$ (or $\varepsilon_\sigma < 0$). When $A < 0$ and the phonon scattering is included in τ^{-1} the resistance should have a minimum when T is increased (see the cases $CeAl_2$ and Eu below). It is important that the coefficient A of T^2 depends on R_0 and is proportional to R_0 at $x \gg 1$, as can be readily seen. A strong dependence of A on R_0 is observed experimentally for α-Ce. In the experiment[2] the residual resistance at pressures $p = 4 - 8$ kbar decreased with increasing pressure at a rate higher by one order of magnitude than in[3], and the coefficient A of T^2 also decreased at a comparable rate. We note that (20) yields at the parameters cited above for α-Ce, together with the experimental value $R_0 = 9 \times 10^{-6}$ Ω-cm, a coefficient $A = 2.7 \times 10^{-9}$ Ω-cm-deg^{-2}, which agrees with the data of [3] at $p = 2$ kbar.

At high temperatures, τ^{-1} in (20) contains a factor linear in T which describes the scattering of s electrons by phonons. In those cases when the hybridization is assumed strong ($x > 1$) it is easily seen that the dependence of b on T in the numerator of (20) can be neglected and it is convenient to express $R(T)$ in a form suitable for further analysis:

$$R = \frac{a_1 + b_1 T\Gamma^{-1}}{1 + c(T)}, \tag{21}$$

where a_1 corresponds to the impurity and hybridization scattering, and $b_1 T\Gamma^{-1}$ to the phonon scattering. Depending on the position of the level ε_f (or ε_σ), on the ratio b_1/a_1 and on the value of Γ, the function $R(T)$ can have a qualitatively different behavior.

At $b_1 \gg a_1$ the plot of $R(T)$ deviates from linearity in a wide temperature range and has negative curvature when $\varepsilon_f > 0$ (or $\varepsilon_\sigma < 0$) and positive curvature when $\varepsilon_f < 0$ (or $\varepsilon_\sigma > 0$). A typical form of $R(T)$ at $\varepsilon_f > 0$ is that of curve 1 of Fig. 1, which describes qualitatively $R(T)$ of Nb_3Sn[9] and corresponds to the values $b_1/a_1 = 15$, $\rho g = 0.055$, $g = 6.5 \cdot 10^3$ K, $\varepsilon_f = 1.4 \cdot 10^3$ K, $\Gamma = 250$ K, $K = 0.7$. A similar behavior of $R(T)$ is observed in a large number of transition metals: γ-Ce, Pr, Nd,[1] $YbAl_3$,[5] $NpRh_3$,[7] Np.[4] We note that, in accord with the behavior of $R(T)$ (curve 1), transitions $|0\rangle \to |\sigma\rangle$ and $\varepsilon_\sigma < 0$ are realized in α-Ce, while in $YbAl_3$ we get transitions $Yb^{13} \to Yb^{14}$ with ~0.9 f holes,[5] i.e., transitions of the type $|\sigma\rangle \to |2\rangle$ with $\varepsilon_f > 0$. For all the rare-earth metals (except Ce) it is assumed that the filled single-electron level ε_n is far enough from the chemical potential, $|\varepsilon_n| \gtrsim 1$ eV, and the width of the conduction band is $2D \approx 8$ eV.[22] If we assume that the transitions $|\varepsilon_n\rangle \to |\varepsilon_{n-1}\rangle (\varepsilon_{n-1} < \varepsilon_n)$, take place in hybridization scattering, then we must choose $g \gtrsim |\varepsilon_n|$ to describe satisfactory the behavior of $R(T)$ of these metals, but then the condition $\rho g^2 \ll |\varepsilon_n|$ may be violated. It is known, however, that at temperatures $T = 600 - 800$ K of the electric resistance, heat capacity, and magnetic susceptibility, the metals Pr, Nd, and Eu have an anomalous behavior attributed to a continuous phase transition in the electron subsystem.[1,23-25] This suggests that these metals have above the Fermi surface an unfilled localized level $\varepsilon_{n+1} \sim 0.1$ eV. The presence of the transtions $|\varepsilon_n\rangle \to |\varepsilon_{n+1}\rangle$ allows us to describe the $R(T)$ relation in Eu (see below), Pr, and Nd within the framework of our model. When the pressure is increased the level ε_{n+1} can move away from the chemical potential. No phase transition with change of valence will be observed in this case. Another assumption that makes it possible to decribe these metals in our model is that the level $|\varepsilon_n| \lesssim 1$ eV.

