Magnetic ordering of impurities in dilute alloys

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The interaction of the conduction electrons of a normal metal with an ordered system of magnetic impurity centers has been investigated. In calculating the electron self-energy component, the most diverging terms were summed. It is shown that in such a system a marked renormalization of the electron spectrum takes place, and in particular, the effective mass at the Fermi surface (and with it the low-temperature electronic heat capacity) increases by several times. The increment in the electronic heat capacity exhibits a broad maximum and depends on the concentration of impurity centers and on the temperature. These dependences are in good qualitative agreement with the experimental ones.

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1. Recently the number of papers devoted to the investigation of the interaction of magnetic impurities in a non-magnetic metallic matrix has increased sharply (see, for example, the reviews[1,2]). This is apparently connected with the fact that even at very low concentrations ($\sim 10^{-4}$–10^{-3} at.%) the interaction of impurities becomes appreciable[3,5] and leads to a marked change in the properties of an alloy.

Magnetic impurities interact with each other through indirect exchange via the conduction electrons. The energy of this interaction in second order perturbation theory was calculated by Ruderman–Kittel–Kasuya–Yosida (RKKY).[6] With increase in impurity concentration the RKKY interaction leads, as was shown in[7–9], to a suppression of the Kondo effect,[10] this occurring at rather low temperatures, but above the temperature for the magnetic ordering of impurities T_c, i.e., the impurity atoms were considered as interacting, but the average moment of each of them was equal to zero. The case of high temperatures ($T \gg \max\{T_c, T_K\}$, T_K being the Kondo temperature) was analyzed by Larkin and his colleagues.[11] Let us note that in all the papers referred to above the RKKY interaction, which is symmetrical with relation to the sign of the exchange constant J, was considered.

In the present paper it is assumed that the alloy is below T_c and magnetic ordering of the impurity atoms has taken place in the system. The results then depend appreciably, as will be shown below, on the sign of the constant J. As was first shown by Kondo,[12] a strong renormalization of the electron spectrum occurs in such a system, leading to an increase of the coefficient in the linear part of the electronic heat capacity by several times. At the same time, according to Kondo the change in the heat capacity does not depend on the concentration of impurity atoms. Despite this, a marked concentration dependence is always observed experimentally.[13–15] As Abrikosov noted in a review,[16] the correction to the electron energy considered by Kondo is the first large term of a series containing powers of $J\ln(\max\{Q, T\}/D)\varepsilon_0^{-1}$ (Q is the energy of an impurity atom in the effective exchange field, T is the temperature, ε_0 is the Fermi energy; the physical meaning of the energy D will be discussed a little later). This correction diverges with increase in $\ln(\max\{Q, T\}/D)$. Moreover, Kondo's results do not depend on the sign of J. With regard to everything that has been said, a theory has been constructed in the present work in which the expansion is not carried out in terms of the constant J, but of a renormalized constant[1)] $J_{\text{eff}} \sim J/[1 - J\ln(\max\{Q, T\}/D)/\varepsilon_0]$. In the case where $J_{\text{eff}} < J$ ($J > 0$), the expansion is improved and the renormalization of the effective masses of the electrons begins to depend on concentration and temperature. The resultant form of the concentration and temperature dependence of the heat capacity is consistent with the experimental results.

