ЖЭТФ, 1999, том 115, вып. 4, стр. 1263-1284

# STRONG COUPLING IN THE KONDO PROBLEM IN THE LOW-TEMPERATURE REGION

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#### Submitted 13 August 1998

The magnetic field dependence of the average spin of a localized electron coupled to conduction electrons with an antiferromagnetic exchange interaction is found for the ground state. In the magnetic field range  $\mu H \sim 0.5T_c$  ( $T_c$  is the Kondo temperature) there is an inflection point, and in the strong magnetic field range  $\mu H \gg T_c$ , the correction to the average spin is proportional to  $(T_c/\mu H)^2$ . In zero magnetic field, the interaction with conduction electrons also leads to the splitting of doubly degenerate spin impurity states.

### 1. INTRODUCTION

In the low-temperature and weak magnetic field region, even a weak interaction of magnetic impurities with a degenerate electron gas becomes strong [1-3]. In this region, perturbation theory is violated. Two scenarios are possible in such a situation. First, an assumption can be made that in the low-temperature region, an increase in the magnetic field takes the system out of a strongly coupled state and into the region of applicability of perturbation theory. This nonobvious conjecture was used in Bethe's ansatz method in the problem under consideration. As the result, in a strong magnetic field  $\mu H \gg T_c$  ( $T_c$  is the Kondo temperature), the correction to the mean spin impurity value has logarithmic behavior [3],

$$\langle S_z \rangle = \frac{1}{2} \left( 1 - \frac{1}{2 \ln(\mu H/T_c)} \right).$$

Such spin dependence of the magnetic field value is too slow, and is inconsistent with the experimental data [4], which yields power-like behavior. The level of spin saturation in the magnetic field in Ref. [4] (Fig. 8) can be reached according to the expression given above only at the magnetic field value  $H \approx 50$  T, instead of the experimental value of 6 T.

The second scenario is connected with the assumption that an increase only in the magnetic field value does not move the system from a strongly coupled state to a weakly perturbed state. The second conjecture is supported by the fact that the correction to the wave function of a system consisting of magnetic impurity plus degenerate Fermi gas, in some state with low energy, contains corrections of two types obtained with the help of perturbation theory. The norm of one of them decreases in an increasing magnetic field, whereas the norm of the other is divergent in the limit  $T \rightarrow 0$  for a finite magnetic field. Consideration of the norm of states in the problem involved is very useful, because it contains direct information about the average value of magnetic spin.

Below we consider in detail the second conjecture and confirm it. In the low-temperature region  $(T \ll T_c)$ , the average spin of magnetic impurities is found for an arbitrary value of

the external magnetic field. States for both signs of interaction constant are investigated. The strong coupled state arises in both cases, but the magnetic field dependence of the average value of spin is substantially different. The definition of Kondo temperature  $T_c$  is also slightly different for different signs of the interaction constant.

### 2. THE MODEL

We will suppose that the interaction of magnetic impurity with the Fermi sea of electrons has an exchange nature. Then the Hamiltonian  $\hat{H}$  of the system under consideration can be taken in the form

$$\hat{H} = \hat{H}_{0} + \int d^{3}r_{1}d^{3}r_{2}V(r_{1} - r_{2})\chi_{\alpha}^{+}(r_{1})\varphi_{\beta}^{+}(r_{2})\chi_{\beta}(r_{2})\varphi_{\alpha}(r_{1}) - \frac{\mu H}{2} \int \left(\varphi_{\uparrow}^{+}(r_{1})\varphi_{\uparrow}(r_{1}) - \varphi_{\downarrow}^{+}(r_{1})\varphi_{\downarrow}(r_{1})\right)d^{3}r_{1}.$$
(1)

In Eq. (1), operators  $\varphi_{\beta}^{+}$ ,  $\chi_{\alpha}^{+}$  are creation operators of an electron in a localized state on a magnetic impurity and in the continuum spectrum respectively. For simplicity, we consider the case with one unpaired electron in the localized state (spin 1/2). The first term in Eq. (1) describes the degenerate electron gas in some external field that leads to creation of one localized state. The spin interaction of electrons in the continuum spectrum with magnetic field leads only to small renormalization of the magnetic moment of a localized electron, and a small shift in the kinetic energy of electrons with spin up and down in such a way that they have the same value of chemical potential (no gap for transfer of electron with spin flip over the Fermi level). For this reason we omit this term in Hamiltonian (1). The last term gives the interaction energy of a localized electron with the magnetic field.

Consider now the limiting case as  $T \to 0$  and H finite. We search for the lowest-energy eigenfunction  $|\psi\rangle$  of Hamiltonian (1) in Fock space in the form

$$\begin{split} |\psi\rangle &= |10;11;11;...\rangle + \sum_{K_{1} < K} C_{2K}^{2L-1} |01; \stackrel{2K}{10}; \stackrel{2L-1}{10} \rangle + \sum_{K_{1} < K} C_{2K-1}^{2L-1} |10; \stackrel{2K-1}{01}; \stackrel{2L-1}{10} \rangle + \\ &+ \sum_{K_{1} < K} C_{2K}^{2L} |10; \stackrel{2K}{10}; \stackrel{2L}{01} \rangle + \sum_{K_{1} < K} C_{2K_{1}}^{2L} \stackrel{2L-1}{2K} \hat{N} |01; \stackrel{2K_{1}}{10}; \stackrel{2K_{2}}{10}; \stackrel{2L-1}{10} \rangle + \\ &+ \sum_{K_{1} < K} C_{2K_{1}-1;2K}^{2L-1} \hat{N} |10; \stackrel{2K_{1}-1}{01}; \stackrel{2K_{2}}{10}; \stackrel{2L-1}{10} \rangle + \sum_{L_{1} < L} C_{2K_{1},2K-1}^{2L-1} \hat{N} |01; \stackrel{2K_{1}-2L-1}{10} \rangle |10; \stackrel{2K_{1}-1}{10} \rangle + \\ &+ \sum_{K_{1} < K; L_{1} < L} C_{2K_{1}-1;2K-1}^{2L_{1}-1} \hat{N} |10; \stackrel{2K_{1}-2K-1}{01}; \stackrel{2K_{2}-1}{10}; \stackrel{2K_{1}-2L-1}{10} \rangle + \\ &+ \sum_{K_{1} < K; L_{1} < L} C_{2K_{1}-2K-1}^{2L_{1}-1} \hat{N} |10; \stackrel{2K_{1}-2K-1}{10}; \stackrel{2K_{1}-2L-1}{10} \rangle + \dots \end{split}$$

$$(2)$$

In Eq. (2), all single-particle states (solutions of Eq. (1) for one particle) are ordered and numbered. Indexes K, L label states under and over the Fermi surface. Each box has two places. The first one means a state with spin up, and the second with spin down. As an example, the state  $\begin{vmatrix} 2K & 2L \\ 10, 01 \end{vmatrix}$  means that the state 2K (spin down) under the Fermi surface

is empty and the state 2L (spin up) over the Fermi surface is filled. The first cell is always reserved for an electron in a localized state. The first term in Eq. (2) gives the ground state of Hamiltonian (1) without interaction (V(r) = 0). The number of upper (or lower) indexes in  $C_{\dots}^{\dots}$  gives the number of excited pairs. For P excited pairs, there are 2P + 1 different symbols  $C_{\dots}^{\dots}$ . Operator  $\hat{N}$  is the ordering operator, and each rearrangement of two neighboring filled states gives a factor (-1). In Eq. (2) in each box below Fermi surface, only one place can be empty and above the Fermi surface in each box, only one place can be filled.

The equation for the wave function  $|\psi\rangle$  is

$$|H\psi\rangle = E|\psi\rangle,\tag{3}$$

where E is the energy of the state.

