Kondo resonances and localized states on magnetic impurities in systems with charge- and spin-density waves

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The Kondo-resonance parameters (self-energy and occupation) in crystals with spin-density waves (SDW) and charge-density waves (CDW) are calculated by Anderson's $1/N$-expansion method for an isolated impurity. The energies of the impurity states localized inside a dielectric gap in such systems are also obtained. It is shown that dielectrization of the spectrum in a phase with an SDW or a CDW does not cause rapid suppression owing to the influence of the square-root singularity in the state density near the edges of the gap. The Kondo-resonance parameters depend on the type of sublattice (with higher or lower charge density) into which the impurity lands in the case of CDW, and do not depend on the type of the magnetic sublattice (with higher or lower spin density) in the case of SDW.

1. INTRODUCTION

The behavior of impurities in materials with charge- and spin-density waves (CDW and SDW) exhibits a number of interesting features due to the restructuring of the electronic and magnetic structures in vicinities on the order of the CDW and SDW correlation lengths. This structure can be self-consistently described only near the phase-transition point, by using the Ginzburg–Landau expansion for the thermodynamic potential $\Omega(\Delta)$ and taking into account the smallness and the slow variation of the order parameter $\Delta(\mathbf{r})$ (a discussion of the corresponding applicability criteria can be found, for example in Ref. 1). Extensive use is made also of non-self-consistent approaches, in which the magnitude and form of $\Delta(\mathbf{r})$, as well as the form of the defect potential $U(\mathbf{r})$ are regarded as given. The validity criteria of the assumptions in question are in general not obvious, but it is obviously necessary to satisfy the requirement that the defect potential be small, $|U| \ll |\Delta|$, and that it be located far from the transition point, i.e., deep in the interior of the ordered phase (see, in particular, one of the first papers[2]).

The restructuring of the electron density near a nonmagnetic point defect was considered in Ref. 3 for a Peierls system with CDS in an approximation with a rigid form of $\Delta(\mathbf{r})$, and in Ref. 4 for a magnetic defect with a frozen-in moment. An analysis similar to that in Ref. 3 was reported in Ref. 5 for a system with CDW. A detailed analysis of the electron spectrum of impurity states, and also of the singularities of the states of systems with SDW in the presence of nonmagnetic defects was carried out in Ref. 6. A similar problem was solved in Ref. 7 for magnetic defects with classical spins.

A common feature of the electronic spectra of defect-containing crystals with SDW and CDW is known to be the onset of localized states inside the energy gap in the ordered phase. The locations, the spin polarizations, and the radii of these states depend on the specific type and value of the potential of the defect in the matrix of the host material, and on the amplitude of the CDW or SDW, but the very presence of localized states in all the discussed structure types can be regarded as established. In fact, the calculations of these states are similar to those in Ref. 8 for the impurity levels in narrow-band A^4B^6 semiconductors. In the latter, the gap in the electron spectrum is determined by a rigorously prescribed "chemical" ionicity parameter, which can be interpreted (naturally, with some relaxed rigor), as the amplitude of a "frozen" CDW.

We intend to describe in this paper the energy spectrum of a single pointlike magnetic defect in a matrix of a commensurable CDW or SDW in the region of the ordered phase, with account taken of the quantum spin fluctuations (Kondo fluctuations). It is assumed that the above criteria of approach to a rigid form of the order parameter $\Delta(\mathbf{r})$ are met. It is assumed in addition that a Kondo state had been formed on the magnetic impurity, and the analysis is carried out for temperatures $T \ll (T_k, T_c)$, where T_c is the transition temperature and T_k is the Kondo temperature. In all the cited discussions of the behavior of magnetic impurities in systems with CDW or SDW, the role of the Kondo scattering was ignored and it was assumed in fact that the singlet state is perturbed (or, equivalently, the temperature range considered was $T \gg T_k$, but generally speaking $T < T_c$). We have recently discussed the role of the lower ("parquet") diagrams in electron–impurity scattering for systems with SDW, under the conditions $T \gg T_k$ and $T_k \ll T_c$. We shall therefore analyze here the case with the temperature relations reversed. We were unable, unfortunately, to consider with any degree of consistency the case $T \approx (T_k, T_c)$.

2. THE MODEL HAMILTONIAN

A system that is unstable to a transition into a CDW or SDW state is described by the standard model of a metal with congruent Fermi-surface segments separated by a distance equal to half the reciprocal lattice vector $\mathbf{Q} = \mathbf{G}/2$ (Ref. 9). The magnetic impurity is described in the context of a two-configuration model, in which the ion fluctuates between the states $f^0 = |0\rangle$ and $f^1 = |m\rangle$, where $m = (J, \ldots, -J)$, $N = 2J + 1$, and N is the degeneracy multiplicity of the state f^1 (the Anderson model of an impurity with N-fold degeneracy in one-center repulsion limit).[10] The interaction of band electrons with localized states of the magnetic ion is specified in the form of single-particle hybridization. The Hamiltonian of the investigated system takes thus the form

$$H = H_1 + H_2 + H_3 - \mu n, \tag{1}$$

where the Hamiltonian H_1 describes the band electrons in

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the mean-field approximation

$$H_1 = \sum_{k,\alpha} \varepsilon(\mathbf{k}) a_\alpha^+(\mathbf{k}) a_\alpha(\mathbf{k}) - \sum_{k,\alpha,\beta} [\Delta_{\beta\alpha} a_\alpha^+(\mathbf{k}) a_\beta(\mathbf{k}+\mathbf{Q}) + \text{c.c.}]. \quad (2)$$

Here $\Delta_{\beta\alpha} = (\Delta_t \sigma)_{\beta\alpha}$ in the SDW case and $\Delta_{\beta\alpha} = \Delta_s \delta_{\beta\alpha}$ for CDW, while Δ_t and Δ_s are the corresponding spin and charge order parameters. The band-electron dispersion law satisfies the "nesting" condition $\varepsilon(\mathbf{k}) = \varepsilon(\mathbf{k}+\mathbf{Q})$, μ is the chemical potential measured from the center of the band, n is the total-fermion-number operator, α and β are the spin indices, and σ is a vector made up of Pauli matrices. For convenience, we shall henceforth reckon the fermion energies directly from the Fermi level of the system, assuming μ to be known (e.g., fixed in the case of a reservoir of infinite size or, in the absence of a reservoir, self-consistently calculated from the condition that the total number of particles in the system is conserved). In the latter case the dependence of μ on Δ_t (Δ_s) is known:

$$\mu^2 = \mu_0^2 + \Delta_{s(t)}^2. \quad (3)$$

To be specific, we assume throughout that $\mu > 0$ (electron doping) and consider the situation at zero temperature ($T = 0$).