The fact of magnetic ordering of impurities at low concentrations is well established experimentally, although the theoretical aspects of the problem have not been exhaustively studied. Let us note in this connection that from the point of view of the RKKY potential usually employed, only ordering of the "spin-glass" type is possible, in which, at each lattice point containing an impurity atom, local magnetization occurs without rigid correlation with neighboring impurity atoms, so that a macroscopic magnetic moment may be absent. Consequently, ferromagnetic ordering, which is often observed experimentally (see, for example,[18]) at quite low concentrations, is in contradiction to the elementary concepts of the mechanism of indirect exchange in metals. This contradiction can, however, be resolved within the framework of the description proposed in a paper by Korenblit and Shender,[19] in which it was shown that for a complex form of the Fermi surface containing small segments with low typical momenta, the occurrence of an oscillating exchange potential with a rather large period is possible. It should be emphasized, however, that the efficiency of such an ordering mechanism is only adequate in good single crystals. On the other hand, typical experiments are being carried out on polycrystalline samples in which, because of the significant angular averaging, the mechanism referred to is of low efficiency. In the present paper we would like to draw attention to one possibility which can be realized even in the isotropic case. The point is that in Kondo's theory there is an energy cutoff parameter D,[20] $2D$ being that range of energies in which the interaction between the conduction electrons and the d-electrons of the impurity is appreciable. If for any reason there is a sufficiently narrow spike in the density of states of the conduction electrons in the neighborhood of the Fermi surface, then electrons with energies in the range of this spike will obviously participate more effectively in the indirect exchange. Such a spike may occur both as a consequence of the specific dispersion law and as a result of the overlap of two bands (a broad and a narrow one), the states of which are entangled in a polycrystal because of potential scattering, as, for example, in the alloy $CuTi_2S_4$. If $D \gtrsim \varepsilon_0$, the effective exchange interaction is the same as the RKKY potential. In the case where $D \ll \varepsilon_0$, the effective interaction assumes the form

$$V(r) = -\left(-\frac{J}{2n}\right)^2 \frac{D}{(p_0 r)^2} \left\{\varphi\left(\frac{r}{r_0}\right) - \psi\left(\frac{r}{r_0}\right) \cos 2p_0 r\right\},$$

$$\varphi(x) = \frac{1}{x} \{2x[\mathrm{Ci}(2x) - \mathrm{Ci}(x)] + 2\sin x - \sin 2x\},$$

$$\psi(x) = \frac{1}{x} \{[\mathrm{Ci}(2x) - \mathrm{Ci}(x)]\sin 2x - \mathrm{Si}(2x)\cos 2x + 2\,\mathrm{Si}(x)\cos^2 x\},$$

where $r_0 = 2\varepsilon_0/Dp_0$, p_0 is the Fermi momentum, and n is the concentration of electrons introduced for the sake of normalization. At large distances ($r \gg r_0$) the value of $V(r)$ coincides with the main term of the RKKY potential ($V(r) \sim \cos 2p_0 r/(2p_0 r)^3$), while for $r \lesssim r_0$, $V(r)$ is an oscillating but not sign-reversing function ($V(r) \sim (\sin p_0 r/p_0 r)^2$), and the interaction has a ferromagnetic character. Consequently, ferromagnetic ordering is possible at concentrations $c \gtrsim r_0^{-3}$.

The mathematical reason which leads to ordering is that contributions from diagrams for the spin Green functions containing closed electron loops are proportional to2) T^{-k} ($k \geq 1$) and consequently at low temperatures perturbation theory in terms of the coupling constant does not lead to sensible results. A theory will therefore be developed below in which the expansion is carried out not for the spin Green functions, but for the spin semi-invariants (they are defined in the next section), for which, when ordering is present, the corresponding diagrams are proportional to $T^{-k}\exp(-kQ/T)$ as $T \to 0$. Such a theory is fully equivalent to the principle of cancellation of "dangerous" diagrams4) developed by Bogolyubov[21] for the case of superconductivity, the value of Q being determined from the condition that diagrams that diverge as $T \to 0$ be cancelled out.

2. Let us examine a system of electrons in exchange interaction with randomly distributed magnetic impurity centers. The Hamiltonian of such a system3) in Vonsovskiĭ's s-d-exchange model approximation[22] is of the form

$$H = \sum_{\mathbf{k}s} \varepsilon_{\mathbf{k}} a_{\mathbf{k}s}^{+} a_{\mathbf{k}s} - \frac{J}{2n} \sum_{j} \sum_{\substack{\mathbf{k}s \\ \mathbf{k}'s'}} a_{\mathbf{k}s}^{+} \boldsymbol{\sigma}_{ss'} a_{\mathbf{k}'s'} \mathbf{S}_j e^{i(\mathbf{k}-\mathbf{k}')\mathbf{r}_j}. \tag{1}$$

Here $a_{\mathbf{k}s}^{+}$ and $a_{\mathbf{k}s}$ are creation and annihilation operators for electrons with quasi-momentum $\mathbf{k}$ and spin s, $\varepsilon_{\mathbf{k}}$ is the free-electron energy, σ are the Pauli matrices, and $\mathbf{r}_j$ are the coordinates of the impurity centers. In what follows we shall omit the spin indices, having in mind that all the electron functions are spin matrices.