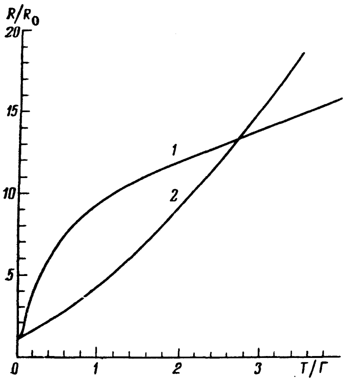

FIG. 1. Temperature dependence of the resistance $R(T)$: R_0—residual resistance, Γ—damping. Curves 1 and 2 describe qualitatively $R(T)$ of Nb_3Sn($\Gamma = 250$ K) and $YbAl_2$($\Gamma = 300$ K).

A deviation of the resistance from linearity is observed, for example, in $YbAl_2$,[5] which has ~0.5 f-holes; this corresponds effectively to the transitions $|\sigma\rangle \to |2\rangle$ with $\varepsilon_f < 0$. Such a behavior of $R(T)$ is represented by curve 2 of Fig. 1, which corresponds to the following parameters in expression (21): $b_1/a_1 = 5$, $\rho g = 0.055$, $g = 5.5 \cdot 10^3$ K, $\varepsilon_f = -1.2 \cdot 10^3$ K, $\Gamma = 300$ K, $K = 0.9$.

Consider now the case when the resistance due to the hybridization interaction and to impurity scattering is of the order of the high-temperature phonon resistance, i.e., $a_1 \sim b_1$. In this case, if K is close to 0.5 ($\varepsilon_f > 0$ or $\varepsilon_\sigma < 0$) the value of $(1 - K^2)$ differs substantially from zero and $R(T)$ can have a minimum at a large hybridization resistance, as noted above. A typical form of such a behavior of $R(T)$ is shown in Fig. 2. Curve 1 of Fig. 2 corresponds to the following parameters in (21): $b_1/a_1 = 2.5$, $\rho g = 0.05$, $g = 5.10^3$ K, $\varepsilon_\sigma = -10^3$ K, $\Gamma = 100$ K, $K = 0.55$. Curve 2 of Fig. 2 corresponds to the case $x = 1.5$ and is obtained from (21) when account is taken of the dependence of b_1 on T [see (20)] and corresponds to the parameters $b_1(T=0)/a_1 = 0.5$, $\rho g = 0.1$, $g = 8 \cdot 10^3$ K, $\varepsilon_f = 5 \cdot 10^3$ K, $\Gamma = 115$ K, $K = 0.58$. Curve 1 on Fig. 2 corresponds to the behavior of $R(T)$ in $CeAl_2$[6] with a minimum at $T = 13$ K and to an almost linear (with a slight bend) $R(T)$ plot at high temperatures. On the other hand, curve 2 of Fig. 2 corresponds qualitatively to the experimental

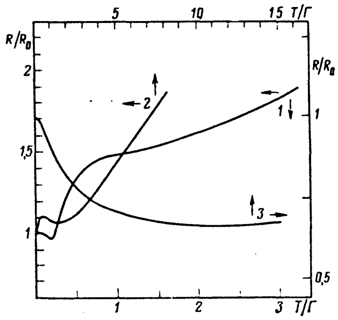

FIG. 2. Temperature dependence of the resistance $R(T)$: R_0—residual resistance, Γ—damping. Curves 1, 2, and 3 describe qualitatively $R(T)$ of $CeAl_2$($\Gamma = 100$ K), Eu($\Gamma = 115$ K), and $PuAl_2$($\Gamma = 20$ K), respectively.

$R(T)$ dependence of Eu[1] above the magnetic-ordering point ($T > 85$ K). We note that $CeAl_2$ exhibits at $T \leqslant 4$ K a resistance decrease that is not described by our approach and may be due to magnetic ordering.