The Hamiltonian H_2 of a magnetic point defect can be expressed with the aid of the Hubbard operators $X_{00} = |0\rangle\langle 0|$, $X_{mm} = |m\rangle\langle m|$ in the form

$$H_2 = \sum_m E_1 X_{mm} + E_0 X_{00}, \quad (4)$$

where E_1 and E_0 are the energies of f^1 and f^0 configurations, respectively.

Single-particle transitions between localized f-orbitals of the impurity and the states of the band electrons (hybridization) are described in terms of the transition operators $X_{0m} = |0\rangle\langle m|$ and $X_{m0} = |m\rangle\langle 0|$ by the Hamiltonian

$$H_3 = \sum_{\mathbf{k},m,\alpha} [V_{m\alpha}(\mathbf{k}) X_{m0} a_\alpha(\mathbf{k}) + \text{c.c.}],$$
$$V_{m\alpha}(k) = V_m(\mathbf{k}) \langle \mathbf{k}, J, m | \mathbf{k}, \alpha \rangle. \quad (5)$$

The operators X_{0m} and X_{m0} do not satisfy the standard commutation relations, so that it is difficult to analyze the Hamiltonian H_3 by traditional diagram-technique methods. One of the most brilliant methods of solving this problem is to change from Hubbard operators to auxiliary boson (b) and fermion (f) operators[11] in accordance with the scheme

$$X_{0m} \to b^+ f_m, \quad X_{m0} \to f_m^+ b,$$
$$X_{mm'} \to f_m^+ f_{m'}, \quad X_{00} \to b^+ b. \quad (6)$$

The operators f_m and b satisfy the standard commutation rules. Expressing H_2 and H_3 in terms of the operators f_m and b we can write

$$H_2 = \sum_m E_1 f_m^+ f_m + E_0 b^+ b, \quad (7)$$

$$H_3 = \sum_{\mathbf{k},m,\alpha} [V_{m\alpha}(\mathbf{k}) f_m^+ b a_\alpha(\mathbf{k}) + \text{c.c.}]. \quad (8)$$

The operator H commutes with the operator of the total number of fermions and bosons on the impurity

$$Q = b^+ b + \sum_m f_m^+ f_m. \quad (9)$$

In our problem, the requirement $Q = 1$ must be rigorously satisfied. Nonphysical states can be formally excluded by adding to the Hamiltonian H the term $\lambda(Q-1)$ and going to the limit $\lambda \to \infty$ in the expressions for the physical mean values.[11]

3. DERIVATION OF BASIC RELATIONS IN THE MEAN-BOSON-FIELD APPROXIMATION AT $N \gg 1$

We use in the Hamiltonian (1) the mean-field approximation with respect to the Boson variable, i.e., we replace b and b^+ by their mean value[12]

$$\langle b^+ \rangle = \langle b \rangle = Z^{1/2}. \quad (10)$$

Equation (1) is then transformed into the single-particle Hamiltonian

$$H = H_1 + \sum_m \tilde{\varepsilon}_f f_m^+ f_m + Z^{1/2} \sum_{\mathbf{k},m,\alpha} [V_{m\alpha}(\mathbf{k}) f_m^+ a_\alpha(\mathbf{k}) + \text{c.c.}] + (\tilde{\varepsilon}_f - E_1)(Z-1) + E_0 Z, \quad (11)$$

where $\tilde{\varepsilon}_f = E_1 + \lambda$. The parameters Z of the theory of the mean field $\tilde{\varepsilon}_f$ are determined from the condition that the free energy of the system with the Hamiltonian (1) be a minimum. Carrying out in (11) a thermodynamic averaging and using the theorem $\partial \langle H(y) \rangle / \partial y = \partial H(y) / \partial y \rangle$, where y is a parameter of the Hamiltonian H, we get

$$Z = 1 - n_f, \quad (12)$$

$$(E_1 - E_0) - \tilde{\varepsilon}_f = -\frac{1}{2} Z^{-1/2} \sum_{\mathbf{k},m,\alpha} [\langle V_{m\alpha}(k) f_m^+ a_\alpha(k) \rangle + \text{c.c.}]. \quad (13)$$

We solve the system (12) and (13) by the Green's function method. The form of this function for fermions localized on site $\mathbf{R}_0$ is

$$G_{mm'}^{-1}(\varepsilon, \mathbf{R}_0) = (\varepsilon - \tilde{\varepsilon}_f)\delta_{mm'} - \Sigma_{mm'}(\varepsilon, \mathbf{R}_0), \quad (14)$$

where the self-energy part $\Sigma_{mm'}(\varepsilon, \mathbf{R}_0)$ can be written in the form

$$\Sigma_{mm'}(\varepsilon, \mathbf{R}_0) = Z \sum_{\mathbf{k},\alpha_1,\alpha_2} V_{m\alpha_1}(\mathbf{k}) \pi(\mathbf{k}, \varepsilon, \mathbf{R}_0) V_{m'\alpha_2}^*(\mathbf{k}) \delta_{mm'}, \quad (15)$$

$$\pi(\mathbf{k}, \varepsilon, \mathbf{R}_0) = G_{\alpha_1\alpha_2}^0(\mathbf{k}, \mathbf{k}, \varepsilon) + G_{\alpha_1\alpha_2}^0(\mathbf{k}, \mathbf{k}+\mathbf{Q}, \varepsilon) \exp i\mathbf{Q}\mathbf{R}_0, \quad (16)$$

$$G_{\alpha_1\alpha_2}^0(\mathbf{k}, \mathbf{k}, \varepsilon) = [\varepsilon + \mu + \varepsilon(\mathbf{k})] [(\varepsilon+\mu)^2 - \varepsilon^2(\mathbf{k}) - \Delta_{s(t)}^2]^{-1} \delta_{\alpha_1\alpha_2}, \quad (17)$$

$$G_{\alpha_1\alpha_2}^0(\mathbf{k}, \mathbf{k}+\mathbf{Q}, \varepsilon) = -B_{\alpha_1\alpha_2}^{s(t)} [(\varepsilon+\mu)^2 - \varepsilon^2(\mathbf{k}) - \Delta_{s(t)}^2]^{-1}, \quad (18)$$

$$B_{\alpha_1\alpha_2}^s = \Delta_s \delta_{\alpha_1\alpha_2}, \quad B_{\alpha_1\alpha_2}^t = \Delta_t \sigma_{\alpha_1\alpha_2}^z \quad (19)$$

for SDW and CDW, respectively. The factor $\exp iQR_0 = \pm 1$ is determined by the position R_0 of the impurity in the lattice relative to nonequivalent sites with maximum or minimum SDW (CDW). The filling of the f-level is determined by the known relation

$$n_f = -\pi^{-1} \sum_m \int f(\varepsilon) \operatorname{Im} G_{mm}(\varepsilon, \mathbf{R}_0) d\varepsilon, \quad (20)$$

where $f(\varepsilon)$ is the Fermi distribution function. A detailed expression for $G_{mm}(\varepsilon, \mathbf{R}_0)$ and n_f is given in the Appendix.