Inserting expression (2) for the wave function  $|\psi\rangle$  into Eq. (3), we obtain a set of linear equations for the quantities  $C_{\dots}$ . Due to the structure of Hamultonian (1), each quantity  $C_{\dots}$  with index P is coupled only with quantities  $C_{\dots}$  with indexes  $P, P \pm 1$ . From the first equation of this system, we obtain the energy of the state,

$$E = E_0 - \mu H/2 - \delta E, \tag{4}$$

$$\delta E = \sum \left( \left( I_{2K-1}^{2L-1} \right)^* C_{2K-1}^{2L-1} - \left( I_{2K}^{2L-1} \right)^* C_{2K}^{2L-1} \right),$$

where  $E_0$  is the energy of the ground state without interaction. For convenience, we leave the magnetic energy of the localized state out of the correction term  $\delta E$ . The quantities  $I_{...}^{...}$  in Eq. (4) are the transition matrix elements. As an example, we have

$$I_{2K}^{2L-1} = \int d^3 r_1 d^3 r_2 \chi_{\uparrow}^*(r_1) \varphi_{\downarrow}^*(r_2) \varphi_{\uparrow}(r_1) \chi_{\downarrow}(r_2) V(r_1 - r_2).$$
(5)

The Hamiltonian (1) possesses deep symmetry properties. To see some of these, we will keep indexes on  $I_{\dots}^{\dots}$  that indicate energy and spin in the initial and final states. The next three equations for the quantities  $C_{\dots}^{\dots}$  are

$$-I_{2K}^{2L-1} + \sum_{k=1}^{2L-1} C_{2K_{1}}^{2L-1} I_{2K}^{2K_{1}} - \sum_{k=1}^{2L-1} C_{2K_{1}-1}^{2L_{1}-1} I_{2K}^{2L_{1}-1} - \sum_{k=1}^{2L-1} C_{2K_{1}}^{2L_{1}} I_{2L_{1}}^{2L_{1}-1} + \\ + (\mu H + \varepsilon_{L} - \varepsilon_{K} - \delta E) C_{2K}^{2L-1} + \sum_{K_{1} < K} C_{2K_{1};2K}^{2L_{1};2L-1} I_{2L_{1}}^{2K_{1}} - \\ - \sum_{K < K_{1}} C_{2K;2K_{1}}^{2L_{1};2L-1} I_{2L_{1}}^{2K_{1}} - \sum_{k=1}^{2L} C_{2K_{1}-1;2K}^{2L_{1};2L-1} I_{2L_{1}}^{2K_{1}-1} = 0,$$

$$I_{2K-1}^{2L-1} - \sum_{k=1}^{2L} I_{2K-1}^{2L-1} C_{2K-1}^{2L-1} + \sum_{L_{1} < L} C_{2K_{1},2K-1}^{2L-1} I_{2L_{1}-1}^{2K_{1}-1} - \sum_{L < L_{1}} I_{2L_{1}-1}^{2K_{1}} I_{2L_{1}-1}^{2K_{1}} + \sum_{L_{1} < L} C_{2K_{1};2K-1}^{2L_{1}-1} I_{2L_{1}-1}^{2K_{1}-1} - \\ - \sum_{L < L_{1}} C_{2K_{1};2K-1}^{2L-1;2L_{1}-1} I_{2L_{1}-1}^{2K_{1}-1} + \sum_{K < K_{1};L_{1} < L} C_{2K_{1}-1;2K-1}^{2L_{1}-1} I_{2L_{1}-1}^{2K_{1}-1} - \\ - \sum_{L < L_{1}} C_{2K_{1};2K-1}^{2L-1;2L_{1}-1} I_{2L_{1}-1}^{2K_{1}-1} + \sum_{K < K_{1};L_{1} < L} C_{2K_{1}-1;2K-1}^{2L_{1}-1} I_{2L_{1}-1}^{2K_{1}-1} - \\ - \sum_{L < L_{1}} C_{2K_{1}-1;2L_{1}-1}^{2L_{1}-1} I_{2L_{1}-1}^{2K_{1}-1} + \sum_{K < K_{1};L_{1} < L} C_{2K_{1}-1;2K-1}^{2L_{1}-1} I_{2L_{1}-1}^{2K_{1}-1} - \\ - \sum_{L < L_{1};K < K_{1}} C_{2K_{1}-1;2K_{1}-1}^{2L_{1}-1} I_{2L_{1}-1}^{2K_{1}-1} + \sum_{K_{1} < K_{1} < K_$$

$$-\sum_{L_{2L_{1}-1}} I_{2L_{1}-1}^{2L} C_{2K}^{2L_{1}-1} + (\varepsilon_{L} - \varepsilon_{K} - \delta E) C_{2K}^{2L} + \sum_{K < K_{1}} C_{2K;2K_{1}}^{2L;2L_{1}-1} I_{2L_{1}-1}^{2K_{1}} - \\ -\sum_{K_{1} < K} C_{2K_{1};2K}^{2L;2L_{1}-1} I_{2L_{1}-1}^{2K_{1}} + \sum_{L_{1}-1} C_{2K_{1}-1;2K}^{2L;2L_{1}-1} I_{2L_{1}-1}^{2K_{1}-1} = 0.$$

In Eqs. (6), the quantities  $\varepsilon_{L,K}$  are the energies of single states. As mentioned above, index L means a state above the Fermi level and index K means a state below the Fermi level. The equations for  $C_{...}^{...}$  are given in Appendix A. Since the equations for  $C_{...}^{...}$  have a special structure, each quantity  $C_{...}^{...}$  with index P is coupled only with quantities  $C_{...}^{...}$  with indexes  $P, P \pm 1$ , it is possible to leave quantities  $C_{2K}^{...}$  with indexes  $P \ge 2$  out of Eqs. (6). As the result, we obtain three equations for the quantities  $C_{2K}^{2L-1}$ ,  $C_{2K-1}^{2L-1}$  and  $C_{2K}^{2L}$ . They have the following form (see Appendix A):

$$-I_{2K}^{2L-1} + \sum_{K} C_{2K_{1}}^{2L-1} I_{2K}^{2K_{1}} - \sum_{K} C_{2K_{1}-1}^{2L-1} I_{2K}^{2K_{1}-1} - \sum_{K} C_{2K}^{2L_{1}} I_{2L_{1}}^{2L-1} + + \left(\mu H + \varepsilon_{L} - \varepsilon_{K} - \delta E - \Sigma_{(K,L)}^{(1)}\right) C_{2K}^{2L-1} = A_{1} \left(C_{2K}^{2L-1}; C_{2K-1}^{2L-1}; C_{2K}^{2L}\right), I_{2K-1}^{2L-1} - \sum_{K} C_{2K_{1}}^{2L-1} I_{2K-1}^{2K_{1}} + \sum_{K} C_{2K_{1}-1}^{2L-1} I_{2K-1}^{2K_{1}-1} - \sum_{K} C_{2K-1}^{2L_{1}-1} I_{2L_{1}-1}^{2L-1} + + \left(\varepsilon_{L} - \varepsilon_{K} - \delta E - \Sigma_{(K,L)}\right) C_{2K-1}^{2L-1} = A_{2} \left(C_{2K}^{2L-1}; C_{2K-1}^{2L-1}; C_{2K}^{2L}\right),$$

$$(7)$$

$$-\sum I_{2L_{1}-1}^{2L}C_{2K}^{2L_{1}-1} + \left(\varepsilon_{L} - \varepsilon_{K} - \delta E - \Sigma_{(K,L)}\right)C_{2K}^{2L} = A_{3}\left(C_{2K}^{2L-1}; C_{2K-1}^{2L-1}; C_{2K}^{2L}\right).$$

The linear operators  $A_{1,2,3}$  do not contain terms proportional to the quantities  $C_{2K}^{2L-1}, C_{2K-1}^{2L-1}, C_{2K}^{2L}$  without integral over one of variable K, L with some function of K, L. These terms form the  $\Sigma_{(K,L)}^{(1)}, \Sigma_{(K,L)}$  terms in Eq. (7). All off-diagonal elements of such a form are equal to zero. The linear operators  $A_{1,2,3}$  also do not contain terms proportional to the convolution of quantities  $C_{...}^{(1)}$  with  $I_{...}^{(1)}$  over one of variable K, L without of denominator with the same variable. In Appendix C, we give the expressions for quantities  $\Sigma_{(K,L)}^{(1)}, \Sigma_{(K,L)}$  in the fourth order of perturbation theory. Quantities  $C_{2K}^{2L-1}, C_{2K-1}^{2L-1}, C_{2K}^{2L}$  in the third order can be found from equations given in Appendix B. It is easy to check that in the fourth order of perturbation theory,

$$-\delta E - \Sigma_{(K,L)}\Big|_{\varepsilon_K = \varepsilon_L = \varepsilon_F} = 0.$$
(8)

This equality holds in all the orders of perturbation theory. Below, we put

$$-\delta E - \Sigma_{(K,L)}\Big|_{\varepsilon_K = \varepsilon_L = \varepsilon_F} = \Delta.$$
<sup>(9)</sup>

In Eq. (9),  $\Delta \equiv \Delta(H)$  is some function of the magnetic field that must be determined from self-consistency. This equation is given below. Very important properties follow from the normalisation of states defined by Eqs. (2) and (7). To simplify the investigation of Eqs. (7), we give also the expression for operators  $A_{1,2,3}$  in the lowest order of perturbation theory in Appendix D. All statements made above are independent of the exact form of spectrum  $\varepsilon_K, \varepsilon_L$  and potential V(r).

