Theory of coexistence between itinerant-electron antiferromagnetism and superconductivity

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The coexistence of spin-density waves and superconductivity has been theoretically analyzed in a two-band model, a case for which the commonly used descriptions for the ternary rare-earth compounds and highly anisotropic organic solids are unapplicable. The phase diagram at $T=0$, the temperature dependence of the order parameters, and the critical transition temperatures have been obtained. The theoretical results are in good agreement with the experiments concerning the Cr alloys.

I. INTRODUCTION

Owing to its theoretical and experimental importance, the interplay of magnetism and superconductivity has attracted much attention especially in the last decade. In this context, ferromagnetism (which usually destroys the superconducting phase) is opposed by other magnetic ordering which coexists with superconductivity.[1] Some exotic examples in this direction are the helical spin systems[2] and the spin glasses.[3] Furthermore, there is no *a priori* reason to exclude the coexistence of antiferromagnetism and superconductivity, because the superconducting coherent length is a hundred times greater than the periodicity of the antiferromagnetic order.[4] As to the itinerant systems only a small region of the Fermi surface is characterized by the nesting property—which gives rise to spin density waves[5] (SDW)—the remaining portion of the Fermi surface being used for superconducting pairing.[6]

So far, experimental evidence for the coexistence between antiferromagnetism and superconductivity has been clearly established for the RMo_6S_8 (Ref. 7) and RMo_6Se_8 (Ref. 8) Chevrel compounds, for the RRh_4B_4 ternary rare-earth borides[9] and for the highly anisotropic organic solids di-tetramethyltetraselenafulvalene salts $(TMTSF)_2X$ (Ref. 10).

One of the first theoretical works on this subject was by Baltensperger and Strassler[11] who proved that an electron gas in an ionic antiferromagnet can also be superconducting; however, in this case the pairing does not involve time-reversed waves. A few years later Petalas and Baltensperger[12] showed that an electron gas in SDW state can simultaneously carry superconductivity.

As a result of the discovery of the antiferromagnetic superconductors in the Chevrel phase and alongside the observation of the H_{c2} dip just below the Néel temperature in these materials,[7] the problem of the coexistence between antiferromagnetism and superconductivity has become of present interest. Starting from the model established by Fulde and Ferrell in one of their papers[13] (in which they proved that under a ferromagnetic molecular field a superconducting pairing state characterized by a spatially varying order parameter is more stable than the usual BCS state), Machida and co-workers[14] point out

that the formation of a similar superconducting pairing (characterized by the Δ_Q order parameter) becomes possible under an antiferromagnetic molecular field. However, Nass, Levin, and Grest,[15] (using a self-consistent treatment and taking into account fluctuation effects) demonstrate that Δ_Q is a vanishing quantity in the absence of an external magnetic field and that the superconducting pairing is of the usual BCS type. The paper of Sakai *et al.*[16] also deals with this problem, namely they consider an electromagnetic interaction, between the superconducting electrons and the localized spins, leaving aside the exchange effects. In the works of Machida,[17] Tachiki,[18] and Machida *et al.*[4] the effect on superconductivity of a staggered magnetic field H_Q produced by antiferromagnetism is studied. Suzumara and Nagi[19] also considered another magnetic field's influence (i.e., the external field) upon the superconducting phase. In this way, they connected the results deduced for $H_Q=0$ (Ref. 20) with the effects obtained in the presence of the staggered magnetic field. The pairbreaking in the superconducting phase, near and below the antiferromagnetic transition, has also been investigated by other authors (see Ref. 21).

The picture of the electronic origin which describes the coexistence of superconductivity and antiferromagnetism in rare-earth ternary compounds[4,14−21] is based on the observation that these materials have partially filled localized $4f$ electrons which are responsible for the antiferromagnetism. These local moments interact very weakly with the d-band conduction electrons which create the superconducting order. Thus, magnetism and superconductivity are carried by different type electrons of different ions. The coexistence in these compounds is described by taking into account a spatially periodic antiferromagnetic molecular field, created by the localized $4f$ electrons which act on the conduction electron system where the BCS coupling is realized. In general terms, the two long-range orders interfere destructively.

For the quasi-one-dimensional highly anisotropic organic structures $(TMTSF)_2X$, in which the superconducting phase coexists with SDW,[10] the theoretical description given by Machida, Fenton, and Psaltakis (see Refs. 6, 22, and 23) take into account a quasi-one-dimensional Fermi surface, characterized by two regions: one, in which the existing nesting condition gives rise to SDW and another

one, for which the electron-electron interaction is sufficiently attractive to cause the appearance of the superconducting phase. Depending on the portion of the Fermi surface opened by the SDW, the superconductivity is more or less supressed.

Recently, Kohara and co-workers[24] have experimentally found an entirely different kind of coexistence between antiferromagnetism and superconductivity in some Cr alloys. In this case, the studied compounds are not quasi-one-dimensional and highly anisotropic, such as $(TMTSF)_2X$, and they represent a typical two-band itinerant system, where the SDW-like itinerant antiferromagnetism is carried by the same d-band conduction electrons which are responsible for the superconducting pairing. Thus, a totally different theoretical description is needed in this case.

In this paper, we try to analyze the possibility of a coexistence between superconductivity and a two-band SDW, such as the one which is characteristic for the Cr alloys.[5,25]

The paper is organized as follows: in Sec. II we describe the Hamiltonian which characterizes the studied system and we deduce the Green's functions, the order-parameter equations, and the expression for the difference between the electron and hole concentration from the two-band (n). The phase diagrams for $T=0$ are obtained in Secs. III and IV for $n=0$ and $n\neq0$, respectively. Section V contains the analysis of the characteristic parameters at $T\neq0$. Section VI is dedicated to discussions and conclusions.