In the absence of SDW (CDW) it is easy to obtain from (20) the known result[12]

$$n_f = N\pi^{-1}\,\mathrm{arcctg}(\tilde{\varepsilon}_f/\Theta), \quad \tilde{\varepsilon}_f > 0, \tag{21}$$

$$\Theta = Z\Theta_0, \quad \Theta_0 = 2\pi N(0)V^2/N, \tag{22}$$

where $N(0)$ is the density of the states of the band electrons and $V_m = VN^{-1/2}$. Since $\tilde{\varepsilon}_f/\Theta \sim N$, we have for $N \gg 1$

$$n_f = N\Theta/\pi\tilde{\varepsilon}_f = (N\Theta_0/\pi\tilde{\varepsilon}_f)[1+(N\Theta_0/\pi\tilde{\varepsilon}_f)]^{-1}.$$

The energy of the resonant level is calculated from relation (13), which can be rewritten in the form

$$(E_1 - E_0) - \tilde{\varepsilon}_f = -Z^{1/2}\pi^{-1}\int f(\varepsilon)\,\mathrm{Im}\,\Phi(\varepsilon, \tilde{\varepsilon}_f, \mathbf{R}_0)\,d\varepsilon. \tag{23}$$

An expression for $\Phi(\varepsilon, \tilde{\varepsilon}_f, R_0)$ is given in the Appendix.

4. ENERGY OF RESONANT LEVEL AND ITS OCCUPATION IN SYSTEMS WITH SDW AND CDW

A. Systems with SDW

It follows from the computation given in the Appendix that, in the lowest (zeroth) order in (N^{-1}), the right-hand sides of Eqs. (20) and (23) for systems with SDW contain no dependences on the position $\mathbf{R}_0$ of the magnetic impurity in the lattice (such a dependence appears only at term values $\sim (N^{-1})^2$. We shall consider below two regimes, dielectric ($\mu < \Delta_t$) and metallic ($\mu > \Delta_t$), and to be specific we shall bear in mind the case of electron alloying ($\mu > 0$). Note that the metallic regime always obtains in a model with a fixed number of particles, where $\mu = (\mu_0^2 + \Delta_t^2)^{1/2}$, and μ_0 is the deviation from half-occupation in the paramagnetic phase. The dielectric regime $\mu < \Delta_t$ is realized in a model with a "reservoir," the role of which can be assumed, for example, by noncongruent sections of the Fermi surface, which do not participate in the formation of SDW (or CDW).

It follows thus from Eqs. (A6), (A7), and (A9), (A10) that the resonance-level parameters ε_f and n_f, where $\varepsilon_f = \tilde{\varepsilon}_f + \mu$ is the energy measured from the half-filled level of the band, does not depend explicitly on μ if $\mu < \Delta_t$. The asymptotic behavior of the quantities ε_f and n_f can in some limiting cases be determined relatively simply. Thus, for $|\varepsilon_f|^2 \gg \Delta_t^2$ we have

$$\varepsilon_f = \varepsilon_0[1 - n_0(\Delta_t/2^{1/2}\varepsilon_0)^2 \ln(2\varepsilon_0/\Delta_t)],$$
$$n_f = n_0 + n_0(1-n_0)(n_0-2)(\Delta_t/2^{1/2}\varepsilon_0)^2 \ln[2\varepsilon_0/\Delta_t], \tag{24}$$

$$\varepsilon_0 = D\exp(-\pi|\varepsilon_1|/N\Theta_0), \tag{25}$$

$$n_0 = (N\Theta_0/\pi\varepsilon_0)(1+N\Theta_0/\pi\varepsilon_0)^{-1}, \tag{26}$$

it being assumed that $\varepsilon_1 = -|\varepsilon_1|$, $|\varepsilon_1| \gg \varepsilon_f, \Delta_t, \mu$, i.e., the single-particle excitation level ε_1 is deeply lower than the Fermi level.

For $|\varepsilon_f|^2 \ll \Delta_t^2$ we have

$$\varepsilon_f = \varepsilon_0[1 - n_1 + n_1(2\Delta_t/\pi\varepsilon_0)\ln[2\varepsilon_0/\Delta_t]] < 0, \tag{27}$$

$$n_f = n_1 = (N\Theta_0/2\Delta_t)(1+N\Theta_0/2\Delta_t)^{-1}. \tag{28}$$

Thus, in the region of low values $\Delta_t \ll \varepsilon_0$, the level ε_f decreases in proportion to $(\Delta_t/\varepsilon_0)^2 \ln(2\varepsilon_0/\Delta_t)$, passes next through the middle of the gap at $^*\Delta_t = 2\varepsilon_0 \exp[n_0/(1-n_0)]$, and with further increase of Δ_t its absolute value increases but stays negative and remains all the time inside the gap. The occupation n_f decreases everywhere with increase of Δ_t, tending to zero at $\Delta_t \gg \varepsilon_0$, i.e., its Kondo state is disturbed.

The analysis of the behavior of ε_f and n_f in the metallic state ($\mu > \Delta_t$) is somewhat more complicated. At $\varepsilon_f, \mu \gg \Delta_t$ (small gap):

$$\varepsilon_f = \mu + \varepsilon_0\left[1 - n_0\left(\frac{\Delta_t}{2^{1/2}(\varepsilon_0+\mu)}\right)^2\left[\frac{\varepsilon_0+\mu}{\mu} + \ln\frac{\varepsilon_0}{\mu}\right]\right], \tag{29}$$

$$n_f = n_0 + n_0(1-n_0)\left(\frac{\Delta_t}{\varepsilon_0+\mu}\right)^2\left[\left(\frac{n_0}{2} - \frac{\varepsilon_0}{\varepsilon_0+\mu}\right)\ln\frac{\varepsilon_0}{\mu} + \frac{(n_0-1)}{2}\frac{(\varepsilon_0+\mu)}{\mu} - 1\right]. \tag{30}$$