## 3. WAVE FUNCTION OF THE GROUND STATE

The average electron spin  $\langle S_z \rangle$  in a bound state at zero temperature can be found by differentiating the energy  $\delta E$  with respect to  $\mu H$ 

$$\langle S_z \rangle = \frac{1}{2} - \frac{\partial \delta E}{\partial \mu H}.$$
 (10)

In accordance with quantum mechanical rules, the quantity  $\langle S_z \rangle$  in the ground state is also given by an expression containing only norms of the states in expansion (2):

$$\langle S_{z} \rangle = \frac{1}{2} \Big\{ 1 + \Big| C_{2K-1}^{2L-1} \Big|^{2} + \Big| C_{2K}^{2L} \Big|^{2} - \Big| C_{2K}^{2L-1} \Big|^{2} + \Big| C_{2K_{1}-1;2K}^{2L_{1};2L-1} \Big|^{2} + \Big| C_{2K_{1}-1;2K-1}^{2L_{1},2L-1} \Big|^{2} + \\ + \Big| C_{2K_{1};2K}^{2L_{1};2L} \Big|^{2} - \Big| C_{2K_{1};2K}^{2L_{1};2L-1} \Big|^{2} - \Big| C_{2K_{1};2K-1}^{2L_{1}-1;2L-1} \Big|^{2} + \\ \times \Big\{ 1 + \Big| C_{2K-1}^{2L-1} \Big|^{2} + \Big| C_{2K}^{2L} \Big|^{2} + \Big| C_{2K}^{2L-1} \Big|^{2} + \Big| C_{2K_{1}-1;2K-1}^{2L_{1}-1} \Big|^{2} + \Big| C_{2K_{1}-1;2K-1}^{2L_{1}-1} \Big|^{2} + \\ + \Big| C_{2K_{1};2K}^{2L_{1};2L} \Big|^{2} + \Big| C_{2K_{1};2K}^{2L_{1}-1} \Big|^{2} + \Big| C_{2K_{1}-1;2K-1}^{2L_{1}-1} \Big|^{2} + \\ \Big| C_{2K_{1};2K}^{2L_{1};2L} \Big|^{2} + \Big| C_{2K_{1};2K}^{2L_{1}-1} \Big|^{2} + \Big| C_{2K_{1};2K-1}^{2L_{1}-1} \Big|^{2} + \\ \Big| C_{2K_{1};2K}^{2L_{1};2L} \Big|^{2} + \Big| C_{2K_{1};2K}^{2L_{1}-1} \Big|^{2} + \Big| C_{2K_{1};2K-1}^{2L_{1}-1} \Big|^{2} + \\ \Big| C_{2K_{1};2K}^{2L_{1};2L} \Big|^{2} + \Big| C_{2K_{1};2K}^{2L_{1}-1} \Big|^{2} + \Big| C_{2K_{1};2K-1}^{2L_{1}-1} \Big|^{2} + \\ \Big| C_{2K_{1};2K}^{2L_{1};2L} \Big|^{2} + \Big| C_{2K_{1};2K}^{2L_{1}-1} \Big|^{2} + \Big| C_{2K_{1};2K-1}^{2L_{1}-1} \Big|^{2} + \\ \Big| C_{2K_{1};2K}^{2L_{1};2L} \Big|^{2} + \Big| C_{2K_{1};2K}^{2L_{1}-1} \Big|^{2} + \Big| C_{2K_{1};2K-1}^{2L_{1}-1} \Big|^{2} + \\ \Big| C_{2K_{1};2K}^{2L_{1};2L} \Big|^{2} + \Big| C_{2K_{1};2K}^{2L_{1}-1} \Big|^{2} + \Big| C_{2K_{1};2K-1}^{2L_{1}-1} \Big|^{2} + \\ \Big| C_{2K_{1};2K}^{2L_{1},2L} \Big|^{2} + \Big| C_{2K_{1};2K}^{2L_{1}-1} \Big|^{2} + \Big| C_{2K_{1};2K-1}^{2L_{1}-1} \Big|^{2} + \\ \Big| C_{2K_{1};2K}^{2L_{1},2L} \Big|^{2} + \Big| C_{2K_{1};2K}^{2L_{1}-1} \Big|^{2} + \Big| C_{2K_{1};2K-1}^{2L_{1}-1} \Big|^{2} + \\ \Big| C_{2K_{1};2K}^{2L_{1}-1} \Big|^{2} + \Big| C_{2K_{1};2K}^{2L_{1}-1} \Big|^{2} + \Big| C_{2K_{1};2K}^{2L_{1}-1} \Big|^{2} + \\ \Big| C_{2K_{1};2K}^{2L_{1}-1} \Big|^{2} + \Big| C_{2K_{1};2K}^{2L_{1}-1} \Big|^{2} + \\ \Big| C_{2K_{1};2K}^{2L_{1}-1} \Big|^{2} + \Big| C_{2K_{1};2K}^{2L_{1}-1} \Big|^{2} + \\ \Big| C_{$$

Below we use both Eqs. (10) and (11). To solve Eqs. (7) and (9), we consider  $\Delta$  as a parameter. Then the right-hand sides of Eqs. (7) can be taken into account in perturbation theory. In the leading approximation we obtain

$$-I_{2K}^{2L-1} + \sum_{2K_{1}} C_{2K_{1}}^{2L-1} I_{2K}^{2K_{1}} - \sum_{2K_{1}-1} C_{2K_{1}-1}^{2L_{1}-1} I_{2K}^{2L_{1}-1} - \sum_{2K_{1}} C_{2K_{1}}^{2L_{1}-1} I_{2L_{1}}^{2L_{1}-1} + (\mu H + \varepsilon_{L} - \varepsilon_{K} + \Delta) C_{2K}^{2L-1} = 0 ,$$

$$I_{2K-1}^{2L-1} - \sum_{2K_{1}} C_{2K_{1}}^{2L-1} I_{2K-1}^{2K_{1}-1} + \sum_{2K_{1}-1} C_{2K_{1}-1}^{2L_{1}-1} - \sum_{2K_{1}-1} C_{2K_{1}-1}^{2L_{1}-1} I_{2L_{1}-1}^{2L-1} + (\varepsilon_{L} - \varepsilon_{K} + \Delta) C_{2K-1}^{2L-1} = 0 ,$$

$$-\sum_{2L_{1}-1} C_{2K_{1}}^{2L_{1}-1} C_{2K_{1}}^{2L_{1}-1} + (\varepsilon_{L} - \varepsilon_{K} + \Delta) C_{2K}^{2L} = 0 .$$
(12)

Below we make the usual assumptions about the energy-independent value of the density of states near the Fermi surface, and that the characteristic energy in transition matrix elements  $I_{\dots}^{\dots}$  is also the Fermi energy  $\varepsilon_F$ . As a result, we can put

$$\sum_{K} I_{2K}^{\dots}(\dots) \to g \int_{0}^{\varepsilon_{F}} dx(\dots), \quad \sum_{L} I_{\dots}^{2L} \to g \int_{0}^{A\varepsilon_{F}} dy(\dots), \qquad (13)$$
$$\varepsilon_{L} - \varepsilon_{F} = y, \qquad \varepsilon_{F} - \varepsilon_{K} = x .$$

In Eqs. (13), g is the dimensionless coupling constant. The potential V(r) in Hamiltonian (1) is in natural units, hence the smallness of the coupling constant g is connected only to the small radius of bound state.

Due to the energy independence of the transition matrix elements  $I_{\dots}^{\dots}$ , Eqs. (12) can be substantially simplified. To do this, we define new quantities that are convolutions of functions  $C_{\dots}^{\dots}$  with overlap integral  $I_{\dots}^{\dots}$  over only one variable, K or L, that is

$$Z_L = \sum_{K_1} I_{2K}^{2K_1} C_{2K_1}^{2L-1}, \qquad Z_K = \sum_{L_1} I_{2L_1-1}^{2L} C_{2K}^{2L_1-1} ,$$

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$$Y_{L} = \sum_{K_{1}} I_{2K}^{2L_{1}-1} C_{2K_{1}-1}^{2L_{-1}} , \qquad Y_{K} = \sum_{L_{1}} I_{2L_{1}-1}^{2L_{-1}} C_{2K-1}^{2L_{1}-1} , \qquad (14)$$
$$X_{L} = \sum_{L} I_{2L_{1}-1}^{2L} C_{2K}^{2L_{1}} , \qquad X_{K} = \sum_{L} I_{2L_{1}}^{2L-1} C_{2K}^{2L_{1}} .$$

Inserting Eqs. (14) into Eqs. (12), we obtain

$$C_{2K}^{2L-1} = \frac{1}{\mu H + y + x + \Delta} \left\{ I - Z_L + Y_L + X_K \right\} ,$$

$$C_{2K-1}^{2L-1} = \frac{1}{y + x + \Delta} \left\{ -I + Z_L - Y_L + Y_K \right\} ,$$

$$C_{2K}^{2L} = \frac{1}{y + x + \Delta} Z_K ,$$
(15)

where I is the value of the transition matrix element  $I_{...}^{...}$  for states near the Fermi surface. Now from Eqs. (14) and (15) we can obtain a complete set of equations for the quantities  $Z_{K,L}, Y_{K,L}, X_{K,L}$  only. In addition, the quantities  $X_{K,L}$  are very simply related to  $Z_{K,L}, Y_{K,L}$ . Eliminating them, we obtain a set of equations for just the quantities  $Z_{K,L}, Y_{K,L}$ .