II. HAMILTONIAN, GREEN'S FUNCTIONS, AND GAP EQUATIONS OF THE MODEL

We start with the following Hamiltonian:

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_1+\mathcal{H}_{BCS}\ ,\tag{1}$$

where

$$\mathcal{H}_0=\sum_{k,\alpha}\zeta_a a_k^{\dagger\alpha}a_k^\alpha+\sum_{k,\alpha}\zeta_b b_k^{\dagger\alpha}b_k^\alpha\ ,\tag{2}$$

$$\mathcal{H}_1=\sum_{k,k'\,\alpha,\beta,\atop\gamma,\delta}(g_c\delta_{\alpha\beta}\delta_{\gamma\delta}+g_s\sigma_{\alpha\beta}\cdot\sigma_{\gamma\delta})(a_k^{\dagger\alpha}b_k^\beta b_k^{\dagger\gamma}a_{k'}^\delta+\text{H.c.})\ ,\tag{3}$$

$$\mathcal{H}_{BCS}=\tfrac{1}{2}\sum_{i,j,k}\sum_{\alpha,\beta}\lambda_{ij}c_{ik}^{\dagger\beta}c_{j-k}^{\dagger\alpha}c_{j-k}^\alpha c_{ik}^\beta\ .\tag{4}$$

The Hamiltonian (2) represents the kinetic energy of the electrons and holes from the two-band, for which $a_k^{\dagger\alpha}$, a_k^α and $b_k^{\dagger\alpha}$, b_k^α are the creation and annihilation operators ($b_k^\alpha\equiv b_{k+Q}^\alpha$). The unperturbed electronic band structure is modeled by $\zeta_a=\epsilon+\delta_\mu$ and $\zeta_b=-\epsilon+\delta_\mu$, where δ_μ is a measure of the electron and hole concentration difference, ζ_a and ζ_b being the kinetic energies of the electrons and holes as characteristic for the Cr alloys.[25] The g_c and g_s coupling constants cause the appearance of the charge density wave (CDW) and spin density wave (SDW) coupling between electrons and holes. In this way, we can define Δ_c the CDW and Δ_s the SDW order parameter [see Eqs. (6)]. $\mathcal{H}_{BCS}$ is a generalized form for the BCS Hamiltonian, whereby it can be described the interband and intraband BCS coupling with different coupling constants λ_{ij}. The band indices i and j can take independently the a and b values, $c_a^\dagger$ and $c_b^\dagger$ ($c_a^\dagger\equiv a^\dagger$, $c_b^\dagger\equiv b^\dagger$) operators denote the creation operators in the two-band (similarly for the annihilation operators).

The Green's functions $G_{ij}^{\alpha\gamma}$ and $F_{ij}^{\dagger\alpha\gamma}$, the order parameters Δ_c, Δ_s, and Δ_{ij} are defined as

$$G_{ij}^{\alpha\gamma}=\langle\langle c_{ik}^\alpha\,|\,c_{jk}^{\dagger\gamma}\rangle\rangle\ ,$$

$$F_{ij}^{\dagger\alpha\gamma}=\langle\langle c_{ik}^{\dagger\alpha}\,|\,c_{j-k}^{\dagger\gamma}\rangle\rangle\ ,\tag{5}$$

$$\Delta_c=\tfrac{1}{2}g_c\beta^{-1}\sum_{\alpha,\gamma}\delta_{\alpha\gamma}\sum_{k,n}G_{ba}^{\alpha\gamma}(k,\omega_n)\ ,$$

$$\Delta_s=\tfrac{1}{2}g_s\beta^{-1}\sum_{\alpha,\gamma}\sigma_{\alpha\gamma}^z\sum_{k,n}G_{ba}^{\alpha\gamma}(k,\omega_n)\ ,\tag{6}$$

$$\Delta_{ij}=\tfrac{1}{2}\lambda_{ij}\beta^{-1}\sum_{\alpha,\gamma}\Pi_{\alpha\gamma}\sum_{k,n}F_{ij}^{\alpha\gamma}(k,\omega_n)\ ,$$

where $\beta=1/k_BT$, α and γ are the spin indices, $\sigma_{ij}^{\alpha\gamma}$ are the Pauli matrices component, and $\Pi_{\alpha\gamma}=i\sigma_{\alpha\gamma}^y$. In Eqs. (6), Δ_c, Δ_s, and Δ_{ij} represent the order parameter for the CDW, SDW,[25] and superconducting pairing, respectively. The equation of motion[26] for the Green's function leads to the following matrix relation in the Nambu formalism:

$$\begin{bmatrix}\epsilon_a^-1 & 0 & -\widehat{\Delta} & 0 & -\widehat{\Delta}_{aa} & -\widehat{\Delta}_{ba} & 0 & 0\\ 0 & \epsilon_a^-1 & 0 & -\widehat{\Delta} & 0 & 0 & -\widehat{\Delta}_{aa} & -\widehat{\Delta}_{ba}\\ -\widehat{\Delta} & 0 & \epsilon_b^-1 & 0 & -\widehat{\Delta}_{ab} & -\widehat{\Delta}_{bb} & 0 & 0\\ 0 & -\widehat{\Delta} & 0 & \epsilon_b^-1 & 0 & 0 & -\widehat{\Delta}_{ab} & -\widehat{\Delta}_{bb}\\ \widehat{\Delta}_{aa}^* & 0 & \widehat{\Delta}_{ab}^* & 0 & \epsilon_a^\dagger1 & 0 & \widehat{\Delta} & 0\\ 0 & \widehat{\Delta}_{aa}^* & 0 & \widehat{\Delta}_{ab}^* & 0 & \epsilon_a^\dagger1 & 0 & \widehat{\Delta}\\ \widehat{\Delta}_{ba}^* & 0 & \widehat{\Delta}_{bb}^* & 0 & \widehat{\Delta} & 0 & \epsilon_b^\dagger1 & 0\\ 0 & \widehat{\Delta}_{ba}^* & 0 & \widehat{\Delta}_{bb}^* & 0 & \widehat{\Delta} & 0 & \epsilon_b^\dagger1\end{bmatrix}\begin{bmatrix}\widehat{G}_{aa}\\ \widehat{G}_{ab}\\ \widehat{G}_{ba}\\ \widehat{G}_{bb}\\ \widehat{F}_{aa}^\dagger\\ \widehat{F}_{ab}^\dagger\\ \widehat{F}_{ba}^\dagger\\ \widehat{F}_{bb}^\dagger\end{bmatrix}=\begin{bmatrix}1\\0\\0\\1\\0\\0\\0\\0\end{bmatrix}\ ,\tag{7}$$

where the caret denotes a matrix in the spin space, 1 is the 2×2 unity matrix in this space, and

$$\hat{\Delta} = \begin{bmatrix} \Delta_c + \Delta_s & 0 \\ 0 & \Delta_c - \Delta_s \end{bmatrix} .$$

We also used the notation $\epsilon_{a(b)}^{\pm} = \omega \pm \zeta_{a(b)}$.