It can be seen that if $\varepsilon_0 \gg \mu$ the qualitative behavior of ε_f and n_f is similar to the one considered above: as Δ_t increases the energy ε_f of the level and its population n_f decrease. If $\varepsilon_0 \ll \mu$, however, as follows from (29) and (30), the picture becomes qualitatively different: Δ_f begins to increase as Δ_t increases, whereas n_f decreases as before. As Δ_t rises (large gap) we obtain in the $|\varepsilon_f| \ll \mu$, Δ_t, regime

$$\varepsilon_f = \varepsilon_0\left[1 - n_2 - n_2\frac{\Delta_t}{\varepsilon_0}\ln\left[\frac{\mu + (\mu^2-\Delta_t^2)^{1/2}}{2\varepsilon_0}\right] \times\left[\frac{\pi}{2} + \mathrm{arctg}\frac{(\mu^2-\Delta_t^2)^{1/2}}{\Delta_t}\right]^{-1}\right], \tag{31}$$

$$n_f = n_2 = \frac{\tilde{g}}{\Delta_t}\Big/\left(1 + \frac{\tilde{g}}{\Delta_t}\right),$$

$$\tilde{g} = \frac{N\Theta_0}{\pi}\left[\frac{\pi}{2} + \mathrm{arctg}\frac{(\mu^2-\Delta_t^2)^{1/2}}{\Delta_t}\right], \tag{32}$$

i.e., a behavior similar to (27) and (28): ε_f increases logarithmically in absolute value, dropping below the middle of the gap but remaining in the gap, while n_f decreases and tends to zero with increase of Δ_t. Thus, in the metallic phase the Kondo-resonance energy can vary nonmonotonically at $\varepsilon_0 \ll \mu$ and have a maximum at $\Delta_t \sim \varepsilon_0$. This effect is due to a competition between two factors-partial dielectrization of the spectrum, which by itself keeps some of the band states the inside the gap from producing Kondo-resonances, and enhancement of the Kondo scattering by the increase of the allowed-states density near the edge of the gap.

B. Systems with CDW

In contrast to systems with SDW, the energy and occupation of a Kondo resonance depend strongly on the location $\mathbf{R}_0$ of the impurity in the lattice relative to the maximum or minimum of the charge-density wave [see Eqs. (A11)–(A14)]. This is due to the singlet structure of the Kondo state formed in an effective potential that is different in sublattices with higher or lower electron density ($\exp i\mathbf{Q}\mathbf{R}_0 = \pm 1$). By analogy with Sec. A, we present for the dielectric regime ($\mu < \Delta_s$), in zeroth order in (N^{-1}), the asymptotic expression

$$\varepsilon_f^{\pm} = \varepsilon_0\left[1 \mp \frac{\Delta_s}{\varepsilon_0} n_0 \ln\frac{2\varepsilon_0}{\Delta_s}\right], \tag{33}$$

$$n_f^{\pm} = n_0\left[1 \mp \frac{\Delta_s}{\varepsilon_0}(1-n_0)^2 \ln\frac{2\varepsilon_0}{\Delta_s}\right] \tag{34}$$

for $|\varepsilon_f^{\pm}|^2 \gg \Delta_s^2$. Evidently, with the increase of Δ_s, depending on the type of sublattice (maximum or minimum of the CDW), the values of $\varepsilon_f^{\pm}$ decrease (upper sign) or increase

(lower sign) with increase of $\varepsilon_f^{\pm}$, i.e., the Kondo resonance is weakened in the former case and strengthened in the latter. With further increase of Δ_s the values of $\varepsilon_f^{\pm}$ pass through zero at

$$\Delta_s = \overset{*}{\Delta}_s{}^{\pm} = 2\varepsilon_0 \exp\{[n_0/(1-n_0)] \mp \pi/2\},$$

(here ε_f^- has a maximum but ε_f^+ does not), after which their moduli increase logarithmically, they become negative, and are always located inside the gap. If $\Delta_s \gg |\varepsilon_f|$, we get

$$\varepsilon_f^{\pm} = \varepsilon_0 \left[1 + n_0(1-n_0)^{-1} \left(\ln \frac{2\varepsilon_0}{\Delta_s} \mp \frac{\pi}{2} \right) \right], \tag{35}$$

$$n_f^{\pm} = \frac{g_{\pm}}{\Delta_s} \left(1 + \frac{g_{\pm}}{\Delta_s} \right)^{-1}, \quad g_{\pm} = \frac{N\Theta_0}{\pi} \left(\frac{\pi}{2} \mp 1 \right). \tag{36}$$

In the metallic regime ($\mu > \Delta_s$) we obtain, just as in Sec. A, if $\varepsilon_f^2 \gg \Delta_s^2$ and $\mu^2 \gg \Delta_s^2$

$$\varepsilon_f^{\pm} = \mu + \varepsilon_0 \left[1 \mp \frac{\Delta_s}{\varepsilon_0 + \mu} \ln \frac{\varepsilon_0}{\mu} \right], \tag{37}$$

$$n_f^{\pm} = n_0 \left[1 \pm (1-n_0) \left(\frac{\Delta_s}{\varepsilon_0 + \mu} \right) \left[1 + \left(n_0 - \frac{\varepsilon_0}{\varepsilon_0 + \mu} \right) \ln \frac{\varepsilon_0}{\mu} \right] \right], \tag{38}$$

and if $\varepsilon_f^2 \ll \Delta_s^2, \mu^2$:

$$\varepsilon_f^{\pm} = \varepsilon_0 (1 - \tilde{n}_f^{\pm}) \left[1 + n_0(1-n_0)^{-1} \left[\ln \frac{2\varepsilon_0}{\mu + (\mu^2 - \Delta_s^2)^{1/2}} \mp \left(\frac{\pi}{2} + \operatorname{arctg} \frac{(\mu^2 - \Delta_s^2)^{1/2}}{\Delta_s} \right) \right] \right], \tag{39}$$

$$\tilde{n}_f^{\pm} = \frac{\tilde{g}_{\pm}}{\Delta_s} \Big/ \left(1 + \frac{\tilde{g}_{\pm}}{\Delta_s} \right), \quad \tilde{g}_{\pm} = \frac{N\Theta_0}{\pi} \left[\frac{\pi}{2} + \operatorname{arctg} \frac{(\mu^2 - \Delta_s^2)^{1/2}}{\Delta_s} \pm \frac{(\mu^2 - \Delta_s^2)^{1/2}}{\mu} \mp 1 \right]. \tag{40}$$

Analysis shows that if $\varepsilon_0 > \mu$ the qualitative behavior of the $\varepsilon_f^{\pm}(\Delta_s)$ and $n_f^{\pm}(\Delta_s)$ dependences in the metallic phase differs little from the "dielectric" case ($\mu < \Delta_s$). If $\varepsilon_0 < \mu$, however, this behavior is strongly altered: sublattices with maxima (upper signs in all the equations) and with minima (lower signs) of the CDW so to speak exchange places, i.e., the value of ε_f^+ increases with increase of Δ_s, passes through a maximum at $\varepsilon_0 \sim \Delta_s$, and then decreases logarithmically, whereas ε_f^- decreases monotonically. Recall that if $\varepsilon_0 > \mu$ the value of ε_f^+ decreases monotonically, while ε_f^- has a maximum at $\varepsilon_0 \sim \Delta_s$.