$$Z_{L}\left(1+g\ln\frac{\varepsilon_{F}}{\mu H+y+\Delta}\right) - Y_{L}g\ln\frac{\varepsilon_{F}}{\mu H+y+\Delta} =$$

$$= Ig\ln\frac{\varepsilon_{F}}{\mu H+y+\Delta} + g^{2}\int_{0}^{\varepsilon_{F}}\frac{dxZ_{K}\ln[A\varepsilon_{F}/(x+\Delta)]}{\mu H+y+x+\Delta} ,$$

$$Z_{K}\left(1-g^{2}\ln\frac{A\varepsilon_{F}}{x+\Delta}\ln\frac{A\varepsilon_{F}}{\mu H+x+\Delta}\right) =$$

$$= Ig\ln\frac{A\varepsilon_{F}}{\mu H+x+\Delta} - g\int_{0}^{A\varepsilon_{F}}\frac{dy(Z_{L}-Y_{L})}{\mu H+y+x+\Delta} ,$$

$$Y_{L}\left(1+g\ln\frac{\varepsilon_{F}}{y+\Delta}\right) - Z_{L}g\ln\frac{\varepsilon_{F}}{y+\Delta} = -Ig\ln\frac{\varepsilon_{F}}{y+\Delta} + g\int_{0}^{\varepsilon_{F}}\frac{dxY_{K}}{y+x+\Delta} ,$$

$$Y_{K}\left(1-g\ln\frac{A\varepsilon_{F}}{x+\Delta}\right) = -Ig\ln\frac{A\varepsilon_{F}}{x+\Delta} + g\int_{0}^{A\varepsilon_{F}}\frac{dy(Z_{L}-Y_{L})}{y+x+\Delta} .$$
(16)

Equations (16) are valid for both signs of the interaction constant g. But their solutions are substantially different for g < 0 and g > 0. Consider first the case g < 0 (attractive interaction in the Kondo problem). In such a case, the quantities  $Z_L$ ,  $Y_L$  are large in comparison with  $Z_K$  and  $Y_K$ . To obtain this, we introduce a formal definition of «Kondo» temperature  $T_c$ ,

$$|g|\ln\frac{\varepsilon_F}{T_c} = \frac{1}{2}.$$
(17)

Now we also put

$$T_L(y) = Z_L - Y_L. \tag{18}$$

Eliminating terms  $Z_K$ ,  $Y_K$  from (16), we obtain one equation the quantity  $T_L$ :

$$T_{L}(y) = \frac{1}{1+g\ln[\varepsilon_{F}/(y+\Delta)] + g\ln[\varepsilon_{F}/(\mu H + y + \Delta)]} \left\{ Ig\left(\ln\frac{\varepsilon_{F}}{y+\Delta} + \ln\frac{\varepsilon_{F}}{\mu H + y + \Delta}\right) + \frac{Ig}{2} \int_{0}^{\varepsilon_{F}} dx \left(\frac{1}{\mu H + y + x + \Delta} + \frac{1}{y+x+\Delta}\right) \left[\frac{g^{2}\ln[A\varepsilon_{F}/(x+\Delta)]\ln[A\varepsilon_{F}/(\mu H + x + \Delta)]}{1-g^{2}\ln[A\varepsilon_{F}/(x+\Delta)]\ln[A\varepsilon_{F}/(\mu H + x + \Delta)]} + \frac{g\ln[A\varepsilon_{F}/(x+\Delta)]}{1-g\ln[A\varepsilon_{F}/(x+\Delta)]}\right] - \frac{g^{2}}{2} \int_{0}^{\varepsilon_{F}} dx \left(\frac{1}{\mu H + y + x + \Delta} + \frac{1}{y+x+\Delta}\right) \times \left[\frac{g\ln[A\varepsilon_{F}/(x+\Delta)]}{1-g^{2}\ln[A\varepsilon_{F}/(x+\Delta)]\ln[A\varepsilon_{F}/(\mu H + x + \Delta)]} \times \left[\frac{g\ln[A\varepsilon_{F}/(x+\Delta)]\ln[A\varepsilon_{F}/(\mu H + x + \Delta)]}{1-g\ln[A\varepsilon_{F}/(x+\Delta)]\ln[A\varepsilon_{F}/(\mu H + x + \Delta)]} \times \int_{0}^{A\varepsilon_{F}} \frac{dy_{1}T_{L}(y_{1})}{\mu H + y_{1} + x + \Delta} + \frac{1}{1-g\ln[A\varepsilon_{F}/(x+\Delta)]} \int_{0}^{A\varepsilon_{F}} \frac{dy_{1}T_{L}(y_{1})}{y_{1} + x + \Delta}\right] \right\}.$$
(19)

It can be shown that the last term in Eq. (19) can be omitted, because it is small in the parameter  $(|g| \ln(1/|g|))$ . We then obtain from Eqs. (17) and (19)

$$T_L(y) = \frac{1}{|g| \ln\left[(y+\Delta)(\mu H + y + \Delta)/T_c^2\right]} \left\{ -I - I \int_0^{1/2} dt \left(\frac{t^2}{1-t^2} - \frac{t}{1-t}\right) \right\}.$$
 (20)

And finally

$$T_L(y) = \frac{-I\beta}{|g|\ln[(y+\Delta)(\mu H + y + \Delta)/T_c^2]}, \qquad \beta = \frac{1}{2}\ln 3 + \ln\frac{3}{2}.$$
 (21)

Inserting Eqs. (18) and (21) into Eqs. (15), we obtain the expressions for coefficients  $C_{2K}^{2L-1}$ ,  $C_{2K-1}^{2L-1}$ .

$$C_{2K}^{2L-1} = -\frac{T_L(y)}{\mu H + y + x + \Delta} , \qquad C_{2K-1}^{2L-1} = \frac{T_L(y)}{y + x + \Delta}.$$
 (22)

Now we can determine the value of  $\Delta$ . Equations (10) and (11) should give the same value for average spin  $\langle S_z \rangle$ . This condition, with the help of Eqs. (4) and (22), gives

$$\beta \int_{0}^{\infty} \frac{dy}{(\mu H + y + \Delta) \ln^{2} \left[ (y + \Delta)(\mu H + y + \Delta)/T_{c}^{2} \right]} \left/ \left( 1 + \frac{\beta^{2}}{\ln \left[ \Delta(\mu H + \Delta)/T_{c}^{2} \right]} \right) = \frac{\partial \Delta}{\partial \mu H} \frac{1}{\ln \left[ \Delta(\mu H + \Delta)/T_{c}^{2} \right]} + \int_{0}^{\infty} \frac{dy}{(\mu H + y + \Delta) \ln^{2} \left[ (y + \Delta)(\mu H + y + \Delta)/T_{c}^{2} \right]}.$$
 (23)

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We seek a solution of Eq. (23) in the form

$$\Delta(\mu H + \Delta) = T_c^2(1+\gamma), \qquad 0 < \gamma \ll 1.$$
(24)

Terms proportional to  $\gamma^{-1}$  cancel on the right-hand side of Eq. (23). This condition yields

$$\frac{\partial \Delta}{\partial \mu H} + \frac{T_c^2}{(\mu H + \Delta)(\mu H + 2\Delta)} = 0.$$
(25)

The solution of this equation is

$$\Delta(\mu H + \Delta) = T_c^2, \tag{26}$$

$$\Delta = -\frac{\mu H}{2} + \left( \left( \frac{\mu H}{2} \right)^2 + T_c^2 \right)^{1/2},$$
(26a)

and confirms our conjecture (24) about it. Of course, Eq. (24) has two solutions for  $\Delta$ . One is given by Eq. (26a) (ground state), and the other is

$$\Delta = -\frac{\mu H}{2} - \left( \left( \frac{\mu H}{2} \right)^2 + T_c^2 \right)^{1/2}.$$
 (26b)

Solution (26b) corresponds to the excited state. In the limit  $\mu H \gg T_c$ , this state transforms to a state with spin orientation along the magnetic field. The excited state is separated from the ground state by a «gap»  $2((\mu H/2)^2 + T_c^2)^{1/2}$ . The gap results in the independence of the position of the maximum of impurity heat capacity from the magnetic field in the range  $\mu H \ll T_c$ (Schottky anomaly). Such a residual Schottky anomaly is always presented in experiments [5]. In Sec. 4 we will show that renormalization of the term  $\mu H$  in (7) leads to a change from  $\mu H$ in Eq. (27) to  $\mu \tilde{H}$  defined by Eq. (43). As a result, we obtain the mean spin  $\langle S_z \rangle$  as an implicit function of the magnetic field  $\mu H$ .

An attempt to obtain such an equation at nonzero temperature was made in Ref. [6]. But the mean field approximation used there is incorrect for the problem considered.