In order to describe the superconducting phase we use only s-wave pairing, because, as far as Cr alloys are concerned, the possibility of an exotic p-wave pair appearance can be neglected.[24] Furthermore, we do not consider a spatially periodic order parameter Δ_Q since it is stable only in the presence of an external magnetic field.[15,19] To solve the matrix equation (7), we take into consideration only real superconducting gaps. In the first approximation, a small variation of the concentration of the carriers in the two-band does not change the modulus of the gap parameters. Thus we have no reason to make a difference between the modulus of the two superconducting gaps Δ_{aa} and Δ_{bb} in the two-band. To simplify things, we consider only $|\Delta_{aa}| = |\Delta_{bb}|$. In this case, one obtains two different solutions.[27] One is called the symmetrical solution with $\Delta_{aa} = \Delta_{bb}$ and $\Delta_{ab} \neq 0$ and the other is an asymmetrical one, with $\Delta_{aa} = -\Delta_{bb}$ and $\Delta_{ab} = 0$, where Δ_{ab} is the interband superconducting gap ($\lambda_{ab} = \lambda_{ba}$). In order to simplify the notations, we denote $\lambda_{aa} = \lambda$ and $\Delta_{aa} = \Delta$. In this way the solutions of Eq. (7) are

$$G_{aa(bb)}^{\alpha\beta} = \frac{(\omega + \delta_+)(\omega^2 - \delta_-^2) + 2\eta \Delta \Delta_\sigma \Delta_{ab} - \Delta^2(\omega + \delta_{+(-)}) - \Delta_\sigma^2(\omega - \delta_{-(+)}) - \eta \Delta_{ab}^2(\omega + \delta_{-(+)})}{[\omega^2 - \omega_+^2(\sigma)][\omega^2 - \omega_-^2(\sigma)]} , \tag{8}$$

$$G_{ab}^{\alpha\beta} = G_{ba}^{\alpha\beta} = \frac{\Delta_\sigma[(\omega + \delta_\mu)^2 - \epsilon^2 - \Delta_\sigma^2 - \eta \Delta_{ab}^2 - \xi \Delta^2] - 2\eta \Delta \Delta_{ab}(\omega + \delta_\mu)}{[\omega^2 - \omega_+^2(\sigma)][\omega^2 - \omega_-^2(\sigma)]} , \tag{9}$$

$$F_{aa}^{\dagger\alpha\beta} = -\sigma \frac{\Delta(\Delta^2 + \xi \Delta_\sigma^2 - \eta \Delta_{ab}^2 - \omega_-^2 - \xi \delta_-^2) - 2\eta \Delta_\sigma \Delta_{ab} \delta_-}{[\omega^2 - \omega_+^2(\sigma)][\omega^2 - \omega_-^2(\sigma)]} , \tag{10}$$

$$F_{ab}^{\dagger\alpha\beta} = F_{ba}^{\dagger\alpha\beta} = -\sigma\eta \frac{\Delta_{ab}[\Delta_{ab}^2 - \Delta^2 + \Delta_\sigma^2 - (\omega + \epsilon)^2 + (\delta_\mu)^2] - 2\Delta \Delta_\sigma \delta_\mu}{[\omega^2 - \omega_+^2(\sigma)][\omega^2 - \omega_-^2(\sigma)]} , \tag{11}$$

where σ is $+1$ and -1 for up and down-spin indices, respectively, in the case of Eqs. (8), and (9) and is $+1$ or -1 for ($\alpha\beta \equiv \downarrow\uparrow$) or ($\alpha\beta \equiv \uparrow\downarrow$), respectively, in the case of Eqs. (10) and (11). Furthermore, ξ is $+1$ and -1 and η is $+1$ and 0 for symmetrical and asymmetrical cases, respectively. We also used the notations

$$\delta_\sigma \equiv \delta_\pm = \delta_\mu \pm \epsilon, \quad \Delta_\sigma \equiv \Delta_\pm = \Delta_c \pm \Delta_s, \quad (\delta\tilde{\mu})^2 = (\delta\mu)^2 + \eta \Delta_{ab}^2, \quad \omega_\pm^2(\sigma) = (E_\sigma \pm \delta\tilde{\mu})^2 + \tilde{\Delta}^2(\sigma), \quad E_\sigma^2 = \epsilon^2 + \tilde{\Delta}_\sigma^2 , \tag{12}$$

where the renormalized gaps are

$$\tilde{\Delta}^2(\sigma) = \frac{\eta}{(\delta\tilde{\mu})^2}(\delta\mu \, \Delta - \Delta_\sigma \Delta_{ab})^2 + \Delta^2(1 - \eta)\left[1 - \frac{\Delta_\sigma^2}{(\delta\mu)^2}\right] ,$$

$$\tilde{\Delta}_\sigma^2 = \frac{\eta}{(\delta\tilde{\mu})^2}(\delta\mu \, \Delta_\sigma + \Delta \Delta_{ab})^2 + \Delta_\sigma^2(1 - \eta)\left[1 + \frac{\Delta^2}{(\delta\mu)^2}\right] . \tag{13}$$

Together with the gap equations we must analyze the $n = \delta n / 4N(0)$ quantity, where δn expresses the difference between the electron and hole concentration, as follows:

$$\delta n = \sum_k \left[2 - \beta^{-1} \sum_n \text{Tr}_\alpha \text{Tr}_i G_{ii}^{\alpha\alpha}(k, \omega_n)\right] . \tag{14}$$

One can consider n as a quantity proportional with the impurity concentration introduced in the system. It can be proved that $\delta\mu = 0$ implies $n = 0$.

Using Eqs. (6), (8)—(11), and (14), for $\delta\mu \neq 0$ one obtains

$$\frac{1}{|\lambda| N(0)} = \sum_{\sigma = \pm 1} \left[I_1^\sigma + \eta \delta\mu \tilde{\Delta}(\sigma) I_2^\sigma + (1 - \eta)\left[\delta\mu - \frac{\Delta_\sigma^2}{\delta\mu}\right] I_2^\sigma\right] , \tag{15}$$

$$\frac{\Delta_c}{g_c N(0)} = \sum_{\sigma = \pm 1} \left[\Delta_\sigma I_1^\sigma - \eta \Delta_{ab} \tilde{\Delta}(\sigma) I_2^\sigma - \frac{1 - \eta}{\delta\mu} \Delta^2 \Delta_\sigma I_2^\sigma\right] , \tag{16}$$