A complete analysis of the behavior of the Kondo-resonance parameters ε_f and n_f at arbitrary relations between the values of ε_0, μ, and $\Delta_{s,t}$ can be carried out only numerically and is not our purpose here. At the same time, many qualitative features (e.g., the dependence of ε_f on the size of the gap) can be already qualitatively understood from the simple estimates above. We shall consider this question in Sec. 6 below.

5. LOCALIZED STATES INSIDE A DIELECTRIC GAP IN A CRYSTAL WITH SDW AND CDW

Beside the Kondo resonances, which exist in principle in the absence of SDW or CDW, the presence of such ordering can give rise to localized single-electron states of special type, due to singularities of the band spectra of crystals with SDW or CDW. These states separate from the (upper or lower) edge of the dielectric gap even in the case of ordinary potential electron-impurity scattering, and lead to a strong spatial (charge and spin) redistribution of the band electrons in a region of the order of the correlation length around the defect. To calculate the energy of such a state it suffices to have an expression for the pole of the matrix of the scattering of band electrons by the defect. Leaving out the simple intermediate calculations, we write the sought relation in the form

$$1 + \overline{U}(\omega)\Gamma_{t,s}(\omega) = 0, \quad |\omega| < \Delta_{s,t}, \tag{41}$$

$$\overline{U}(\omega) = U(\omega - \varepsilon_f)^{-1} = U_0(1-n_f)/(\omega - \varepsilon_f), \quad U_0 = \Theta_0 N,$$

$$U = U_0(1-n_f), \tag{42}$$

$$\Gamma_t(\omega) = \omega(\Delta_t^2 - \omega^2)^{-1/2}, \tag{43}$$

$$\Gamma_s(\omega) = (\omega \mp \Delta_s)(\Delta_s^2 - \omega^2)^{-1/2}. \tag{44}$$

Equation (41) is similar to the analogous expression given in Refs. 6–8, but the effective scattering potential $\overline{U}(\omega)$ depends now on the frequency ω, making the analysis of the solution (41) more complicated. Solutions (41) can in principle be written in the form of roots of a cubic equation. For a qualitative assessment of the feasibility of a localized state and for asymptotic estimates it is more convenient to use a graphic method.

A. Systems with SDW

It is easy to verify that the equation

$$\varepsilon_f - \omega = U\omega(\Delta_t^2 - \omega^2)^{-1/2}, \tag{45}$$

always has a unique solution $\omega = \omega_0$ in the interval $|\omega| \ll \Delta_t$. For $\varepsilon_f \gg \Delta_t$, neglecting terms proportional to Δ_t/ε_f, we get

$$\omega_0 = \Delta_t(1 + U^2/\varepsilon_f^2)^{-1/2} < \Delta_t. \tag{46}$$

If $|\varepsilon_f| \ll \Delta_t$ we have for both positive and negative ε_f

$$\omega_0 = \varepsilon_f(1 + U/\Delta_t)^{-1}. \tag{47}$$

B. Systems with CDW

The equation

$$\varepsilon_f - \omega = U(\omega \mp \Delta_s)(\Delta_s^2 - \omega^2)^{-1/2}, \tag{48}$$

does not always have a real solution in the region $|\omega| \ll \Delta_s$. It is easily shown that for a site with a maximum CDW [upper sign in Eq. (48)] no such solution exists at $\varepsilon_f^+ > \Delta_s$, appears jumpwise at $\varepsilon_f^+ = \Delta_s$ ($\omega_0 \to \Delta_s$ for $\varepsilon_f^+ = \Delta_s, -\varepsilon$, where ε is an infinitesimal positive quantity), and exists in the entire $\varepsilon_f^+ < \Delta_s$ region regardless of the sign of ε_f^+. For a site with minimum CDW [lower sign in (48)] the situation is different, i.e., a real solution is absent at $\varepsilon_f^- < -\Delta_s$, appears jumpwise at $\varepsilon_f^- = -\Delta_s$, and exists next for all $\varepsilon_f^- > -\Delta_s$. We have not considered the case of hole doping, when a situation $\varepsilon_f^{\pm} < -\Delta_s$ can arise, so that formally a localized state always exists for electron doping in sites with minimum CDW, while in sites with maximum CDW it exists only in a bounded region of the model parameters.

In the case of hole doping, the sublattices with minimum and maximum CDW change places from the standpoint of formation of localized states, and all the arguments above remain valid apart from interchange of the terms "maximum CDW" and "minimum CDW." We present a

few asymptotic estimates.

For $\varepsilon_f \ll \Delta_s$ we have

$$\omega_0^- \approx \Delta_s(1-U^2/\varepsilon_f^2)(1+U^2/\varepsilon_f^2)^{-1} < \Delta_s, \tag{49}$$

and there is no ω_0^+. For $\varepsilon_f \ll \Delta_s$

$$\omega_0^\pm = \varepsilon_f \pm U, \quad U \ll \Delta_s, \tag{50}$$

$$\omega_0^\pm = \pm\Delta_s \mp 2\Delta_s(\Delta_s/U)^2, \quad U \gg \Delta_s. \tag{51}$$

For $\varepsilon_f \to \Delta_s$ but $\varepsilon_f \leqslant \Delta_s$ we have

$$\begin{aligned} &\omega_0^+ \to \Delta_s, \quad U \ll \Delta_s, \\ &\omega_0^- \to \Delta_s - (2\Delta_s)^{1/3}U^{2/3}, \quad U \ll \Delta_s, \end{aligned} \tag{52}$$

$$\begin{aligned} &\omega_0^+ \to \Delta_s, \quad U \gg \Delta_s, \\ &\omega_0^- \to -\Delta_s + (2\Delta_s)^3/U^2, \quad U \gg \Delta_s. \end{aligned} \tag{53}$$

A localized state in a system with SDW is always located above the middle of the electric gap, and its energy does not depend explicitly on the character of the doping and on the type of the sublattice containing the defect. In systems with CDW, depending on the defect parameters, a localized state can lie either above or below the middle of the gap, and its energy is determined essentially by the sublattice type and by the character of the doping (electron or hole). In particular, in the case of a strong Kondo resonance, when $|\varepsilon_f| > \Delta_s$ no bound state is produced at all for one of the sublattices.

6. DISCUSSION OF RESULTS

The analysis above permits three important qualitative statements to be made.