Let us define the single-particle temperature Green function

$$G_{\mathbf{k}\mathbf{k}'}(t, t'; \mathbf{U}) = i^{-1}\langle \hat{T} P a_{\mathbf{k}}(t) a_{\mathbf{k}'}^{+}(t')\rangle / \langle \hat{T} P\rangle. \tag{2}$$

In formula (2) the angle brackets denote thermodynamic averaging, and the Heisenberg representation is taken for the dependence of the operators on time. The operator P is defined by the equality

$$P = \exp[-i\mathbf{S}(t)\mathbf{U}(t)].$$

Here and in what follows the integration with respect to the twice-encountered t-variables is carried out from 0 to $-i\beta$ ($\beta = 1/T$), and $\mathbf{U}(t)$ is an arbitrary vector function of time which will be put equal to zero at the end of the calculation.

It is necessary to note that since the Green function (2) takes account of the interaction of electrons with impurity centers, it depends on the coordinates of all the impurity atoms. However, the impurity atoms are randomly distributed throughout the metal and consequently the Green function must be averaged with respect to the positions of the impurity atoms. This operation can be easily carried out if correlations between electrons in various scattering acts are ignored, and the interaction of impurity atoms is taken into account in only the molecular-field approximation. It is then sufficient to consider the Green function in the single-impurity approximation, and to define the self-energy part of the averaged Green function by the relationship

$$\Sigma_{\mathbf{k}}(t-t') = n_i T_{\mathbf{k}\mathbf{k}}(t, t'; \mathbf{U}=0), \tag{3}$$

n_i is the number of impurity centers per electron, $n_i = c/n$. The T-matrix in the local s–d-exchange model does not depend on the momenta and is connected with the Green function (2) by the formal relationship

$$G_{\mathbf{k}\mathbf{k}'}(t, t'; \mathbf{U}) = G_{0\mathbf{k}}(t-t')\delta_{\mathbf{k}\mathbf{k}'} + n^{-1} G_{0\mathbf{k}}(t-t_1) T(t_1, t_2; \mathbf{U}) G_{0\mathbf{k}'}(t_2-t'). \tag{4}$$

Here $\mathbf{G}_{0\mathbf{k}}$ is the Green function for electrons without interaction with impurities. Using the equation for the G-function, it is easy to derive an expression for the T-matrix:

$$T(t, t', \mathbf{U}) = -\frac{J}{2} \sum_{\mathbf{k}} \sigma(\langle \hat{T} P \mathbf{S}(t) a_{\mathbf{k}}(t) a_{\mathbf{k}'}^{+}(\bar{t})\rangle / \langle \hat{T} P\rangle) G_{0\mathbf{k}'}^{-1}(\bar{t}-t'). \tag{5}$$

It is not necessary here to integrate with respect to the variable t.

Using the method proposed by Martin and Schwinger[23] as modified by Kadanoff and Baym,[24] the equation

$$T(t, t'; \mathbf{U}) = T_0(t, t'; \mathbf{U}) - \lambda D(t, t_1; \mathbf{U}) \hat{\Pi}(t_1, t_2; \mathbf{U}) T(t_2, t'; \mathbf{U}), \tag{6}$$

can be derived for $T(t, t'; \mathbf{U})$, where $\lambda = JN(0)/n = 3J/4\varepsilon_0$ ($N(0)$ is the density of states at the Fermi surface),

$$\begin{gathered} T_0(t, t'; \mathbf{U}) = -{}^1/_2 J D(t, t'; \mathbf{U}) \boldsymbol{\sigma} \mathbf{M}(t), \\ \mathbf{M}(t) = \langle \hat{T} P \mathbf{S}(t)\rangle / \langle \hat{T} P\rangle; \\ D^{-1}(t, t'; \mathbf{U}) = \delta(t-t') + \lambda R(t-t') \boldsymbol{\sigma} \mathbf{M}(t), \\ R(t) = \frac{1}{N(0)} \sum_{\mathbf{k}} G_{0\mathbf{k}}(t); \\ \hat{\Pi}(t, t'; \mathbf{U}) = R(t-t') \boldsymbol{\sigma} i \frac{\delta}{\delta \mathbf{U}(t)}. \end{gathered} \tag{7}$$