$$\frac{\Delta_s}{g_s N(0)} = \sum_{\sigma = \pm 1} \left[\sigma \Delta_\sigma I_1^\sigma - \eta \sigma \Delta_{ab} \tilde{\Delta}(\sigma) I_2^\sigma - \sigma \frac{1 - \eta}{\delta\mu} \Delta^2 \Delta_\sigma I_2^\sigma\right] , \tag{17}$$

$$\frac{\Delta_{ab}}{|\lambda_{ab}|N(0)} = \eta \sum_{\sigma=\pm 1}\left[\frac{\delta\mu}{\delta\widetilde{\mu}}\widetilde{\Delta}(\sigma)\widetilde{\Delta}_\sigma I_2^\sigma - \frac{\Delta_{ab}}{\delta\widetilde{\mu}}I_3^\sigma\right],\tag{18}$$

$$n = \sum_{\sigma=\pm 1}\left[I_3^\sigma - \eta(\widetilde{\Delta}^2(\sigma)-\Delta^2)I_2^\sigma + (1-\eta)\left|\frac{\Delta\Delta_\sigma}{\delta\mu}\right|^2 I_2^\sigma\right].\tag{19}$$

The integrals which appear in Eqs. (15)–(19) are given in the Appendix.

III. PHASE DIAGRAM AT EQUAL CONCENTRATION OF ELECTRONS AND HOLES

We are interested in finding a domain in which superconductivity can coexist with SDW. We have $\delta\mu=0$ and if we make an analysis at $T=0$, from Eqs. (6), (8)–(11), and (14), a simple form for the gap equations is reached, which after some algebra yields, in the asymmetrical case,

$$4\ln\frac{\Delta_{c0}}{\Delta_0} = \left[\frac{\Delta_c}{\Delta}-\frac{\Delta}{\Delta_c}\right]\ln\left|\frac{(\Delta-\Delta_c)^2-\Delta_s^2}{(\Delta+\Delta_c)^2-\Delta_s^2}\right| + \frac{\Delta_s}{\Delta}\ln\left|\frac{(\Delta-\Delta_s)^2-\Delta_c^2}{(\Delta+\Delta_s)^2-\Delta_c^2}\right| - \frac{\Delta_s}{\Delta_c}\ln\left|\frac{(\Delta_c-\Delta_s)^2-\Delta^2}{(\Delta_c+\Delta_s)^2-\Delta^2}\right|,$$

$$4\ln\frac{\Delta_{s0}}{\Delta_0} = \left[\frac{\Delta_s}{\Delta}-\frac{\Delta}{\Delta_s}\right]\ln\left|\frac{(\Delta-\Delta_s)^2-\Delta_c^2}{(\Delta+\Delta_s)^2-\Delta_c^2}\right| + \frac{\Delta_c}{\Delta}\ln\left|\frac{(\Delta-\Delta_c)^2-\Delta_s^2}{(\Delta+\Delta_c)^2-\Delta_s^2}\right| - \frac{\Delta_c}{\Delta_s}\ln\left|\frac{(\Delta_s-\Delta_c)^2-\Delta^2}{(\Delta_s+\Delta_c)^2-\Delta^2}\right|,\tag{20a}$$

and in the symmetrical case,

$$4\ln\frac{\Delta_0}{\Delta_{c0}} = \frac{\Delta_s}{\Delta_c}\ln\frac{\Delta^2+(\Delta_c-\Delta_s)^2}{\Delta^2+(\Delta_c+\Delta_s)^2},$$

$$4\ln\frac{\Delta_0}{\Delta_{s0}} = \frac{\Delta_c}{\Delta_s}\ln\frac{\Delta^2+(\Delta_c-\Delta_s)^2}{\Delta^2+(\Delta_c+\Delta_s)^2}\tag{20b}$$

where Δ_{c0}, Δ_{s0}, and Δ_0 are the order parameters for pure CDW, SDW, and BCS phases, respectively:

$$\Delta_0 = 2\Omega\exp[-1/|\lambda|N(0)],$$

$$\Delta_{c0} = 2\Omega\exp[-1/g_cN(0)],\tag{21}$$

$$\Delta_{s0} = 2\Omega\exp[-1/g_sN(0)],$$

where Ω is the cutoff energy.

In both asymmetrical and symmetrical cases, the gap equations allow a coexistence domain, but in the symmetrical case, this domain is not energetically stable. The energetical stability was done with the use of standard methods.[28,29] In the asymmetrical case, the phase diagram is presented in Fig. 1. As it can be seen, a stable coexistence domain is found only between three phases, a situation in which Δ_c, Δ_s, and Δ are all nonvanishing quantities. So SDW will coexist with superconductivity only in the presence of a CDW phase. We have to mention that this situation is not characteristic for the available experimental data[24] where, due to the Re impurities in Cr, we have $\delta\mu\neq 0$.

Further on, it will be interesting to make some comments upon the coexistence of the CDW and the superconducting phase, which has some features which are also characteristic for the SDW superconducting phase coexistence. The investigation starts from the discovery of the martensitic transition in $A15$ compounds,[30,31] which led Gor'kov to suggest[32] that the observed cubic to tetragonal transition is driven by a Peierls instability. The experiments revealed a number of compounds which exhibit a

CDW superconductor coexistence, such as dichalcogenides,[33] trichalcogenides,[34] organic superconductors,[35] and one-dimensional (1D) polymers.[36] The theoretical approach starts from the Gor'kov model,[32,37] which shows that, at the center of the face of the simple cubic Brillouin zone, the CDW gap separates the energy band, depopulating the area of the Fermi surface and reducing the number of electrons available for the BCS pairing. Thus, a great part of the electronic density of states at Fermi level can be removed by the CDW gap, which leads to a marked decrease of the superconducting transition temperature. Further on, Levin et al.[38] studied the possibility of the coexistence of CDW and superconducting gaps in
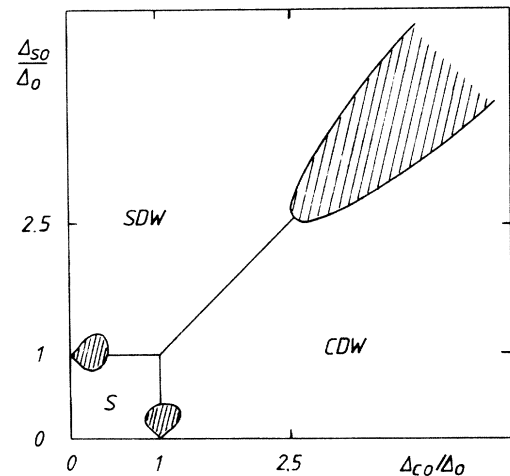

FIG. 1. Phase diagram at $T=0$ and $n=0$ as a function of the reduced parameters Δ_{s0}/Δ_0 and Δ_{c0}/Δ_0. In the dashed regions energetically stable coexistence phase occurs, besides the pure BCS (S), SDW, and CDW phases.