1. Dielectrization of the spectrum in systems with CDW and SDW influences the suppression of the Kondo resonance quite weakly (logarithmically weakly even at large values of the parameter $\Delta/\varepsilon_0 \gg 1$). The reason is the partially compensating influence of the singularities in the density of the band states near the gap edge. As a result, the Kondo resonance is preserved even deeply in the dielectric phase and lies inside the gap in the electron spectrum.

2. The location of the Kondo resonance in a normal metallic phase is known to be determined by the location of the Fermi level. In the dielectric phase this resonance is rigidly connected to the position of the gap edges 2Δ. In systems with SDW, the Kondo-level energy and density are equal for both sublattices (with spin density "up" or "down"), while in systems with CDW they are unequal, depending on the type of sublattice (with excess or shortage of charge density).

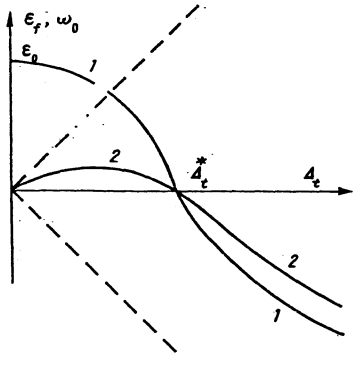

FIG. 1. Qualitative dependences of impurity-state energy levels on SDP amplitude: *1*—$\varepsilon_f(\Delta_t)$, *2*—$\omega_0(\Delta_t)$.

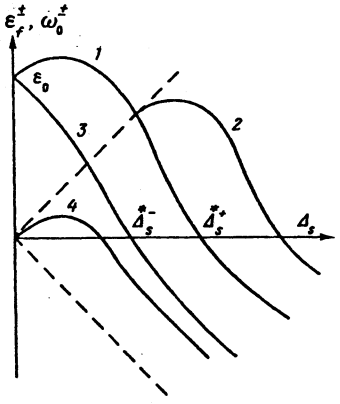

FIG. 2. Qualitative dependences of impurity-state energy levels on CDP amplitude: *1*—$\varepsilon_f^+(\Delta_s)$, *2*—$\omega_0^+(\Delta_s)$, *3*—$\varepsilon_f^-(\Delta_s)$, *4*—$\omega_0^-(\Delta_s)$.

3. Single-particle localized states of band electrons are produced inside the dielectric gap in systems with Kondo impurities alongside with Kondo resonances. In systems with SDW this takes place independently of the position of the impurity in any of the sublattices, whereas in systems with CDW the localized states have different energies for different sublattices, and may even be absent from one of them under certain conditions.

By way of illustration, Figs. 1 and 2 show approximate dependences of ε_f and ω_0 on $\Delta_{t,s}$ for crystals with SDW and CDW in the dielectric phase ($\mu = 0$, half-filled bands). The dependences of ε_f and ω_0 on the doping level can also be plotted, but account must then be taken of the dependence of $\Delta_{t,s}$ on μ. The main qualitative feature of doped systems with CDW and SDW, which follows from the equations of Sec. 4, is that at $\mu > \varepsilon_0$ the value of ε_f can exceed the corresponding value in the normal phase (i.e., metallic without SDW or CDW). The functions $\varepsilon_f(\mu)$ and $\omega_0(\mu)$ themselves are nonmonotonic and have characteristic maxima at certain values of μ. Figures 3 and 4 show as examples approximate plots of $\varepsilon_f(\mu_0)$ for systems with fixed numbers of particles (the SDW and CDW cases, respectively), when

$$\mu^2 = \mu_0^2 + \Delta^2, \quad \Delta^2 = \Delta_0(\Delta_0 - 2\mu_0),$$

and Δ_0 is the amplitude of the SDW (or CDW) in the absence of doping.

We consider in conclusion the possibility of applying our results to some actual objects. The SDW model is known[13] to describe fairly well antiferromagnetism in a

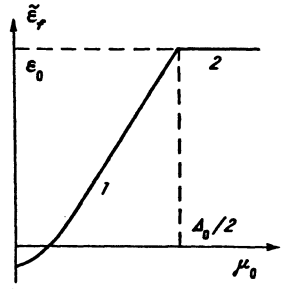

FIG. 3. Qualitative dependence of reduced Kondo-resonance energy $\tilde{\varepsilon}_f$ on the band occupation: *1*—in a phase with SDP; *2*—in a normal phase.

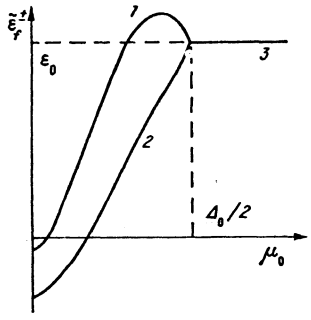

FIG. 4. Qualitative dependence of reduced Kondo-resonance energy $\tilde{\varepsilon}_f$ on the band occupation: *1*, *2*—in phase with CDW for different sublattices, *3*—in normal phase.

number of band magnets. Suitable candidates for our problem may be dilute Cr–Fe(Co)–V alloys with low Néel temperature, $T_N < T_k$ (it is known that weak V doping suppresses strongly the T_N of pure chromium, and according to certain data[14] T_k for Fe in Cr is < 50 K, so that at V densities close to 3–4% one can hope to satisfy the criteria called for by our theory). One can furthermore hope that addition of Fe to the band ferromagnet NiMn is a Kondo impurity in a system with SDW (Ref. 15). It can be assumed that other transition-metal and rare-earth-metal impurities, or nonstoichiometry defects in ordered alloys such as Pt_3Fe, FeRh, and the already mentioned NiMn can be qualitatively described in the framework of the proposed model. Possible examples of systems with CDW and Kondo impurities are apparently A^4B^6 semiconductors with rare earths (such as Gd) and transition metals (such as Mn). It would be of interest to track the behavior of the Kondo resonance ε_f and of the local levels $\omega_0^{\pm}$, for example of optical measurements, when the ionicity parameter Δ (Ref. 8) (an "analog" of Δ_s) in ternary systems with substitution of a nonmagnetic metal (for example, $Pb_{1-x}Sn_xTe$:Gd). It would be of interest to investigate from this viewpoint of Kondo anomalies also traditional Peierls quasi-one-dimensional and layered systems with transition or rare-earth magnetic metals as impurities.

In closing, one more important class of objects to which the proposed model may be applicable comprises magnetic impurities (or magnetic-metal films) on reconstructed surfaces. For example, a magnetic impurity on a W(001) or Mo(001) surface can apparently be an example of a situation with CDW (Ref. 16), while a magnetic impurity on an Si(III) surface can be an example of a situation with SDW, if one accepts a statement made by a number of workers[17] that the reconstruction mechanism in this system is of "antiferromagnetic" origin.