Integrating (6), we obtain a series for $T(t, t'; \mathbf{U})$ in powers of λ and of the semi-invariants $M^{\alpha_1 \cdots \alpha_n}(t_1, \ldots, t_n)$ which are defined by the relationship

$$M^{\alpha_1 \ldots \alpha_n}(t_1, \ldots, t_n) = i^n \frac{\delta^n}{\delta U^{\alpha_1}(t_1) \ldots \delta U^{\alpha_n}(t_n)} \ln \langle \hat{T}P \rangle. \tag{8}$$

Calculation of the various terms in the series shows that their order is determined not only by the powers of λ, but also by the quantities containing powers of $\lambda \ln(\max\{Q, T\}/D)$ which may prove to be appreciable because of the large logarithm. In this connection let us re-group the terms in equation (6) so that the resultant series in λ does not contain divergences in the limit as $\ln(\max\{Q, T\}/D) \to \infty$. For this purpose we put $T(t, t'; \mathbf{U})$ in the form:

$$T(t, t'; \mathbf{U}) = T_0(t, \bar{t}; \mathbf{U}) \tilde{L}_0(\bar{t}, t'; \mathbf{U}). \tag{9}$$

Making use of the relationship (6), we obtain the following equation for $\tilde{L}_0$

$$\tilde{L}_0 = L_0 + L_0 (\boldsymbol{\sigma}\mathbf{M})^{-1} \hat{\Pi} T_0 \overset{\searrow}{\tilde{L}}_0, \tag{10}$$

$$L_0 = [I - (\boldsymbol{\sigma}\mathbf{M})^{-1} \hat{\Pi} T_0]^{-1}. \tag{10a}$$

All the functions in expressions (10) and (10a) are matrices in the time and spin variables, and the arrow in (10) identifies the quantity on which the variational derivative in the operator $\hat{\Pi}$ acts.

If we now iterate Eq. (10) with L_0 as the initial approximation, we obtain a series in powers of λL_0, where $L_0 \sim [1 - \lambda \ln(\max\{Q, T\}/D)]^{-1}$, i.e., the constant $\lambda_{\text{eff}} = \lambda L_0$ will replace λ everywhere in the expansion. In an exactly analogous way the constant λ_{eff} can also be improved by putting $\tilde{L}_0$ in the form:

$$\tilde{L}_0(t, t'; \mathbf{U}) = L_0(t, \bar{t}; \mathbf{U}) \tilde{L}_1(\bar{t}, t'; \mathbf{U}).$$

Continuing this procedure, we finally obtain:

$$T = T_0 \prod_{i=0}^{\infty} L_i. \tag{11}$$

In Eq. (11), the matrices L_i must be arranged in order of increasing i:

$$L_i(t, t', \mathbf{U}) = [\delta(t - t') - N_i(t, t'; \mathbf{U})], \tag{12}$$

where N_0 is determined by the equality (10a), and the remaining N_i's are found from the recurrence relations

$$N_i = (\boldsymbol{\sigma}\mathbf{M})^{-1} \hat{\Pi} T_0 L_0 L_1 \ldots \overset{\searrow}{L}_{i-1}. \tag{13}$$

The quantities N_0 and N_i are of the order of

$$N_0 \sim \lambda \ln(\max\{Q, T\}/D), \quad N_1 \sim (\lambda L_0)^2 \ln(\max\{Q, T\}/D). \tag{14}$$