1D systems, using coupled gap equations in mean-field treatment. Also they analyzed the simultaneous fluctuations in both order parameters using the Ginzburg-Landau free-energy functional. They proved that the two phases are generally incompatible and that the ordered state is mixed only when the bare transition temperatures are nearly equal. The coexistence in two dimensions was studied by Balseiro and Falikov.[39] They considered the importance of a detailed band structure in such an analysis and took into account a two-dimensional square lattice model which works for layered compounds. The conclusion was that in general terms, the two order parameters interfere destructively while the coexistence is possible only for a small region of the electron-electron interaction $\lambda \in [0.21w, 0.27w]$ (w is the bandwidth for the analyzed system). Under these circumstances the pure CDW exhibits no gap in the quasiparticle spectrum and the superconducting gap remains practically unchanged, due to the competition between the increasing λ and the decreasing density of states at the Fermi level.

McMillan and co-workers[37,40,41] analyzed the CDW state[40] and the structural Peierls transition influence on superconducting transition[37] and described the CDW and superconducting coexistence. They concluded[41] that the details of the band structure are unimportant for the energetics of the phase transition and that we only need to know the densities of states of the carriers which participate in the transition and the relevant coupling constants. They prove that the two energy gaps compete for the same portion of the Fermi surface inhibiting one another. In their model, the CDW gap opens a portion of the Fermi surface which causes the decrease of the superconducting transition temperature.[41]

Machida et al.[42] argued that, in the above-mentioned works, only one uniform order parameter $\Delta(0)$ was taken into account for the superconducting state. They neglected the reaction of the CDW state caused by superconductivity and they characterized the latter with $\Delta(0)$ and a supplementary spatially periodic order parameter $\Delta(Q)$. This superconducting phase turned out to be more likely to coexist with CDW, as compared to the ordinary BCS, state.

We cannot use a $\Delta(Q)$ order parameter approach because of the presence of the SDW phase,[15] which strongly disfavors it. Coexistence is possible only in a small region of the space of the characteristic parameter since, even if $\delta\mu = 0$, the nesting property is stronger between the electron jack and hole octahedron. This favors the SDW and CDW gap formation which opens up only a small fraction of the Fermi surface. It will be interesting to analyze the resulting coexistence because, according to Volkov et al.[28] the SDW and CDW coexistence means excitonic itinerant ferromagnetism. Its coexistence with superconductibility could eventually explain some recent experimental data concerning superconductibility and weak itinerant electron ferromagnetism mixing.[43]

Returning to our phase diagram we have to mention that the real coexistence domains were obtained (from the energy minimum condition) using a numerical transformation from the (z_1, z_2) plane to the $(\Delta_0, \Delta_{s0}, \Delta_{c0})$ space, where z_1 and z_2 are the solutions of

$$G(z_1, z_2) = \ln(1 + z_1^2 + z_2^2)$$
$$+ \frac{1}{2}\left[(z_1 + z_2)\ln\left|\frac{1 - z_1 - z_2}{1 + z_1 + z_2}\right| \right.$$
$$+ (z_1 - z_2)\ln\left|\frac{1 - z_1 + z_2}{1 + z_1 - z_2}\right|$$
$$\left. - \ln\left|1 + z_1^4 + z_2^4 - 2(z_1^2 + z_1^2 z_2^2 + z_2^2)\right| \right] = 0.$$

$$(22)$$

The three separate stable coexistence domains are determined by the $G(z_1, z_2) > 0$ condition:

$$G(z_1, z_2) = \ln[(F_{\text{coex}} - F_N)/(F_S - F_N)] ,$$

where F_{coex}, F_S, and F_N are the free energies of the coexistence, simple, and normal phases, respectively. In Eq. (22), z_1 and z_2 take the Δ_c/Δ and Δ_s/Δ, Δ/Δ_c and Δ_s/Δ_c, and Δ/Δ_s and Δ_c/Δ_s values, respectively. Because of the complexity of the phase diagram in the $(\Delta_0, \Delta_{s0}, \Delta_{c0})$ space, in Fig. 1 we give it as a function of the reduced parameters Δ_{s0}/Δ_0 and Δ_{c0}/Δ_0.

We must remark that the asymmetrical solution has a lower ground-state energy then the symmetrical one (in agreement with earlier works[27]). So in a system characterized by $\delta\mu = 0$, the asymmetrical solution will be realized practically.

At $T \neq 0$ in the case of small λ value, the transition temperature for the coexistence phase (T_{tr}) can be approximated by

$$\ln\frac{T_{S0}}{T_{\text{tr}}} = \psi\left[\frac{1}{2} + \frac{\Delta_0}{2\sqrt{2}\pi T_{\text{tr}}}\right] - \psi\left[\frac{1}{2}\right] , \qquad (23)$$

where $\psi(x)$ is the digamma function, T_{S0} is the transition temperature of the BCS superconductor which, as it can be seen from Eq. (23), is always greater than T_{tr}. Thus, in order to explain the coexistence found experimentally,[24] we must analyze the $\delta\mu \neq 0$ case, which will be done in the following section.

IV. PHASE DIAGRAM AT $T = 0$ AND $n \neq 0$

As we have seen in the preceding section, for $n = 0$, a stable coexistence domain is obtained between SDW and superconductivity only if $\Delta_c \neq 0$. In the case of different electron and hole concentration, the coexistence domain can be stabilized with the use of the $n \neq 0$ parameter, rather than with Δ_c. The physical reason of this process is given by the fact that $\delta\mu$ can be considered also as a measure of the nesting imperfection between the two-band [see the expressions ζ_a and ζ_b following Eq. (4)]. If $\delta\mu$ is sufficiently small, and therefore n also [see Eq. (30)], the nesting is almost perfect, and thus strongly favors the SDW formation.[25] If we increase $\delta\mu$, the nesting becomes more and more imperfect, which decreases the SDW stability and, above a critical n value, makes possible the superconducting phase formation. In this way, we will analyze only the $\Delta_c = 0$ plane of the phase diagram. This study is presented in this section at $T = 0$.