APPENDIX

The function $G_{mm}(\varepsilon,R_0)$ is given by

$$G_{mm}(\varepsilon,\mathbf{R}_0)=[\varepsilon-\mu-\varepsilon_f+i\Theta\,\mathrm{sign}\,\varepsilon D_{t,s}^m(\varepsilon,\mathbf{R}_0)]^{-1}, \quad (A1)$$

$$D_t^m(\varepsilon,\mathbf{R}_0)=(\varepsilon^2-\Delta_t^2)^{-1/2}\left(\varepsilon\mp\frac{m}{J+1}\Delta_t\right), \quad (A2)$$

$$D_s^m(\varepsilon,\mathbf{R}_0)=(\varepsilon^2-\Delta_s^2)^{-1/2}(\varepsilon-\Delta_s\exp i\mathbf{Q}\mathbf{R}_0). \quad (A3)$$

The energy ε is measured from the middle of the band. The integration in the expression for n_f is in the intervals $\{-D,-\Delta_t(\Delta_s)\}$ and $\{\Delta_t(\Delta_s),\mu\}$, if $\mu>\Delta_t(\Delta_s)$, and in the interval $\{-D,-\Delta_t(\Delta_s)\}$ if $0<\mu<\Delta_t(\Delta_s)$. The function $\Phi(\varepsilon,\varepsilon_f,\mathbf{R}_0)$ is obtained from the relation

$$Z^{1/2}\Phi(\varepsilon,\varepsilon_f,\mathbf{R}_0)=\sum_m G_{mm}(\varepsilon,\mathbf{R}_0)\,(-i\Theta_0\,\mathrm{sign}\,\varepsilon D_{t,s}^m(\varepsilon)). \quad (A4)$$

The intergration over ε in (23) is as in (20) for n_f.

In the lowest order of the expansion in $1/N$, calculation of the integral over the energy in (20) yields for SDW

$$n_f=\frac{N\Theta}{\pi}F_t(\Delta_t,\mu,\varepsilon_f), \qquad \varepsilon_f=\tilde{\varepsilon}_f+\mu. \quad (A5)$$

For $\varepsilon_f^2>\Delta_t^2$ we have

$$F_t(\Delta_t,\mu,\varepsilon_f)=\left[\frac{\varepsilon_f}{\varepsilon_f^2-\Delta_t^2}-\frac{\Delta_t^2}{(\varepsilon_f^2-\Delta_t^2)^{3/2}}\times\ln\left|\frac{\varepsilon_f+(\varepsilon_f^2-\Delta_t^2)^{1/2}}{\Delta_t}\right|\right]\Theta(\Delta_t-\mu)$$
$$+\left[\frac{\varepsilon_f}{\varepsilon_f^2-\Delta_t^2}\left[1-\frac{(\mu^2-\Delta_t^2)^{1/2}}{\mu-\varepsilon_f}\right]-\frac{\Delta_t^2}{(\varepsilon_f^2-\Delta_t^2)^{3/2}}\times\ln\left|\frac{(\varepsilon_f+(\varepsilon_f^2-\Delta_t^2)^{1/2})(\mu\varepsilon_f-\Delta_t^2-(\mu^2-\Delta_t^2)^{1/2}(\varepsilon_f^2-\Delta_t^2)^{1/2})}{(\varepsilon_f-\mu)\Delta_t^2}\right|\right]$$
$$\times\Theta(\mu-\Delta_t). \quad (A6)$$

For $\varepsilon_f^2<\Delta_t^2$ we have

$$F(\Delta_t,\mu,\varepsilon_f)=\left[\frac{\varepsilon_f}{\varepsilon_f^2-\Delta_t^2}+\frac{\Delta_t^2}{(\Delta_t^2-\varepsilon_f^2)^{3/2}}\mathrm{arctg}\left[\frac{\Delta_t^2-\varepsilon_f^2}{\varepsilon_f^2}\right]^{1/2}\right]\Theta(\Delta_t-\mu)$$
$$-\left[\frac{\varepsilon_f}{\varepsilon_f^2-\Delta_t^2}\left[1-\frac{(\mu^2-\varepsilon_f^2)^{1/2}}{\mu-\varepsilon_f}\right]+\frac{\Delta_t^2}{(\Delta_t^2-\varepsilon_f^2)^{3/2}}\times\left[\mathrm{arctg}\left[\frac{\Delta_t^2-\varepsilon_f^2}{\varepsilon_f^2}\right]^{1/2}+\mathrm{arctg}\,\frac{(\Delta_t^2-\varepsilon_f^2)^{1/2}(\mu^2-\Delta_t^2)^{1/2}}{|\Delta_t^2-\varepsilon_f\mu|}\right]\right]$$
$$\Theta(\mu-\Delta_t). \quad (A7)$$

A similar calculation of the integral over the energy in (23) yields for SDW ($\varepsilon_1=E_1-E_0+\mu$):

$$\varepsilon_1-\varepsilon_f=-\frac{N\Theta_0}{\pi}G_t(\Delta_t,\mu,\varepsilon_f). \quad (A8)$$

For $\varepsilon_f^2>\Delta_t^2$ we have

$$G_t(\Delta_t,\mu,\varepsilon_f)=\left[\ln\frac{2D}{\Delta_t}-\frac{\varepsilon_f}{(\varepsilon_f^2-\Delta_t^2)^{1/2}}\times\ln\left|\frac{\varepsilon_f+(\varepsilon_f^2-\Delta_t^2)^{1/2}}{\Delta_t}\right|\right]\Theta(\Delta_t-\mu)$$
$$+\left[\ln\frac{2D}{\mu+(\mu^2-\Delta_t^2)^{1/2}}-\frac{\varepsilon_f}{(\varepsilon_f^2-\Delta_t^2)^{1/2}}\ln\left|\frac{(\varepsilon_f+(\varepsilon_f^2-\Delta_t^2)^{1/2})}{\Delta_t^2}\times\frac{(\Delta_t^2-\mu\varepsilon_f+(\varepsilon_f^2-\Delta_t^2)^{1/2}(\mu^2-\Delta_t^2)^{1/2}}{\mu-\varepsilon_f}\right|\right]\Theta(\mu-\Delta_t). \quad (A9)$$