In calculating N_1 two terms arise: the first one contains the product of two semi-invariants $M^{\alpha_1 \alpha_2}$ and is of the order of $[\lambda L_0 \ln(\max\{Q, T\}/D)]^2$, and a member of the same order enters in the second term, which contains the semi-invariant $M^{\alpha_1 \alpha_2 \alpha_3}$, but these members completely cancel each other. As a result of the cancellation there remain members of the order indicated in (14). As regards the other N_i's, it is not difficult to see that the estimate for them will not in any case be worse than

$$N_i \sim \lambda N_0^i \prod_{k=0}^{i-1} L_k^{i-k+1}.$$

However, it is quite possible that for N_i the estimates will be even more favorable since it is not out of the question that the main members in them also cancel each other as in N_1.

The condition for the convergence of the infinite product (11) is the inequality

$$|N_0 L_0| < 1. \tag{15}$$

In what follows we shall assume that the condition

$$|(\lambda L_0)^2 \ln(\max\{Q, T\}/D)| \ll 1 \tag{16}$$

is satisfied. In this approximation we have $L_i \approx 1$ for $i \geqslant 1$, and consequently

$$T(t, t'; \mathbf{U}) \approx T_0(t, \bar{t}; \mathbf{U}) L_0(\bar{t}, t'; \mathbf{U}). \tag{17}$$

This approximation amounts to summing all the terms of the infinite series which, for each power of the constant λ, contain the maximum power of the large logarithm $\ln(\max\{Q, T\}/D)$, which is formally realized mathematically in the form of an expansion of the T-matrix with respect to the renormalized constant $\lambda_{\text{eff}} = \lambda L_0$. Let us note that this expansion works well only for the ferromagnetic interaction constant $\lambda > 0$, since in that case $N_0 < 0$, $L_0 < 1$, and the inequality (15) is always satisfied. For $\lambda < 0$, the opposite situation arises, i.e., $L_0 > 1$, and although the most divergent terms are summed in the T-matrix, the expansion parameter becomes in fact poorer. For convergence of the produce (11), the more severe inequality $N_0 < \frac{1}{2}$ must be satisfied. In this connection, the results given below are quantitatively applicable only to the case $\lambda > 0$. Nevertheless, some qualitative conclusions can also be drawn for the antiferromagnetic constant on the basis of an analysis of the perturbation-theory series with allowance for the lowest-order terms containing logarithms.

From formulae (7), (10a), and (17) it is not difficult to derive an expression for T:

$$T(\omega_0) = -\frac{J}{2} \boldsymbol{\sigma}\mathbf{M} \left\{ 1 + \lambda i T \sum_{\omega_0'} R(\omega_0') \sigma^\alpha \sigma^\beta M^{\alpha\beta}(\omega_0' - \omega_0) \boldsymbol{\sigma}\mathbf{M}/M^2 \right\}^{-1}. \tag{18}$$

Here ω_0 and ω_0' run through a discrete set of values $\omega_0 = (2n+1) i\pi T$, and the magnitude of $M^{\alpha\beta}$ is determined from the relation (8):

$$M^{\alpha\beta}(t - t') = \langle \hat{T} S^\alpha(t) S^\beta(t') \rangle - M^\alpha M^\beta. \tag{19}$$

In deriving formula (18), the function $\mathbf{U}$ was put equal to zero after taking the variational derivatives.

3. Calculation of expression (18) requires computation of the semi-invariants M^{α} [Eq. (7)] and $M^{\alpha\beta}$ [Eq. (19)]. With the aid of the technique developed above, chains coupled equations can be written for them. In order not to unduly complicate the problem, we confine ourselves to the molecular-field approximation (MFA). In this approximation the spin correlators can be computed even without using the corresponding equations, but an analysis of these equations permits an assessment of the MFA accuracy, which is determined by a quantity of the order of $\eta = \lambda D/3\varepsilon_0 n_i$. Although in a typical experimental situation η may reach unity, the MFA will nevertheless not distort the final results qualitatively even in that case. Thus, for the semi-invariants we have the expressions (see, for example, [25])

$$\mathbf{M} = M\boldsymbol{\tau} = SB_s(S\beta Q)\boldsymbol{\tau}, \tag{20}$$

$$M^{\alpha\beta}(\omega_0) = -i\delta_{\omega_0,0}\tau^{\alpha}\tau^{\beta}\beta\left[S(S+1) - M^2 - M\operatorname{cth}\frac{\beta Q}{2}\right] + iM\frac{\omega_0 i e_{\alpha\beta\gamma}\tau^{\gamma} + Q(\delta_{\alpha\beta} - \tau^{\alpha}\tau^{\beta})}{\omega_0^2 - Q^2}. \tag{21}$$