The phase diagram which one obtains is presented in Fig. 2, where only those separation lines are plotted which really exist. As it can be seen, three different energetically stable phases come true: the pure superconducting phase (S) with $\Delta = \Delta_0 \neq 0$ and $\Delta_s = 0$, the symmetrical coexistence phase (CS) between the (a) and (b) curves $(\Delta = \Delta_{aa} = \Delta_{bb} \neq 0$ and $\Delta_s \neq 0)$, and the asymmetrical coexistence phase (CA) below the (b) curve $(\Delta = \Delta_{aa} = -\Delta_{bb} \neq 0$ and $\Delta_s \neq 0)$. The analytical expressions for the (a) and (b) lines can be obtained from the gap equations, Eqs. (15), (17), and (19). Their equations are

$$(a): \quad \ln\frac{x}{y} = (1+4y^2)^{-1/2}\ln\frac{1+(1+4y^2)^{1/2}}{2y} \tag{24}$$

and

$$(b): \quad \ln\frac{x}{y} = (1+4y^2)^{1/2}\ln\frac{1+(1+4y^2)^{1/2}}{2y} \ , \tag{25}$$

where $y = \Delta_0/2n$ and $x = \Delta_{s0}/2n$.

We have to mention that the gap equations permit also two metastable solutions. There exists a (c) curve between the (a) and (b) lines, which surrounds a metastable asymmetrical coexistence domain. This domain is unstabilized by the symmetrical coexistence solution. For the small superconducting coupling constant one obtains, close to the $\Delta_{s0}/2n$ axis, a separation curve (d), below which a simple metastable SDW phase occurs. This is unstabilized by the asymmetrical coexistence phase.

From the gap equations one can deduce the analytical expression of the (c) and (d) lines:

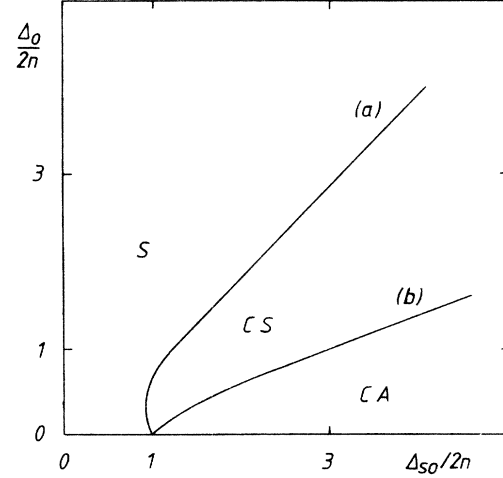FIG. 2. Phase diagram at $T=0$ and $n\neq 0$ for $\Delta_c = 0$, as a function of the reduced parameters $\Delta_0/2n$ and $\Delta_{s0}/2n$. S, CS, and CA denote the pure superconducting, the symmetrical coexistence, and the asymmetrical coexistence phases, respectively.

$$(c): \quad \ln\frac{x}{y} = \left[2y\ln\frac{x}{y} - 1\right]^{1/2}\arcsin\left[2y\ln\frac{x}{y}\right]^{-1} \tag{26}$$

and

$$(d): \quad y = x\exp\left[-K\frac{(x-\frac{1}{2})^2}{x(x-1)}\right] , \tag{27}$$

where $K = 1/|\lambda_{ab}|N(0)$; x and y were defined above.

The $T=0$ gap values for the CS and CA phases are given in Eq. (28) and Eq. (29), respectively:

$$\Delta(0) = \frac{4n^2}{\Delta_{s0}}\exp\left[-\frac{n}{\Delta_{s0}-n}\frac{\ln\frac{\Delta_{s0}}{\Delta_0}}{1-|\lambda_{ab}|N(0)\frac{\tilde{\Delta}_{s0}^2}{(\Delta_{s0}-n)^2}\ln\frac{\Delta_{s0}}{\Delta_0}}\right] ,$$

$$\Delta_s(0) = \tilde{\Delta}_{s0}\left[1-|\lambda_{ab}|N(0)\frac{\Delta_0^2}{n(n^2+\Delta_0^2)^{1/2}}\ln\frac{n+(n^2+\Delta_0^2)^{1/2}}{\Delta_0}\right] , \tag{28}$$

$$\Delta_{ab}(0) = |\lambda_{ab}|N(0)\Delta_0\tilde{\Delta}_{s0}\frac{1}{(n^2+\Delta_0^2)^{1/2}}\ln\frac{n+(n^2+\Delta_0^2)^{1/2}}{\Delta_0} ,$$

and

$$\Delta(0) = \frac{\Delta_{s0}-n}{n}\frac{4n^2}{\Delta_{s0}}\exp\left[-\frac{\Delta_{s0}-n}{n}\ln\frac{\Delta_{s0}}{\Delta_0}\right] ,$$

$$\Delta_s(0) = \tilde{\Delta}_{s0}\left[1-\frac{\Delta_0^2}{2n^2}\exp\left[-\frac{\Delta_{s0}^2}{2n}\frac{1}{(n^2+\Delta_0^2)^{1/2}}\ln\frac{n+(n^2+\Delta_0^2)^{1/2}}{n}\right]\right] , \tag{29}$$

where $\tilde{\Delta}_{s0}^2 = \Delta_{s0}(\Delta_{s0} - 2n)$, with $\Delta(0)$ and $\Delta_s(0)$ we denoted $\Delta(T=0)$ and $\Delta_s(T=0)$. We have to remark that $\Delta(0)$ and $\Delta_s(0)$ are always smaller than the pure phases gaps and from Eqs. (28) and (29), in the case of $\Delta_0 = 0$ or $\Delta_{s0} \leq 2n$, one reobtains the classical SDW gap $\tilde{\Delta}_{s0}$ (Ref. 25) or the BCS gap Δ_0. Concerning $\delta\mu$, it can be approximated in the coexistence domains by

$$\delta\mu = n \left\{ 1 + \frac{1}{2} \left[\frac{\Delta_s}{n} \right]^2 \left[1 - F \left[\frac{\Delta_0}{n} \right] \right] \right\} , \qquad (30)$$

where, for example, in the CA region,

$$F(\Delta_0/n) = (\Delta_0/n)^2 \ln 2 + O[(\Delta_0/n)^4] .$$

Because of the magnitude difference between T_N and T_c values (where T_c is the critical transition temperature for the coexistence phase and T_N is the Néel temperature), determined experimentally,[24] the materials measured in Ref. 24 seem to be situated close to the $\Delta_{s0}/2n$ axis within the CA domain (see Fig. 2). Indeed, as the above presented analysis showed, in this region the coexistence between SDW and superconductivity becomes possible. So, for this region of the phase diagram, it is interesting to analyze the $T \neq 0$ extension of the asymmetrical coexistence domain. This analysis must be made, because it will reveal the critical transition temperatures. This study will be presented in the following section.