For $\varepsilon_f^2<\Delta_t^2$ we have

$$G_t(\Delta_t,\mu,\varepsilon_f)=\left[\ln\frac{2D}{\Delta_t}-\frac{\varepsilon_f}{(\Delta_t^2-\varepsilon_f^2)^{1/2}}\mathrm{arctg}\left[\frac{\Delta_t^2-\varepsilon_f^2}{\varepsilon_f^2}\right]^{1/2}\right]\Theta(\Delta_t-\mu)$$
$$+\left[\ln\frac{2D}{\mu+(\mu^2-\Delta_t^2)^{1/2}}-\frac{\varepsilon_f}{(\Delta_t^2-\varepsilon_f^2)^{1/2}}\left[\mathrm{arctg}\left[\frac{\Delta_t^2-\varepsilon_f^2}{\varepsilon_f^2}\right]^{1/2}+\mathrm{arctg}\,\frac{(\Delta_t^2-\varepsilon_f^2)^{1/2}(\mu^2-\Delta_t^2)^{1/2}}{|\Delta_t^2-\mu\varepsilon_f|}\right]\right]\Theta(\mu-\Delta_t). \quad (A10)$$

The relations for F_s and G_s for systems with CDW are

$$F_s^{\pm}(\Delta_s, \mu, \varepsilon_f)$$
$$= \left[\frac{\varepsilon_f \pm \Delta_s}{\varepsilon_f^2 - \Delta_s^2} - \frac{\Delta_s(\Delta_s \pm \varepsilon_f)}{(\varepsilon_f^2 - \Delta_s^2)^{3/2}} \ln\left|\frac{\varepsilon_f + (\varepsilon_f^2 - \Delta_s^2)^{1/2}}{\Delta_s}\right|\right] \Theta(\Delta_s - \mu)$$
$$+ \left[\frac{(\varepsilon_f \pm \Delta_s)}{\varepsilon_f^2 - \Delta_s^2}\left[1 - \frac{(\mu^2 - \Delta_s^2)^{1/2}}{\mu - \varepsilon_f}\right]\right.$$
$$- \frac{\Delta_s(\Delta_s \pm \varepsilon_f)}{(\varepsilon_f^2 - \Delta_s^2)^{3/2}} \ln\left|\frac{(\varepsilon_f + (\varepsilon_f^2 - \Delta_s^2)^{1/2}}{\Delta_s^2}\right.$$
$$\left.\left. \times \frac{(\Delta_s^2 - \varepsilon_f\mu + (\varepsilon_f^2 - \Delta_s^2)^{1/2}(\mu^2 - \Delta_s^2)^{1/2})}{\mu - \varepsilon_f}\right|\right] \Theta(\mu - \Delta_s), \quad \text{(A11)}$$

for $\varepsilon_f^2 > \Delta_s^2$,

$$F_s^{\pm}(\Delta_s, \mu, \varepsilon_f) = \left[\frac{\varepsilon_f \pm \Delta_s}{\varepsilon_f^2 - \Delta_s^2} + \frac{\Delta_s(\Delta_s \pm \varepsilon_f)}{(\Delta_s^2 - \varepsilon_f^2)^{3/2}}\right.$$
$$\left. \times \operatorname{arctg}\left[\frac{\Delta_s^2 - \varepsilon_f^2}{\varepsilon_f^2}\right]^{1/2}\right] \Theta(\Delta_s - \mu)$$
$$+ \left[\frac{\varepsilon_f \pm \Delta_s}{\varepsilon_f^2 - \Delta_s^2}\left[1 - \frac{(\mu^2 - \Delta_s^2)^{1/2}}{\mu - \varepsilon_f}\right]\right.$$
$$\left. + \frac{\Delta_s(\Delta_s \pm \varepsilon_f)}{(\Delta_s^2 - \varepsilon_f^2)^{3/2}}\left[\operatorname{arctg}\left[\frac{\Delta_s^2 - \varepsilon_f^2}{\varepsilon_f^2}\right]^{1/2}\right.\right.$$
$$\left.\left. + \operatorname{arctg}\frac{(\Delta_s^2 - \varepsilon_f^2)^{1/2}(\mu^2 - \Delta_s^2)^{1/2}}{|\Delta_s^2 - \varepsilon_f\mu|}\right]\right] \Theta(\mu - \Delta_s), \quad \text{(A12)}$$

for $\varepsilon_f^2 < \Delta_s^2$,

$$G_s^{\pm}(\Delta_s, \mu, \varepsilon_f) = \left[\ln\frac{2D}{\Delta_s} - \frac{\varepsilon_f \pm \Delta_s}{(\varepsilon_f^2 - \Delta_s^2)^{1/2}}\right.$$
$$\left. \times \ln\frac{\varepsilon_f + (\varepsilon_f^2 - \Delta_s^2)^{1/2}}{\Delta_s}\right] \Theta(\Delta_s - \mu)$$
$$+ \left[\ln\frac{2D}{\mu + (\mu^2 - \Delta_s^2)^{1/2}} - \frac{\varepsilon_f \pm \Delta_s}{(\varepsilon_f^2 - \Delta_s^2)^{1/2}} \ln\left|\frac{[\varepsilon_f + (\varepsilon_f^2 - \Delta_s^2)^{1/2}]}{\Delta_s^2}\right.\right.$$
$$\left.\left. \times \frac{[\Delta_s^2 - \mu\varepsilon_f + (\varepsilon_f^2 - \Delta_s^2)^{1/2}(\mu^2 - \Delta_s^2)^{1/2}]}{\mu - \varepsilon_f}\right|\right] \Theta(\mu - \Delta_s) \quad \text{(A13)}$$

for $\varepsilon_f^2 > \Delta_s^2$, and

$$G_s^{\pm}(\Delta_s, \mu, \varepsilon_f) = \left[\ln\frac{2D}{\Delta_s} - \frac{(\varepsilon_f \pm \Delta_s)}{(\Delta_s^2 - \varepsilon_f^2)^{1/2}}\right.$$
$$\left. \times \operatorname{arctg}\left[\frac{\Delta_s^2 - \varepsilon_f^2}{\varepsilon_f^2}\right]^{1/2}\right] \Theta(\Delta_s - \mu)$$
$$+ \left[\ln\frac{2D}{\mu + (\mu^2 - \Delta_s^2)^{1/2}} - \frac{(\varepsilon_f \pm \Delta_s)}{(\Delta_s^2 - \varepsilon_f^2)^{1/2}}\left[\operatorname{arctg}\left[\frac{\Delta_s^2 - \varepsilon_f^2}{\varepsilon_f^2}\right]^{1/2}\right.\right.$$
$$\left.\left. + \operatorname{arctg}\frac{(\Delta_s^2 - \varepsilon_f^2)^{1/2}(\mu^2 - \Delta_s^2)^{1/2}}{|\Delta_s^2 - \mu\varepsilon_f|}\right]\right] \Theta(\mu - \Delta_s), \quad \text{(A14)}$$

for $\varepsilon_f^2 < \Delta_s^2$.

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