In Appendix D we show that the right-hand side of (7) leads to renormalization of the coefficients in Eqs. 16, but does not alter the main result of the paper, Eqs. (27) and (43). Of course, renormalization changes Eqs. (17) for the Kondo temperature. The quantity  $\gamma$  can be found only from correction terms to Eqs. (20) and (22). Fortunately, we do not need these correction terms, because in the leading approximation,  $\gamma$  also drops out of Eq. (11) for the spin value. With the help of Eqs. (11), (22), and (24), we obtain

$$\langle S_{z} \rangle = \frac{\mu H}{2} \int_{0}^{\infty} \frac{dy}{(y+\Delta)(y+\mu H+\Delta)(\gamma+y(\mu H+2\Delta)/T_{c}^{2})^{2}} / \frac{1}{\gamma} = \frac{\mu H}{4 \left(T_{c}^{2}+(\mu H/2)^{2}\right)^{1/2}}.$$
(27)

Equation (27) is in good agreement with the experimental data of Ref. [4].

# 4. FERROMAGNETIC CASE (g > 0)

As mentioned above, Eqs. (16) are valid for both signs of the «interaction» constant g. In the case g > 0, we can define the characteristic energy of the problem from the relation

$$g\ln\frac{A\varepsilon_F}{T_c} = 1$$
(28)

for Kondo temperature  $T_c$ . For g > 0, the quantities  $Z_K$ ,  $Y_K$ ,  $X_K$  are large in comparison with  $Z_L$ ,  $Y_L$ ,  $X_L$ . We can eliminate  $Z_L$ ,  $Y_L$  from Eqs. (16). As a result, we have

$$\begin{aligned} Z_{K} \left( 1 - g^{2} \ln \frac{A\varepsilon_{F}}{x + \Delta} \ln \frac{A\varepsilon_{F}}{\mu H + x + \Delta} \right) &= Ig \ln \frac{A\varepsilon_{F}}{\mu H + x + \Delta} - \\ -g \int_{0}^{A\varepsilon_{F}} \frac{dy}{\mu H + y + x + \Delta} \frac{1}{1 + g \ln[\varepsilon_{F}/(y + \Delta)] + g \ln[\varepsilon_{F}/(\mu H + y + \Delta)]} \left[ Ig \ln \frac{\varepsilon_{F}^{2}}{(y + \Delta)(\mu H + y + \Delta)} + \\ + g^{2} \int_{0}^{\varepsilon_{F}} \frac{dx_{1} Z_{K}(x_{1}) \ln[A\varepsilon_{F}/(x_{1} + \Delta)]}{\mu H + y + x_{1} + \Delta} - g \int_{0}^{\varepsilon_{F}} \frac{dx_{1} Y_{K}(x_{1})}{y + x_{1} + \Delta} \right], \end{aligned}$$

$$\begin{aligned} Y_{K} \left( 1 - g \ln \frac{A\varepsilon_{F}}{x + \Delta} \right) &= -Ig \ln \frac{A\varepsilon_{F}}{x + \Delta} + \\ + g \int_{0}^{A\varepsilon_{F}} \frac{dy}{y + x + \Delta} \frac{1}{1 + g \ln[\varepsilon_{F}/(y + \Delta)] + \ln[\varepsilon_{F}/(\mu H + y + \Delta)]} \left[ Ig \ln \frac{\varepsilon_{F}^{2}}{(y + \Delta)(\mu H + y + \Delta)} + \\ + g^{2} \int_{0}^{\varepsilon_{F}} \frac{dx_{1} Z_{K}(x_{1}) \ln[A\varepsilon_{F}/(x_{1} + \Delta)]}{\mu H + y + x_{1} + \Delta} - g \int_{0}^{\varepsilon_{F}} \frac{dx_{1} Y_{K}(x_{1})}{y + x_{1} + \Delta} \right]. \end{aligned}$$

In the range  $x \ll \varepsilon_F$ , Eqs. (29) yield the following values for  $Y_K$ ,  $Z_K$ :

$$Y_K = -\frac{ID}{g\ln[(x+\Delta)/T_c]} , \qquad Z_K = \frac{ID}{g\ln[(x+\Delta)(\mu H + x + \Delta)/T_c^2]} , \qquad (30)$$

where D is a number of order unity. Inserting Eqs. (30) into Eqs. (15), we obtain

$$C_{2K}^{2L-1} = \frac{1}{\mu H + y + x + \Delta} \frac{ID}{g \ln[(x + \Delta)(\mu H + x + \Delta)/T_c^2]},$$

$$C_{2K-1}^{2L-1} = -\frac{1}{y + x + \Delta} \frac{ID}{g \ln[(x + \Delta)/T_c]},$$

$$C_{2K}^{2L} = \frac{1}{y + x + \Delta} \frac{ID}{g \ln[(x + \Delta)(\mu H + x + \Delta)/T_c^2]}.$$
(31)

In the same way as in the case g < 0, with the help of Eqs. (10), (11), and (31), we obtain

$$\frac{\partial \Delta}{\partial \mu H} \left[ \frac{1}{\ln(\Delta/T_c)} + \frac{1}{\ln[\Delta(\mu H + \Delta)/T_c^2]} \right] = -\left[ 1 - \frac{D^2}{1 + D^2 \left( \frac{1}{\ln(\Delta/T_c)} + \frac{1}{\ln[\Delta(\mu H + \Delta)/T_c^2]} \right)} \right] \int_0^\infty \frac{dx}{(x + \Delta + \mu H) \ln^2 \left[ (x + \Delta)(\mu H + x + \Delta)/T_c^2 \right]}.$$
 (32)

The solution of this equation is

$$\Delta \equiv T_c. \tag{33}$$

Relation (33) means that in the leading approximation, the spin value in the magnetic field is saturated,

$$\langle S_z \rangle = \frac{1}{2}.\tag{34}$$

Correction terms to Eq. (34) come only from an energy range  $\varepsilon$  of order  $\varepsilon \propto \varepsilon_F \exp(-1/g^2)$ . Note that a similar energy scale also arises in the problem considered by Nozieres and Dominicis [7]. Our conjecture is that in temperature range

$$T_c^2/\varepsilon_F \ll T \ll T_c, \tag{35}$$

the leading correction to the average spin arises from the cutoff of integrals with respect to energy in expression (11) over an energy range of order T. If such an assumption is true, then the average spin in the magnetic field  $\mu H \gg T$  is

$$\langle S_z \rangle = \frac{1}{2} - \frac{T}{T_c} \int_0^\infty \frac{dx}{(x+1+\mu H/T_c) \ln^2 \left[ (1+x)(x+1+\mu H/T_c) \right]} = \frac{1}{2} - \frac{T}{4T_c} \int_{\ln(1+\mu H/T_c)}^\infty \frac{dz}{\left[ z + (1/2) \ln[1-(\mu H/T_c)e^{-z}] \right]^2}.$$
 (36)

In the limiting cases of weak ( $\mu H \ll T_c$ ) and strong ( $\mu H \gg T_c$ ) magnetic fields, the average spin is

$$\langle S_z \rangle = \frac{1}{2} \left( 1 - \frac{T}{\mu H} \right), \qquad T \ll \mu H \ll T_c,$$

$$\langle S_z \rangle = \frac{1}{2} \left( 1 - \frac{T}{2T_c \ln(\mu H/T_c)} \right), \qquad \mu H \gg T_c.$$

$$(37)$$

# 5. SELF-ENERGY TERMS $\Sigma^{(1)}_{(K,L)},\ \Sigma_{(K,L)}$ IN PERTURBATION THEORY

As mentioned in the Sec. 1, there are two self-energy terms in the problem under consideration,  $\Sigma_{(K,L)}^{(1)}$  and  $\Sigma_{(K,L)}$ . In second-order perturbation theory, they coincide. They

start to differ in third-order in the coupling constant. In third-order perturbation theory, we obtain from Appendix C

$$\Sigma_{(K,L)}^{(1)} - \Sigma_{(K,L)} = I_{2L_1}^{2K_1} I_{2L_2}^{2L_1} I_{2K_1}^{2L_2} \times \\ \times \left( \frac{1}{(\mu H + \varepsilon_L + \varepsilon_{L_1} - \varepsilon_K - \varepsilon_{K_1})(\mu H + \varepsilon_L + \varepsilon_{L_2} - \varepsilon_K - \varepsilon_{K_1})} - \frac{1}{(\varepsilon_L + \varepsilon_{L_1} - \varepsilon_K - \varepsilon_{K_1})(\varepsilon_L + \varepsilon_{L_2} - \varepsilon_K - \varepsilon_{K_1})} \right).$$
(38)

A simple calculation of sums in Eq. (38) leads to

$$\left(\Sigma_{(K,L)}^{(1)} - \Sigma_{(K,L)}\right)_{\varepsilon_L = \varepsilon_K = \varepsilon_F} = -\mu H g^3 \ln^2\left(\frac{\varepsilon_F}{\varepsilon_c}\right),\tag{39}$$

where  $\varepsilon_c$  is the cutoff energy. In Appendix C, we obtain the following term in expansion (39) for the self-energy:

$$\left(\Sigma_{(K,L)}^{(1)} - \Sigma_{(K,L)}\right)_{\varepsilon_K = \varepsilon_L = \varepsilon_F} = -\mu H g^3 \ln^2\left(\frac{\varepsilon_F}{\varepsilon_c}\right) + 2\mu H g^4 \ln^3\left(\frac{\varepsilon_F}{\varepsilon_c}\right) - \dots$$
(40)

Comparison with the expression for  $\delta E$  obtained in perturbation theory shows that

$$\delta \Sigma = \left( \Sigma_{(K,L)}^{(1)} - \Sigma_{(K,L)} \right)_{\varepsilon_K = \varepsilon_L = \varepsilon_F} = \mu H g \ln \left( \frac{\varepsilon_F}{\varepsilon_c} \right) \left[ -\frac{\partial \delta E}{\partial \mu H} \right] = -\frac{\mu H}{2} \left( -\frac{1}{2} + \langle S_z \rangle \right) . \tag{41}$$

To obtain Eq. (41) we used Eqs. (17), (10), and an assumption that  $\varepsilon_c \sim T_c$ .