V. COEXISTENCE AT $T \neq 0$

The asymmetrical coexistence domain at $T \neq 0$ can be characterized by the coupled solutions of Eqs. (15), (17),

and (19). In the high-temperature region, where only the SDW phase exists, the last two terms from Eq. (17) vanish, thus the gap equation for $\Delta_s(T)$ after some algebra, becomes

$$\ln \frac{T}{T_N} = -\operatorname{Re}\left[\psi \left[\frac{1}{2} + i \frac{\delta\mu}{2\pi T} \right] - \psi \left[\frac{1}{2} \right] \right] - \frac{7\zeta(3)}{8\pi^2} \frac{\Delta_s^2(T)}{T^2} , \qquad (31)$$

where $\zeta(x)$ is the zeta function. From Eq. (31) one obtains the Néel temperature T_N,

$$k_B T_N = 2\Omega \frac{\gamma}{\pi} \exp\left[-\frac{1}{g_s N(0)} \left[1 - \frac{(\delta\mu)^2}{T_{N0}^2} \right]^{-1/2} \right] , \qquad (32)$$

and the SDW gap,

$$\Delta_s(T) = k_B T_N \pi \left[\frac{8}{7\zeta(3)} \right]^{1/2} \left[1 - \frac{T}{T_N} \right]^{1/2} , \qquad (33)$$

where T_{N0} is the transition temperature of the pure $(\Delta = 0, n = 0)$ SDW phase.

At low temperature, just above the coexistence phase appearance, for $\Delta_s(T)$, one obtains

$$\Delta_s(T) = \tilde{\Delta}_{s0} - (2\pi \tilde{\Delta}_{s0} k_B T)^{1/2} e^{-\Delta_{s0}/k_B T} \cosh \frac{\delta\mu}{k_B T} , \qquad (34)$$

where $\tilde{\Delta}_{s0}$ was defined after Eq. (29). In the coexistence domain, just below T_c, the $\Delta_s(T)$ expression becomes

$$\Delta_s(T) = \tilde{\Delta}_{s0} - (2\pi \tilde{\Delta}_{s0} k_B T)^{1/2} \exp\left[-\frac{\Delta_{s0}}{k_B T} \left[1 - \frac{\Delta^2(T)}{\Delta_{s0}^2 - (\delta\mu)^2} \right] \right] \cosh \frac{\delta\mu}{k_B T} . \qquad (35)$$

The superconducting gap $\Delta(T)$, for $T \leq T_c$ is

$$\Delta(T) = k_B T_c \pi c_1 \left[1 - \frac{T^2}{T_c^2} \right]^{1/2} , \qquad (36)$$

where T_c is the critical transition temperature for the coexistence phase and is given by

$$T_c = c_2(n - n_c)^{1/2} . \qquad (37)$$

n_c is the critical n value (proportional to the critical concentration) above which the superconducting phase can appear:

$$n_c = \Delta_{s0} \left[2 + \ln \frac{T_{N0}}{T_{s0}} \right] . \qquad (38)$$

The c_1 and c_2 constants have the form

$$c_1^{-2} = \frac{\pi^2 T_c^2}{2n^2} \left[\frac{5}{2} + \frac{n^2}{(\Delta_{s0} - n)^2} \right]$$

$$+ \frac{n^4}{\Delta_{s0}(\Delta_{s0} - n)^3} + \frac{n^2(\Delta_{s0} + n)}{\Delta_{s0}^2(\Delta_{s0} - n)} , \qquad (39)$$

$$c_2^2 = \frac{2n_c^4}{\pi^2(\Delta_{s0} - n)^3} \ln \frac{T_{N0}}{T_{s0}} .$$

For n, at low temperatures the following equality stands:

$$n(T) = [(\delta\mu)^2 - \Delta_s^2(T)]^{1/2} - \frac{\pi^2}{6} \frac{T^2 \Delta_s^2(T)}{[(\delta\mu)^2 - \Delta_s^2(T)]^{3/2}} . \qquad (40)$$

The expression of $\Delta(T)$ and T_c can be deduced from Eqs. (15), (17), and (40). The proof is based on the observation that in the studied temperature region,
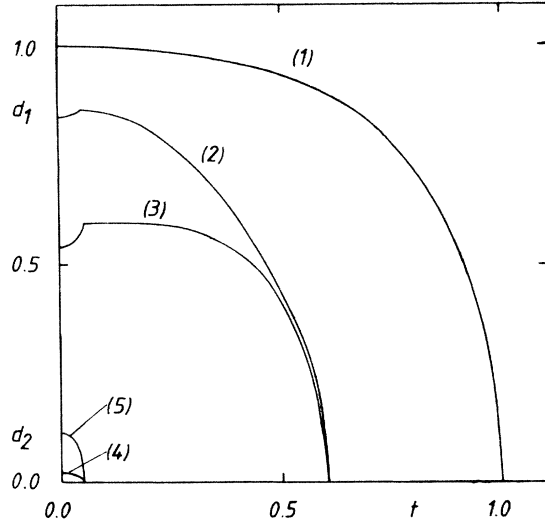
FIG. 3. Temperature dependence of the order parameters $[\Delta(T),\Delta_s(T)]$ as a function of $t=T/T_{N0}$ is plotted $d_1=\Delta_s(T)/\Delta_{s0}$ as curve (1) for pure SDW; curve (2), $\Delta_{s0}/\Delta_0=10$; curve (3), $\Delta_{s0}/\Delta_0=3$ and $d_2=\Delta(T)/\Delta_{s0}$; in curve (4), $\Delta_{s0}/\Delta_0=10$; and curve (5), $\Delta_{s0}/\Delta_0=3$. For T_N and T_c the measured values (Ref. 24) has been used.

$$I_2^\sigma(\widetilde{\Delta},\Delta_s,\delta\mu)=2\frac{(\delta\mu)^3}{(\delta\mu)^2-\Delta_s^2}\frac{\partial^2}{\partial\Delta^2}I_1^\sigma(\widetilde{\Delta},\Delta_s,\delta\mu)\ ,\qquad(41)$$

and I_1^σ can be computed with use of Fermi integrals.