Here $\boldsymbol{\tau}$ is the direction of the spin angular momentum of the impurity ($\boldsymbol{\tau}^2 = 1$), $B_s(x)$ is a Brillouin function, ω_0 assumes even values $\omega_0 = 2ni\pi T$, and $e_{\alpha\beta\gamma}$ is a fully antisymmetric third rank tensor.

At this stage it is necessary to take account of the fact that the internal field Q is formed by the impurity subsystem on account of indirect exchange via the conduction electrons, i.e., the field Q depends in fact on the lattice point at which the impurity is situated. In this connection it is necessary to specify concretely the nature of the field distribution, since until now we have not stipulated what type of ordering has established itself in the impurity subsystem. Two extreme cases are possible here: 1) the orientation of the magnetic moments of the various impurities are rigidly correlated; 2) no perceptible correlation exists between the directions of the magnetic moments of the different impurities. The first case covers ferromagnetic or antiferromagnetic ordering as well as various helicoidal structures. The second type of ordered state is customarily termed "spin glass." It appears that at sufficiently low impurity concentrations the spin-glass type structure is realized; with increase in concentration this is transformed into a more or less correlated phase. In the present work we have confined ourselves to the case of ferromagnetic ordering. This obviates an analysis of the specific properties of the discrete crystal lattice, which is needed for a correct calculation of antiferromagnetic ordering and of helicoidal structures. Moreover, for purely ferromagnetic ordering there are also considerable computational advantages because the directions of all the magnetic moments coincide. In a certain sense ordering of the spin-glass type also possesses a similar simplicity (in this case the T-matrix in formula (3) must be averaged over all possible directions of the vector $\boldsymbol{\tau}$). The functional dependence of the thermodynamic variables on the system parameters for spin-glass and ferromagnetic ordering is identical.

The internal exchange field $\mathbf{Q}_j = Q\boldsymbol{\tau}_j$ acting on an impurity at the point $\mathbf{r}_j$ is connected with the Green function by the relationship

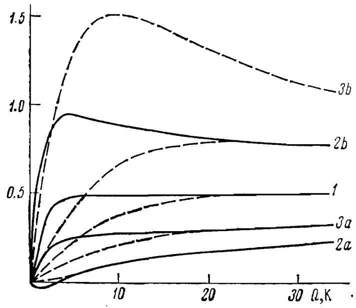

FIG. 1. The dependence of the right-hand side of Eq. (23) (arbitrary units) on Q; the following notation has been adopted in this and the next figure: 1—logarithmic corrections not taken into consideration, 2—perturbation theory, 3—present theory; the symbols a and b correspond to $\lambda = 0.2$ and $\lambda = -0.2$; the continuous lines correspond to $T = 1$ K, the dashed lines to $T = 5$ K; $S = 0.5$, $D = 500$ K.

$$Q_j = -\frac{J}{2n} i\,\mathrm{Sp}_s\,\sigma\bar{G}(\mathbf{r}_j, t; \mathbf{r}_j, t^+); \tag{22}$$

$\bar{G}$ is the Green function averaged over the locations of all the impurities except the one situated at the point $\mathbf{r}_j$, and $t^+ = t + 0$. Making use of relationship (22) and performing the calculations at the adopted accuracy, we find that Q satisfies the equation

$$Q = -\lambda\int d\omega\left(-\frac{\partial f(\omega)}{\partial\omega}\right)\operatorname{Re}F(\omega, Q), \tag{23}$$

$$F(\omega, Q) = -\frac{Jn_iM(\beta Q)}{2} \times \frac{1 - \lambda g(Q+\omega) + i\pi\lambda[f(Q+\omega) + S(S+1)/2M(\beta Q) - {}^1/_2]}{[1 - \lambda g(Q+\omega)]^2}, \tag{24}$$

$$g(\Omega) = \int d\omega\frac{f(\omega) + \nu(Q)}{\omega - \Omega}. \tag{25}$$

Here $f(\omega)$ and $\nu(Q)$ are the Fermi and Bose distribution functions. The logarithmic divergence in relationship (24) is cut off in the usual way at $\omega = D$.