$R(T)$ behaves differently when the phonon scattering remains relatively weak ($b_1 \ll a_1$) even at high temperatures, and the configuration of the localized electrons is not closed. Curve 3 of Fig. 2 shows such an $R(T)$ plot, pertains to $PuAl_2$[4] and corresponds to the following parameters in (21): $b_1/a_1 = 0.014$, $\rho g = 0.025$, $g = 2400$ K, $\varepsilon_f = 600$ K, $\Gamma = 20$ K, $K = 0.57$. At high temperature this $R(T)$ tends to decrease, in analogy with the experimental results for $PuAl_2$. At $T < 10$ K there is a steep decrease of the resistance and it can be assumed that magnetic ordering sets in at these temperatures. A variation of $R(T)$ similar to the one shown, with a smooth decrease of R with rising temperature, is observed for a number of transition metals and their compounds, for example Pu,[4] $PuZn_2$,[7] $CeAl_3$.[6]

In those cases, however, when a sharp decrease of the resistance is observed as $T \to 0$ but no magnetic order sets in (as, probably, in Pu), our approach can not explain the temperature dependence of the resistance. It can be assumed that this situation corresponds to proximity of the single-electron level of the localized electrons to the chemical potential, and then consideration of the higher orders in ρg at low temperatures can lead to a situation similar to the onset of paramagnons.[26]

We call attention to the interesting high-temperature behavior of $UP_{1-x}S_x$,[8] where an increase of the concentration x is accompanied by a simultaneous change of the character of the magnetic order (at $T < 200$ K) and of the curvature of $R(T)$ in the paramagnetic region. This behavior can be attributed to passage of the localized level through the Fermi surface with increasing x. When the sign of the effective exchange interaction is reversed, our model calls for a change of curvature of $R(T)$ in the paramagnetic region.

The presented $R(T)$ curves are only qualitative. For a correct description of the $R(T)$ dependence of a number of concrete metals it would be necessary to take into account, primarily, the degeneracy of the ε_f level. It is seen nevertheless that the considered hybridization scattering of the s electrons by the internal degrees of freedom of a strongly-correlating f-electron level close to the Fermi surface can explain a large class of temperature dependences of the resistance. The difference in the behavior of $R(T)$ is determined by the logarithmic temperature dependence of the renormalizations, by the population of the localized level (which determines the sign of the logarithmic singularity), by the degree of hybridization (i.e., by the value of g^2/ε_f^2), and finally by the ratio of the residual and phonon resistances.

We note in conclusion that the obtained logarithmic temperature dependence has nothing in common with the Kondo logarithm, which appears only in third order in the s–f exchange interaction, equivalent to order g^6 or to second order in the small parameter ρg of our problem.

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APPENDIX

The equation for the Green's function $F_{01}^{(5)}$ is of the form

$$(z+\varepsilon_{0f}) \sum_{\sigma_1} F_{01}^{(5)} = -i\lambda_{01}^{(5)} + gN^{-1}[\overline{\langle X_1^+ X_1 \rangle} F_0^{(1)} + f_0^{(1)} F_1^{(3)} - f_0^{(2)} F_1^{(2)} - f_1^{(2)} F_0^{(2)}]$$

$$+gK \sum_{\sigma_1} F_{01}^{(4)} - gKN^{-1} \sum_{2} F_{02}^{(4)}. \qquad \text{(A.1)}$$

We have left out of (A.1) Green's functions of the type (11) and the functions $\langle\langle \overline{X_0^+ R'_{01} X_1} | B \rangle\rangle$, $\sum_2 \langle\langle a_0^+ \overline{R'_{01} R'_{12}} a_2 | B \rangle\rangle$, which lead to the order $(\rho g)^2$ in the equation for $F_0^{(1)}$.

The system of equations (7–10) and (A.1) is closed. Substituting (A.1) in 10 and summing over k_1, we get $\sum_1 F_{01}^{(4)}$ and consequently $\sum_{\sigma 1} F_{01}^{(4)}$ and $\sum_{\sigma 1} F_{01}^{(5)}$ in terms of $F_0^{(1)} F_0^{(2)}, F_0^{(3)}$. Substitution of $\sum_{\sigma 1} F_{01}^{(4)}, F_{01}^{(5)}$ in Eqs. (8) and (9) yields a rather cumbersome system for $F_0^{(1-3)}$. When grouping the terms in (8) and (9) we make use essentially of the following relations that follow from (8) and (12):

$$\varepsilon_{0f} \operatorname{Re} F_0^{(2)} = KgF_0^{(1)} - gF_0^{(3)} + O(\rho g),$$

$$\varepsilon_{1f} f_1^{(2)} + gf_1^{(3)} - Kgf_1^{(1)} + O(\rho g) = 0. \qquad \text{(A.2)}$$

We take the imaginary part of (8), substitute the real and imaginary parts of $f_0^{(2)}$ from (7) and (A.2) in (8) and (9), and omit terms of order $(\rho g)^2$. We see then that the coefficients of $f_0^{(3)}$ in (8) and (9) agree to within a factor, and we arrive at expression (14) for $F_0^{(1)}$.