Equation (41) means that some corrections should be made in the first of Eqs. (12). Specifically,  $\mu H$  in the first of Eqs. (12) should be corrected by  $\delta \Sigma$ :

$$\mu H \to \mu H - \delta \Sigma = \mu H. \tag{42}$$

The main result of this correction is a decrease in the initial slope of the magnetic field dependence of the average spin value by 3/4. This phenomenon was probably found in the experimental Ref. [4] (Figs. 8 and 9). The average spin  $\langle S_z \rangle$  is given by Eq. (27) with the substitution

$$\mu H \to \mu \tilde{H} = \mu H - \frac{\mu H}{2} \left( \frac{1}{2} - \langle S_z \rangle \right). \tag{43}$$

This equation determines  $\langle S_z \rangle$  as an implicit function of  $\mu H$ . From Eqs. (27) and (43), we find that  $\langle S_z \rangle$  as a function of  $\mu H$  has an a inflection point at  $\mu H/2T_c = 0.2426$ . Such an inflection point was obtained in Ref. [4].

### 6. CONCLUSION

Thus, we show that at zero temperature and finite magnetic field  $\mu H \ll \varepsilon_F$ , a singularity exists in the convolution of amplitudes  $C_{2K_1}^{2L-1}$  and  $C_{2K_1-1}^{2L-1}$  over energy  $\varepsilon_{K_1}$  with amplitude  $I_{2K}^{2K_1}$ . As a result, in the high magnetic field region,  $\mu H \gg T_c$ , the correction to the spin impurity value is proportional to  $(T_c/\mu H)^2$  instead of  $1/\ln(\mu H/T_c)$ , as predicted in Refs. [1–3]. We also find that renormalization of the magnetic field discussed in Sec. 4 leads to an inflection point in the dependence of spin impurity on the magnetic field. The initial slope is a function of z, which enters into the definition of the Kondo temperature (see Appendix D). Our consideration shows that the interaction of the spin of an impurity with an electron gas does not lead to the appearance of the localized state, as assumed in Refs. [8–10]. The Kondo temperature  $T_c$  is given by Eq. (D.7), where z is the root of the equation

$$f(z) = 0. \tag{44}$$

We find here three terms in the expansion of f in Taylor series (Eq. (D.8)). This equation was also studied in Refs. [8, 11]. Our result for the first two terms in Eq. (44) coincide with the result of Ref. [11], because this is also the result of parquet approximation. But, our consideration (Eq. (44)) is conceptually closer to the Ref. [8]. The difference even in the second term is probably related to the assumption of Ref. [8] that in the problem under consideration there is a localized state with spin 1/2.

In fact, such a localized state does not exist. Without interaction there are two states associted with impurity spin 1/2. In zero magnetic field, these two states are degenerate. Interaction removes such a degeneracy and the splitting energy is  $2T_c$ . Of course, interaction does not change the number of states, as in our consideration, and is not fulfilled in Ref. [8]. Note also that the driving term is missing in Refs. [8–10].

Nevertheless, the average value of spin of impurity  $\langle S_z \rangle$  as a function of magnetic field found in Refs. [9, 10] coincides with our result except for the effect of renormalization of the magnetic field (Sec. 4) and the expression for the Kondo temperature.

The authors thank Prof. P. Fulde and Prof. A.I. Larkin for helpful discussions. We thank Prof. P. Fulde for hospitality at the Max-Planck-Institute for Complex Systems (Dresden). The research of Yu. N. O. was supported by CRDF (grant  $\mathbb{N} \mathbb{RP}1$ -194). The research of A.M.D. is supported by INTAS and the Russian Foundation for Basic Research (grant  $\mathbb{N} 95$ -553).

### APPENDIX A

The wave function of a system consisting of one localized electron plus degenerate electron gas can be taken in the form

$$\begin{split} |\psi\rangle &= |10;11;11...\rangle + \sum_{L} C_{2K}^{2L-1} |01;\stackrel{2K}{10};\stackrel{2L-1}{10} \rangle + \\ &+ \sum_{L} C_{2K-1}^{2L-1} |10;\stackrel{2K-1}{01};\stackrel{2L-1}{10} \rangle + \sum_{L} C_{2K}^{2L} |10;\stackrel{2K}{10};\stackrel{2L}{10} \rangle + \\ &+ \sum_{K_{1} < K} C_{2K_{1};2K}^{2L_{1};2L-1} \hat{N} |01;\stackrel{2K_{1}}{10};\stackrel{2K}{10};\stackrel{2L-1}{10} \rangle + \sum_{L} C_{2K_{1}-1;2K}^{2L_{1};2L-1} \hat{N} |10;\stackrel{2K_{1}-1}{0};\stackrel{2L}{10} \rangle + \\ &+ \sum_{L_{1} < L} C_{2K_{1};2K-1}^{2L_{1}-1;2L-1} \hat{N} |01;\stackrel{2K_{1}}{10};\stackrel{2K-1}{01};\stackrel{2L-1}{10} \rangle + \\ &+ \sum_{L_{1} < L} C_{2K_{1};2K-1}^{2L_{1}-1;2L-1} \hat{N} |01;\stackrel{2K_{1}}{10};\stackrel{2K-1}{01};\stackrel{2L-1}{10} \rangle + \\ &+ \sum_{K_{1} < K;L_{1} < L} C_{2K_{1}-1;2L-1}^{2L_{1}-1} \hat{N} |10;\stackrel{2K_{1}-1}{01};\stackrel{2K-1}{10};\stackrel{2L-1}{10} \rangle + \\ \end{split}$$

The notations here are the same as in the text. As we note above, there are (2P + 1) different symbols  $C_{...}^{...}$  of order P. Inserting Eq. (A.1) into Eq. (3) for the wave function, some simple but tedions calculations yield a set of equations for the coefficients  $C_{...}^{...}$ . The five equations for the  $C_{...}^{...}$  are

$$\begin{split} &C_{2K}^{2L-1}I_{2K_{1}}^{2L_{1}} - C_{2K_{1}}^{2L-1}I_{2K}^{2L_{1}} - C_{2K}^{2L_{1}}I_{2K_{1}}^{2L-1} + C_{2K_{1}}^{2L_{1}}I_{2K}^{2L-1} + \\ &+ (\mu H + \varepsilon_{L} + \varepsilon_{L_{1}} - \varepsilon_{K} - \varepsilon_{K_{1}} - \delta E)C_{2K_{1};2K}^{2L_{1};2L-1} + \\ &+ \left(\sum_{K_{2} < K} C_{2K_{2};2K}^{2L_{1};2L-1}I_{2K_{2}}^{2K_{2}} - \sum_{K < K_{2}} C_{2K_{2};2K_{2}}^{2L_{1};2L-1}I_{2K_{2}}^{2K_{2}}\right) + \\ &+ \left(\sum_{K_{1} < K_{2}} C_{2K_{1};2K}^{2L_{1};2L-1}I_{2K_{2}}^{2K_{2}} - \sum_{K_{2} < K_{1}} C_{2K_{2};2K_{1}}^{2L_{1};2L-1}I_{2K_{2}}^{2K_{2}}\right) - \\ &- \sum C_{2K_{1};2K}^{2L_{2};2L-1}I_{2L_{2}}^{2L_{1}} + \left(\sum_{L_{2} < L_{1}} C_{2K_{1};2K}^{2L_{2};2L_{1}}I_{2L_{2}}^{2L-1} - \sum_{L_{1} < L_{2}} C_{2K_{1};2K}^{2L_{1};2L_{2}}I_{2L_{2}}^{2L-1}\right) - \\ &- \left(\sum C_{2K_{2}-1;2K}^{2L_{1};2L-1}I_{2K_{1}}^{2K_{2}-1} - \sum C_{2K_{2}-1;2K_{1}}^{2L_{1};2L-1}I_{2K_{2}}^{2K_{2}-1}\right) - \\ &- \sum_{K_{1} < K < K_{2};L_{2} < L_{1}} C_{2K_{1};2K;2K}^{2L_{2};2L_{1};2L-1}I_{2K_{2}}^{2K_{2}} + \\ &+ \sum_{K_{1} < K < K_{2};L_{2} < L_{1}} C_{2K_{1};2K_{2};2K_{1}}^{2L_{2};2L_{1};2L-1}I_{2L_{2}}^{2K_{2}} - \sum_{K_{2} < K_{1};L_{2} < L_{1}} C_{2K_{2};2K_{1};2K}^{2L_{2};2L_{1};2L-1}I_{2L_{2}}^{2K_{2}} + \\ &+ \sum_{K_{1} < K_{2} < K;L_{2} < L_{1}} C_{2K_{1};2K_{2};2K_{1}}^{2L_{2};2L_{1};2L-1}I_{2L_{2}}^{2K_{2}} - \sum_{K_{2} < K_{1};L_{2} < L_{1}} C_{2K_{2};2K_{1};2K}^{2L_{2};2L_{1};2L-1}I_{2L_{2}}^{2K_{2}} + \\ &+ \sum_{K_{1} < K_{2} < K;L_{2} < L_{1}} C_{2K_{1};2K_{2};2K_{1}}^{2L_{2};2L_{1};2L-1}I_{2L_{2}}^{2K_{2}} - \sum_{K_{2} < K_{1};L_{2} < L_{1}} C_{2K_{2};2K_{1};2K}^{2L_{2};2L_{1};2L-1}I_{2L_{2}}^{2K_{2}} + \\ &+ \sum_{K_{1} < K_{2} < K;L_{2} < L_{1}} C_{2K_{1};2K_{2};2K_{1}}^{2L_{2};2L_{1};2L-1}I_{2L_{2}}^{2K_{2}} - \sum_{K_{2} < K_{1};L_{2} < L_{1}} C_{2K_{2};2K_{1};2K}^{2L_{1}}I_{2L_{2}}^{2K_{2}} + \\ &+ \sum_{K_{1} < K_{2} < K;L_{2} < L_{1}} C_{2K_{1};2K_{2};2K_{1}}^{2L_{1}}I_{2L_{2}}^{2K_{2}} - \sum_{K_{2} < K_{1};L_{2} < L_{1}} C_{2K_{2};2K_{1};2K}^{2L_{2}}I_{2L_{2}}^{2K_{2}} + \\ &+ \sum_{K_{1} < K_{2} < K;L_{2} < L_{1}} C_{2K_{2};2K_{2};2K_{2}}^{2L_{2};2L_{1}}I_{2L_{2}}^{2K_{2}} - C_{2K_{2};2K_{2};2K_{1}}^{2L_{$$