From (23) it is possible to determine the critical temperature of the transition to the ordered state for any given concentration. In contrast to the situation where the logarithmic corrections are neglected, T_c is lowered for the ferromagnetic constant and increased for the antiferromagnetic constant. For small values of λ this change in T_c has the form:

$$\Delta T_c/T_c \approx \lambda\ln(T_c/D).$$

Although relationships (23) and (24) are only good in the case where $\lambda > 0$, this conclusion is nevertheless also correct for $\lambda < 0$ since it follows from the usual perturbation theory in λ.

In Fig. 1 are shown curves for the right-hand side of (23) at positive and negative λ (the curves corresponding to $\lambda < 0$ have a purely illustrative character since, as already noted, the results for the antiferromagnetic constant are valid only qualitatively) and for two values of temperature. For comparison, the right-hand sides of this equation without the logarithmic terms are shown in the same figure, as are the relations derived from perturbation theory. The solutions of Eq. (23), of the

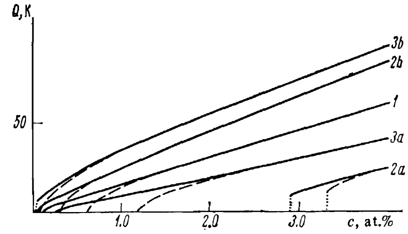

FIG. 2. The dependence of Q on the impurity concentration. Curves 2a and 3b show that a first-order phase transition takes place in the system (the field Q appears jumpwise), but these results are not reliable since $|\lambda \ln(\max\{Q, T\}/D)| \sim 1$ in the region where $T \sim T_c$, and consequently the conditions for applicability of both perturbation theory and the theory presented here are violated for $\lambda < 0$.

analogous perturbation-theory equation, and finally, of the equation in which the logarithmic terms are discarded, are shown as functions of the concentration in Fig. 2.

4. Let us now examine the electron spectrum. From (3), (18), and (21) it is not difficult to find the self-energy part of the Green function averaged over a random impurity distribution:

$$\Sigma_+(\omega+i\delta)=F(\omega, Q),$$
$$\Sigma_-(\omega+i\delta)=-F^*(-\omega, Q). \tag{26}$$

Σ_+ and Σ_- are the self-energy terms for electrons with spin directions parallel to (+) and antiparallel (−) to the field Q, and the function F is defined by Eq. (24). In the limit as $Q \to 0$ formula (26) leads to the corresponding self-energy terms in the Abrikosov[17] approximation.

From (24) and (26) it is evident that in the neighborhood of the Fermi surface the electron spectrum in the range $\omega \sim Q$ is considerably renormalized, the renormalization being substantially more clearly manifest for (−) electrons. In addition, the effective mass of the electrons at the Fermi surface increases sharply (this increase is identical for both (−) and for (+) electrons). For the increase in effective mass the following formula can be obtained:

$$\frac{\Delta m}{m}=\frac{8n_i M\varepsilon_0}{3T_K}\frac{u}{u^2+\xi^2}\frac{1}{\ln^2(u^2+\xi^2)}, \tag{27a}$$

where $u = Q/T_K$, $\xi = 4T/\pi T_K$, T_K being the Kondo temperature defined by the relationship $T_K = D\exp(1/\lambda)$. For the limit $|\lambda \ln(Q/D)| \ll 1$ and $T \ll Q$ it is not difficult to derive from (27a) the result previously found by Kondo.[12] It should, however, be noted that the estimate $\Delta m/m \approx 5$ obtained in[12] is only valid for the antiferromagnetic coupling constant, whereas for the ferromagnetic constant $\Delta m/m \lesssim 2$, as can be seen by using (23) to transform (27a) into

$$\frac{\Delta m}{m}=\frac{2u^2}{u^2+\xi^2}\frac{1}{|\lambda \ln(u^2+\xi^2)|}. \tag{27b}$$

The fact that Δm depends on the concentration and on the temperature distinguishes this result from that derived in[12], in which these dependences are absent.