Note that a finite relaxation time in the nonequilibrium distribution function $F_0^{(3)}$ of the f electrons, and hence also in $F_0^{(1)}$, stems from (A.1) and is proportional to $(\rho g^2)^{-1}$. Allowance for the last term in (A.1) allows us to describe correctly the region of strong hybridization $\varepsilon_{0f} = 0$.

Let us show how the field terms $\lambda_{01}^{(4)}$ and $\lambda_{01}^{(5)} = -\overline{\lambda}_{01}^{(5)}$ reduce to $\lambda^{(2)}$ and $\lambda^{(3)}$. To find the equilibrium mean values $f_{01}^{(4)}$ and $\overline{f}_{01}^{(5)}$ corresponding to $\lambda_{01}^{(4)}$ and $\overline{\lambda}_{01}^{(5)}$ we obtain the Green's functions $\sum_{\sigma 1} \langle\langle a_1 | a_0^+ R'_{01} \rangle\rangle$, $\sum_{\sigma 1} \langle\langle a_0 | X_1^+ R'_{10} \rangle\rangle$, and $\langle\langle a_0 | X_0^+ \rangle\rangle$. Taking into account the further summation over $\mathbf{k}_1$, we can seek these functions in our approximation in the zeroth order in ρg. Carrying out the decouplings in the same order, we obtain the following equations for the Green's functions:

$$(z-\varepsilon_1) \sum_{\sigma_1} \langle\langle a_1 | a_0^+ R_{01}' \rangle\rangle = g \sum_{\sigma_1} \langle\langle X_1 | a_0^+ R_{01}' \rangle\rangle,$$

$$(z-\varepsilon_1) \sum_{\sigma_1} \langle\langle a_1 | X_0^+ R_{01}' \rangle\rangle = g \sum_{\sigma_1} \langle\langle X_1 | X_0^+ R_{01}' \rangle\rangle,$$

$$(z-\varepsilon_f) \sum_{\sigma_1} \langle\langle X_1 | a_0^+ R_{01}' \rangle\rangle = N^{-1} \langle a_0^+ X_1 \rangle + Kg \sum_{\sigma_1} \langle\langle a_1 | a_0^+ R_{01}' \rangle\rangle,$$

$$(z-\varepsilon_f) \sum_{\sigma_1} \langle\langle X_1 | X_0^+ R_{01}' \rangle\rangle = N^{-1} [K(1-K) + \langle Z_{\mathbf{m}}^{\sigma_0 \sigma_0} \rangle + f_0^{(3)}]$$

$$+Kg \sum_{\sigma_1} \langle\langle a_1 | X_0^+ R_{01}' \rangle\rangle,$$

$$(z-\varepsilon_0) \langle\langle a_0 | X_0^+ \rangle\rangle = g \langle\langle X_0 | X_0^+ \rangle\rangle, \quad (z-\varepsilon_f) \langle\langle X_0 | X_0^+ \rangle\rangle = K + gK \langle\langle a_0 | X_0^+ \rangle\rangle.$$

Determining from this the Green's functions, and with their aid the mean values of interest to us, we get the following expressions which enable us, when account is taken of (13), to express $\lambda_{01}^{(4)}, \bar{\lambda}_{01}^{(5)}$ in terms of $\lambda^{(2)}, \lambda^{(3)}$:

$$f_{01}^{(4)} = K^{-1}N^{-1}f_0^{(2)}\bar{f}_1^{(2)},$$

$$\bar{f}_{01}^{(5)} = (NK)^{-1}[f_1^{(3)} - \langle Z_m{}^{22}\rangle]f_0^{(2)}.$$

[1] V. P. Zinov'ev, P. V. Gel'd, and A. L. Sokolov, Fiz. Tverd. Tela (Leningrad) 18, 1329 (1976) [Sov. Phys. Solid State 18, 764 (1976)].

[2] H. Katzman and J. A. Myodosh, Phys. Rev. Lett. 29, 998 (1972).

[3] G. Oomi and T. Mitsui, J. Phys. Soc. Jpn. 41, 705 (1976).

[4] A. J. Arko, M. B. Brodsky, and W. J. Nellis, Phys. Rev. B 5, 4564 (1972).

[5] E. E. Havinga, K. N. J. Buschow, and H. J. Van Daal, Solid State Commun. 13, 621 (1973).

[6] I. Peschel and P. Fulde, Z. Phys. 238, 99 (1970).