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+	$\sum_{K_1 \le K \le K_2; L_1 \le L_2} C_{2K_1; 2K_2; 2K_2}^{2L_1; 2L_2; 2L_2 - 1} I_{2L_2}^{2K_2} -$	
_	$\sum_{K_1 < K_2 < K; L_1 < L_2} C_{2K_1; 2K_2; 2K}^{2L_1; 2L_2; 2L-1} I_{2L_2}^{2K_2} + \sum_{K_2 < K_1 < K; L_1 < L_2} C_{2K_2; 2K_1; 2K}^{2L_1; 2L_2; 2L-1} I_{2L_2}^{2K_2} +$	
+	$\sum_{L_2 < L_1; K_1 < K} C_{2K_2 - 1; 2K_1; 2K}^{2L_2; 2L_1; 2L - 1} I_{2L_2}^{2K_2 - 1} - \sum_{L_1 < L_2; K_1 < K} C_{2K_2 - 1; 2K_1; 2K}^{2L_1; 2L - 1} I_{2L_2}^{2K_2 - 1} = 0 ,$	
_	$I_{2K_{1}-1}^{2L_{1}}C_{2K}^{2L-1} + C_{2K}^{2L_{1}}I_{2K_{1}-1}^{2L-1} - \sum_{K_{2} < K} C_{2K_{2};2K}^{2L_{1};2L-1}I_{2K_{1}-1}^{2K_{2}} + \sum_{K < K_{2}} C_{2K;2K_{2}}^{2L_{1};2L-1}I_{2K_{1}-1}^{2K_{2}} + \sum_{K < K_{2}} C_{2K;2K_{2}}^{2L_{1};2L-1}I_{2K_{2}-1}^{2K_{2}} + \sum_{K < K_{2}} C_{2K;2K_{2}}^{2L_{1};2L-1}I_{2K_{2}-1}^{2K_{2}} + \sum_{K < K_{2}} C_{2K;2K_{2}}^{2L_{1};2L-1}I_{2K;2K_{2}-1}^{2K_{2}} + \sum_{K < K_{2}} C_{2K;2K_{2}-1}^{2K_{2}} + \sum_{K < K_{2}} C_{2K;2K_{2}-1}^{2K_{2}} + \sum_{K < K_{2}} C_{2K;2K_{2}-1}^{2K_{2}} + \sum_{K < K_{2}} C_{2K;2K_{2}-1}^{2K_{2}-1} + \sum_{K < K_{2}} C_{2K;2K_{2}-1$	
+(	$\varepsilon_{L} + \varepsilon_{L_{1}} - \varepsilon_{K} - \varepsilon_{K_{1}} - \delta E)C_{2K_{1}-1;2K}^{2L_{1};2L-1} + \sum C_{2K_{2}-1;2K}^{2L_{1};2L-1}I_{2K_{1}-1}^{2K_{2}-1} - \sum C_{2K_{1}-1;2K}^{2L_{1};2L_{2}-1}I_{2L_{2}-1}^{2L-1} + $	
+	$\sum_{L_2 < L} C_{2K;2K_1 - 1}^{2L_2 - 1;2L - 1} I_{2L_2 - 1}^{2L_1} - \sum_{L < L_2} C_{2K;2K_1 - 1}^{2L - 1;2L_2 - 1} I_{2L_2 - 1}^{2L_1} +$	(A.2)
+	$\sum_{L_2 < L; K < K_2} C_{2K; 2K_2; 2K_1 - 1}^{2L_1; 2L_2 - 1; 2L - 1} I_{2L_2 - 1}^{2K_2} - \sum_{L_2 < L; K_2 < K} C_{2K_2; 2K; 2K_1 - 1}^{2L_1; 2L_2 - 1; 2L - 1} I_{2L_2 - 1}^{2K_2} -$	
	$\sum C_{2K;2K_2;2K_1-1}^{2L_1;2L_2-1} I_{2L_2-1}^{2K_2} + \sum_{L < L_2;K_2 < K} C_{2K_2;2K;2K_1-1}^{2L_1;2L_2-1} I_{2L_2-1}^{2K_2} - $	
_	$\sum_{L_2 < L; K_1 < K_2} C_{2K_1 - 1; 2K; 2K_2 - 1}^{2L_1; 2L_2 - 1; 2L - 1} I_{2L_2 - 1}^{2K_2 - 1} + \sum_{L_2 < L; K_2 < K_1} C_{2K_2 - 1; 2K; 2K_1 - 1}^{2L_1; 2L_2 - 1; 2L - 1} I_{2L_2 - 1}^{2K_2 - 1} +$	
+	$\sum_{L < L_2; K_1 < K_2} C_{2K_1 - 1; 2K; 2K_2 - 1}^{2L_1; 2L - 1; 2L_2 - 1} I_{2L_2 - 1}^{2K_2 - 1} - \sum_{L < L_2; K_2 < K_1} C_{2K_2 - 1; 2K; 2K_1 - 1}^{2L_1; 2L - 1; 2L_2 - 1} I_{2L_2 - 1}^{2K_2 - 1} = 0 ,$	
(	$C_{2K-1}^{2L-1}I_{2K_1}^{2L_1-1} - C_{2K-1}^{2L_1-1}I_{2K_1}^{2L-1} + \sum_{2K-1}C_{2K-1;2K_1}^{2L_2;2L-1}I_{2L_2}^{2L_1-1} - \sum_{2K-1;2K_1}C_{2K-1;2K_1}^{2L_2-1}I_{2L_2}^{2L-1} +$	
	+ $(\mu H + \varepsilon_L + \varepsilon_{L_1} - \varepsilon_K - \varepsilon_{K_1} - \delta E)C_{2K_1;2K-1}^{2L_1-1;2L-1} + \sum_{2K_2;2K-1}C_{2K_2;2K-1}^{2L_1-1;2L-1}I_{2K_1}^{2K_2} +$	
	$+\sum_{K$	<sup>2</sup> <sub>2</sub>
	$-\sum_{K_2 < K_1} C_{2K_2;2K_1;2K-1}^{2L_2;2L_1-1;2L-1} I_{2L_2}^{2K_2} - \sum_{K < K_2} C_{2K-1;2K_1;2K_2-1}^{2L_2;2L_1-1;2L-1} I_{2L_2}^{2K_2-1} +$	
	+ $\sum_{K_2 < K} C_{2K_2 - 1; 2K_1; 2K - 1}^{2L_2; 2L_1 - 1; 2L_1 - 1} I_{2L_2}^{2K_2 - 1} = 0$ ,	
(	$(\varepsilon_L + \varepsilon_{L_1} - \varepsilon_K - \varepsilon_{K_1} - \delta E)C_{2K_1;2K}^{2L_1;2L} + \sum_{2K_1;2K} C_{2K_1;2K}^{2L;2L_2-1}I_{2L_2-1}^{2L_1} - \sum_{2K_1;2K} C_{2K_1;2K}^{2L_1;2L_2-1}I_{2L_2-1}^{2L_1} - \sum_{2K_1;2K} C_{2K_1;2K}^{2L_1;2L_2-1}I_{2L_2-1}^{2L_2-1} - \sum_{2K_1;2K} C_{2K_1;2K}^{2L_1;2L_2-1}I_{2L_2-1}^{2L_2-1}I_{2L_2-1}^{2L_2-1} - \sum_{2K_1;2K} C_{2K_1;2K}^{2L_2-1}I_{2L_2-1}^{2L_2-1}I_{2L_$	-
	$-\sum_{K_1 < K < K_2} C_{2K_1;2K;2K_2}^{2L_1;2L_2;2L_2-1} I_{2L_2-1}^{2K_2} + \sum_{K_1 < K_2 < K} C_{2K_1;2K_2;2K}^{2L_1;2L_2;2L_2-1} I_{2L_2-1}^{2K_2} -$	
	$-\sum_{K_2 < K_1 < K} C_{2K_2;2K_1;2K}^{2L_1;2L_2-1} I_{2L_2-1}^{2K_2} + \sum_{K_2 < L_1;2L_2;2L_2-1} C_{2K_2-1;2K_1;2K}^{2L_1;2L_2-1} I_{2L_2-1}^{2K_2-1} = 0 ,$	
	$-I_{2K_{1}-1}^{2L_{1}-1}C_{2K-1}^{2L-1} + C_{2K_{1}-1}^{2L_{1}-1}I_{2K-1}^{2L_{1}-1} + C_{2K-1}^{2L_{1}-1}I_{2K_{1}-1}^{2L-1} - C_{2K_{1}-1}^{2L_{1}-1}I_{2K-1}^{2L-1} +$	
	$+(\varepsilon_L+\varepsilon_{L_1}-\varepsilon_K-\varepsilon_{K_1}-\delta E)C_{2K_1-1;2K-1}^{2L_1-1;2L-1}-$	