In Fig. 3 the numerical solution of the gap equations are plotted. As it can be seen a diminution of $\Delta_s(T)$ appears below T_c, for comparision we also give the pure SDW gap's value. Furthermore, as we mentioned earlier, n can be considered as a monotonous increasing function
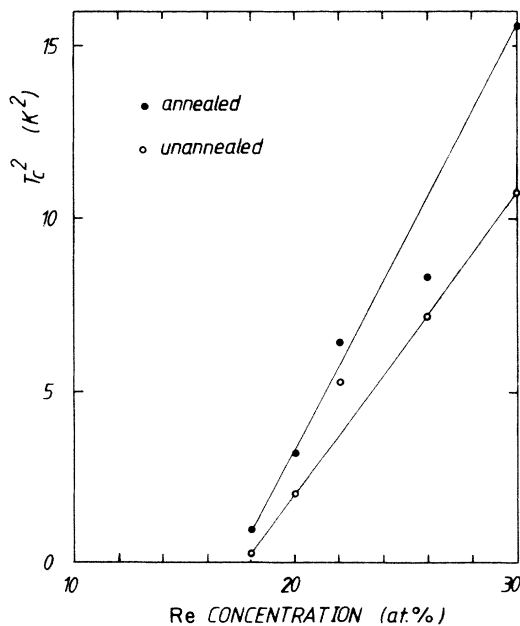

FIG. 4. Experimental data (from Ref. 24) for T_c^2 vs the Re concentration.

of the impurity concentration within the system. In this way from Eq. (37) one obtains the experimental observations[24] that below a critical concentration, the superconducting phase does not appear and that T_c grows as the Re concentration in the Cr alloy increases. If we plot, using the experimental data published by Nishihara et al.,[24] T_c^2 as a function of the Re impurity concentration we obtain a straight line (see Fig. 4), the slope of which depends on the annealing condition. This figure shows that, above the critical concentration (which allows the appearance of the superconducting phase), the superconducting critical temperature is proportional with the square of the concentration, as our description predicts [see Eq. (37)].

VI. DISCUSSIONS AND CONCLUSIONS

Until recent measurements (presented in Ref. 24), the coexistence of SDW and superconductivity has been experimentally found in rare-earth ternary alloys[7-9] (RE) and quasi-one-dimensional, highly anisotropic organic structures[10] $(TMTSF)_2X$. For RE, the theoretical descriptions[14-21] are based on the observation that the localized $4f$ electrons (which are responsible for antiferromagnetism) interact very weakly with the d-band conduction electrons (which create the superconducting order). For $(TMTSF)_2X$, the theoretical studies[22,23] use the quasi-one-dimensional Fermi surface which is characterized by two regions, one of which presents the nesting property (which gives rise to the SDW formation) while the other one allows the superconducting pairing.

The recent experiments[24] which reveal the coexistence between SDW and superconductivity in Cr alloys need a different explanation since in this case the studied materials are not quasi-one-dimensional and the observed antiferromagnetic order is a typical two-band itinerant one which is carried by the same d-band conduction electrons that are responsible for the superconducting pairing. This paper provides a theoretical description of this process. The procedure we use is based on the Green's function equation of motion, as is characteristic for Cr alloys.[25]

We demonstrated that SDW and superconductivity can coexist, while the phase is stable for different electron and hole concentrations $(\delta\mu\neq0)$. The physical origin of this process can be explained starting from the fact that $\delta\mu$ is a measure of the nesting imperfection between the electron jack and the hole octahedron in Cr alloys. If the impurity concentration is relatively small, the nesting is nearly perfect and thus strongly favors the SDW formation which acts destructively upon the superconducting pairing. If the impurity concentration is situated above a critical value (proportional to n_c) the nesting imperfection increases, affecting the SDW, and thus the superconducting phase can appear.

In Sec. II, we obtain from Eq. (7) the characteristic Green's functions and the order-parameter equations. To solve exactly the matrix equation (7) is a rather difficult problem. Thus we take into account two presumptions usually used in the literature [26-28] for this kind of equation. First we consider real gap parameters (this because the Hamiltonian must be invariant under calibration

transformation for s-wave pairing). Concerning the modulus of the superconducting gaps we consider $|\Delta_{aa}| = |\Delta_{bb}|$, because (in the first approximation) a small variation of the concentration of the carriers from the two-band does not change the modulus of the two superconducting gaps in such a way, that the difference $|\Delta_{aa}| - |\Delta_{bb}|$ could be considered vanishing. (The validity of these two presumptions are verified by the agreement of our results with the experimental data.) In Sec. III, the phase diagram, the gap expressions, and the critical temperatures are obtained. As can be seen from Eq. (37), the superconducting critical temperature vanishes below a critical impurity concentration, being proportional with the square of the concentration (in agreement with Fig. 4). We also study the possibility of the coexistence from an energetical point of view.

In our attempt to explain the coexistence of SDW and superconductivity in Cr alloys, we use a weak-coupling description which yields a $\Delta(T=0)/T_c$ ratio which is quite similar to the experimentally measured value. How-

ever, in the future other contributions and effects can be taken into account in the theoretical description to refine this analysis.

APPENDIX: INTEGRALS APPEARING IN THE GAP EQUATIONS

In Eqs. (15)—(19) we made the following notations:

$$I_1^\sigma = \frac{1}{4} \int_0^\Omega \frac{d\epsilon}{E_\sigma} \sum_{\nu=\pm 1} \frac{E_\sigma + \nu\delta\mu}{\omega_\nu(\sigma)} \tanh\left[\frac{\beta}{2}\omega_\nu(\sigma)\right], \quad \text{(A1)}$$

$$I_2^\sigma = \frac{1}{4} \int_0^\Omega \frac{d\epsilon}{E_\sigma} \sum_{\nu=\pm 1} \frac{\nu}{\omega_{-\nu}(\sigma)} \tanh\left[\frac{\beta}{2}\omega_{-\nu}(\sigma)\right], \quad \text{(A2)}$$

$$I_3^\sigma = \frac{1}{4} \int_0^\Omega d\epsilon \sum_{\nu=\pm 1} \nu \frac{E_\sigma + \nu\delta\mu}{\omega_\nu(\sigma)} \tanh\left[\frac{\beta}{2}\omega_\nu(\sigma)\right], \quad \text{(A3)}$$

where Ω is the cutoff energy.

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