[7] M. B. Brodsky, Phys. Rev. B 9, 1381 (1974).

[8] M. Kamimoto, Y. Takahashi, and T. Mukaibo, J. Phys. Chem. Solids 37, 719 (1976).

[9] R. W. Cohen, G. D. Cody, and J. J. Halloran, Phys. Rev. Lett. 19, 840 (1967).

[10] B. Cournut and B. Coqblin, Phys. Rev. B 5, 4541 (1972).

[11] R. Jullien, M. T. Beal-Monod, and B. Coqblin, Phys. Rev. B 9, 1441 (1974).

[12] A. F. Barabanov, K. A. Kikoin, and L. A. Maksimov, Solid State Commun. 18, 1527 (1976).

[13] D. Wohlleben J. Phys. (Paris) 37, C4-232 (1976).

[14] C. M. Varma, Rev. Mod. Phys. 48, 219 (1976).

[15] J. R. Schrieffer and P. A. Wolff, Phys. Rev. 149, 491 (1966).

[16] E. V. Kuz'min, G. A. Petrakovskiĭ, and E. A. Zavadskiĭ, Fizika magnitouporyadochennykh veshchestv (Physics of Magnetically Ordered Substances), Nauka, Novosibirsk, 1976.

[17] A. F. Barabanov, K. A. Kikoin, and L. A. Maksimov, Teor. Mat. Fiz. 20, 364 (1974).

[18] E. S. Alekseev and A. F. Barabanov, Fiz. Tverd. Tela (Leningrad) 18, 1686 (1976) [Sov. Phys. Solid State 18, 979 (1976)].

[19] J. Hubbard, Proc. R. Soc. London Ser. A 285, 542 (1965).

[20] R. Kubo, J. Phys. Soc. Jpn. 12, 570 (1957).

[21] D. N. Zubarev, Usp. Fiz. Nauk 71, 71 (1960) [Sov. Phys. Usp. 3, 320 (1960)].

[22] M. Darby and K. N. Taylor, Physics of Rare-Earth Solids, Halsted, 1972.

[23] Yu. N. Smirnov and I. A. Prokhorov, Zh. Eksp. Teor. Fiz. 67, 1017 (1974) [Sov. Phys. JETP 40, 504 (1975)].

[24] V. M. Polovov, Zh. Eksp. Teor. Fiz. 65, 1557 (1973) [Sov. Phys. JETP 38, 775 (1974)].

[25] V. M. Polovov and L. G. Maĭstrenko, Zh. Eksp. Teor. Fiz. 68, 1418 (1975) [Sov. Phys. JETP 41, 707 (1975)].

[26] S. Doniach, Proc. of Seventeenth Conf. on Magnetism and Magnetic Materials, Chicago, 1971, AIP, New York, 1972.

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Many-particle impurity complexes in silicon doped with boron, phosphorus, and antimony

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Recombination radiation emitted at helium temperatures from silicon doped with boron, phosphorus, and antimony was investigated experimentally as a function of the photoexcitation conditions and uniaxial compression. The results obtained confirmed the formation of many-particle impurity complexes and were interpreted using the shell model of these complexes.

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1. INTRODUCTION

The recombination radiation spectra of silicon doped with group III and V elements exhibit, at helium temperatures, a series of narrow lines[1-3] located on the low-energy side directly beyond the bound-exciton peak.[4,5] The spectral positions of these lines in the series are characteristic for each of the dopants and the lines themselves appear in decreasing order of their energy as the excitation rate is increased. On this basis, it has been concluded[1-3] that the new lines are due to the radiative decay of many-particle complexes formed as a result of the consecutive capture of one, two, or more excitons by an impurity atom. We shall denote these complexes by $B_1, B_2, \ldots$ and the corresponding recombination radiation lines by $\alpha_1, \alpha_2, \ldots$, and so on.[6] Thus, a complex B_m consists of a singly charged impurity atom, m carriers of the same sign, and $m+1$ carriers of the opposite sign. A system of this kind is basically different from an ordinary atomic or molecular system because the latter contains light particles of just one sign.

The proposed explanation[1-3] of the origin of these α lines has been confirmed in a number of investigations[7-9] of the kinetics of formation and decay of many-particle complexes. Later investigations[10,11] have been concerned with the splitting of the α lines in a magnetic field and as a result of uniaxial deformation of silicon. According to these authors, the results obtained cannot be explained by any model of many-particle impurity complexes. It is suggested[10,11] that the

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