As already noted, ReΣ and ImΣ are non-monotonic functions of ω in the neighborhood of the Fermi surface. The form of these functions can be reconstructed directly from tunnel experiments (see[26]).

Since the low-temperature electronic heat capacity C is proportional to the effective mass of electrons on the Fermi surface, it is evident that a change in effective mass will result in a change in heat capacity.

$$\Delta C = C\Delta m/m.$$

The dependence of ΔC on concentration and temperature is shown in Fig. 3. The plots agree well qualitatively with the experimental data (see, for example, [13,14]). No quantitative comparison was made, since it is difficult to deduce the alloy parameters from the experiments. Let us note that there is a broad maximum in the temperature dependence of the electronic heat capacity. A corresponding singularity associated with a second-order phase transition is present in the impurity component of the heat capacity, which is, however, proportional to the impurity concentration and is not appreciable at the concentrations under consideration ($n_i \lesssim 10^{-2}$). Anderson suggested[27] that the broad maximum in the heat capacity can be attributed to a "slow" phase change in which small impurity-center clusters first become ordered, and the critical transition temperature is averaged over the clusters. However, as is evident from Fig. 3, the proposed model guarantees a smooth behavior of the heat capacity even for complete ferromagnetic ordering of the impurity-center subsystem.

5. In conclusion let us dwell once more on the approximations made in this paper:

1) the self-energy part is written with an accuracy defined by the inequality (16);

2) the averaging over the random impurity distribution is carried out in a way such that Σ is calculated in an approximation linear in the concentration;

3) the impurity correlators are calculated in the molecular-field approximation.

Thus, the solution obtained reduces to the Kondo effect in a magnetic field, except that the field is defined self-

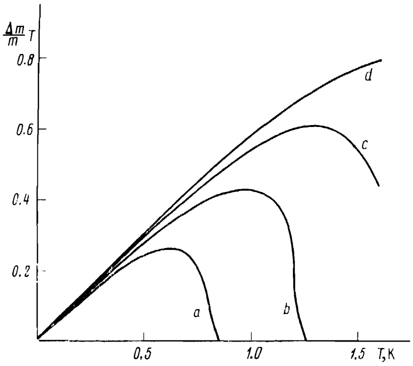

FIG. 3. The dependence of $T\Delta m/m$ on temperature at concentrations of a) 0.4 at.%, b) 0.6 at.%, c) 0.8 at.%, and d) 1.0 at.%; $\lambda = 0.2$; $S = 0.5$; $D = 500$ K.

consistently. Generalization of the problem to the case where there is an external magnetic field presents no difficulty.

From the foregoing analysis it follows that in investigating the interaction of impurity centers in dilute magnetic alloys at low temperatures one must not confine oneself to the RKKY approximation, since the RKKY Hamiltonian only depends on the square of the exchange interaction constant, whereas, as shown above, the results obtained depend appreciably on the sign of the constant.

We have explained here the concentration and temperature dependences of the electronic heat capacity, have shown that for a ferromagnetic coupling constant the heat capacity cannot increase by more than three times, and consequently, if a larger increase in heat capacity is observed experimentally, it is evident that the coupling constant has a negative sign.

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1)It should be noted that the analytical theory developed below in terms of Abrikosov's[17] "parquet" diagram technique is equivalent to summing the most divergent diagrams.

2)Attention was kindly drawn to this circumstance by A. I. Larkin.

3)To simplify the notation we set the volume of the system equal to unity.

4)For a treatment of these diagrams see N. M. Hugenholtz, Physica **23**, 481 (1957) (Translator).

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