$$\begin{split} &- \left( \sum_{k_1 < k_2} C_{2k_1;2k-1}^{2L_1-1;2L-1} I_{2k_1-1}^{2K_2} - \sum_{k_1 < k_1} C_{2k_1;2k-1}^{2L_1-1;2L-1} I_{2k_1-1}^{2K_2} \right) + \\ &+ \left( \sum_{k_1 < k_2} C_{2k_1-1;2L-1}^{2L_1-1} I_{2k_1-1}^{2K_1-1} - \sum_{k_1 < k_1} C_{2k_1-1;2L-1}^{2L_1-1} I_{2k_1-1}^{2K_1-1} \right) - \\ &- \left( \sum_{k < k_2} C_{2k_1-1;2L-1}^{2L_1-1} I_{2k_1-1}^{2L_1-1} - \sum_{k_1 < k_2} C_{2k_1-1;2L-1}^{2L_1-1} I_{2k_1-1}^{2L_1-1} \right) - \\ &- \left( \sum_{k < k_2} C_{2k_1-1;2L-1}^{2L_1-1} I_{2L_1-1}^{2L_1-1} - \sum_{k_1 < k_2} C_{2k_1-1;2L-1}^{2L_1-1} I_{2L_2-1}^{2L_1-1} \right) + \\ &+ \left( \sum_{k < k_2} C_{2k_1-1;2L-1}^{2L_1-1} I_{2L_1-1}^{2L_1-1} - \sum_{k_1 < k_2} C_{2k_1-1;2L-1}^{2L_1-1} I_{2L_2-1}^{2L_1-1} \right) - \\ &- \sum_{k_2 < k_1 < k_2} C_{2k_1-1;2L-1}^{2L_1-1} I_{2L_2-1}^{2L_1-1} - \sum_{k_1 < k_2} C_{2k_1-1;2L-1}^{2L_1-1} I_{2L_2-1}^{2L_1-1} \right) - \\ &- \sum_{k_1 < k_2 < k_1 < k_2} C_{2k_1-1;2L-1}^{2L_1-1} I_{2L_2-1}^{2L_1-1} - \sum_{k_1 < k_2} C_{2k_1-1;2L-1}^{2L_1-1} I_{2L_2-1}^{2L_1-1} - \\ &- \sum_{k_1 < k_2 < k_1 < k_2 < k_1 < k_2 < k_$$

Equations (A.2) are exact.

# APPENDIX B

Our purpose is to obtain an expression for the self-energy terms  $\Sigma_{(K,L)}^{(1)}$  and  $\Sigma_{(K,L)}$  in fourth-order perturbation theory. To do this we should obtain equations on the quantities  $C_{\dots}$  in the «leading» approximation. Really, we need only six equations in the six quantities entering into Eqs. (A.2). The required system can be obtained from Eqs. (3) and (A.1). These equations are

$$\begin{aligned} (\mu H + \varepsilon_L + \varepsilon_{L_1} + \varepsilon_{L_2} - \varepsilon_K - \varepsilon_{K_1} - \varepsilon_{K_2}) C_{2K_2;2K_1;2K}^{2L_2;2L_1;2L-1} - \\ &- \left\{ C_{2K_1;2K}^{2L_1;2L-1} I_{2K_2}^{2L_2} - C_{2K_2;2K}^{2L_1;2L-1} I_{2K_1}^{2L_2} + C_{2K_2;2K_1}^{2L_1;2L-1} I_{2K}^{2L_2} - \\ &- C_{2K_1;2K}^{2L_2;2L-1} I_{2K_2}^{2L_1} + C_{2K_2;2K}^{2L_2;2L-1} I_{2K_1}^{2L_1} - C_{2K_2;2K_1}^{2L_2;2L-1} I_{2K}^{2L_2} \right\} - \\ &- \left\{ C_{2K_1;2K}^{2L_2;2L_1} I_{2K_2}^{2L-1} - C_{2K_2;2K}^{2L_2;2L-1} I_{2K_1}^{2L-1} + C_{2K_2;2K_1}^{2L_2;2L_1} I_{2K}^{2L-1} \right\} = 0 \end{aligned}$$



Fig. 1. Relation between various terms  $C_{\dots}$ . Dashed lines represent scattering process

$$\begin{split} &(\varepsilon_{L}+\varepsilon_{L_{1}}+\varepsilon_{L_{1}}-\varepsilon_{K}-\varepsilon_{K_{1}}-\varepsilon_{K_{1}})C_{2K_{1}-1;2K_{1};2K_{1}}^{2L_{1};2L_{1};2L_{1}-1} \\ &+C_{2K_{1};2K}^{2L_{2};2L_{1}}I_{2L_{1}-1}^{2L_{1}}+\left\{C_{2K_{1};2K}^{2L_{1};2L-1}I_{2K_{1}-1}^{2L_{2}}-C_{2K_{1};2K}^{2L_{2};2L-1}I_{2K_{1}-1}^{2L_{1}}\right\}=0,\\ &(\mu H+\varepsilon_{L}+\varepsilon_{L_{1}}+\varepsilon_{L_{2}}-\varepsilon_{K}-\varepsilon_{K_{1}}-\varepsilon_{K_{2}})C_{2K_{1};2L_{1}-1}^{2L_{2};2L_{1}-1}I_{2K_{1}-1}^{2L_{1}-1}-\\ &-\left\{C_{2K_{1}-1;2K_{1}}^{2L_{1}-1}I_{2K_{2}}^{2L_{2}-1}-C_{2K_{1}-1;2K_{1}}^{2L_{2};1L_{1}-1}-C_{2K_{1}-1;2K_{1}}^{2L_{2};L_{1}-1}I_{2K_{2}}^{2L_{2}-1}+C_{2K_{1}-1;2K_{1}}^{2L_{2};L_{1}-1}I_{2K_{1}}^{2L_{1}-1}-\right.\\ &-\left\{C_{2K_{1}-1;2K_{1}}^{2L_{1}-1}I_{2K_{2}}^{2L_{2}}-C_{2K_{1}-1;2K_{1}}^{2L_{1}-1}I_{2K_{1}}^{2L_{2}}\right\}=0,\\ &(\varepsilon_{L}+\varepsilon_{L_{1}}+\varepsilon_{L_{2}}-\varepsilon_{K}-\varepsilon_{K_{1}}-\varepsilon_{K_{2}})C_{2K_{2}-1;2K_{1}}^{2L_{2};2L_{1}-1}I_{2K_{2}-1}^{2L_{2}-1}+C_{2K_{2}-1;2K_{1}}^{2L_{2};2L_{1}-1}I_{2K_{1}-1}^{2L_{2}-1}+\right.\\ &+\left\{C_{2K_{1}-1;2K_{1}}^{2L_{1}-1}I_{2K_{2}-1}^{2L_{2}-1}-C_{2K_{2}-1;2K_{1}}^{2L_{2}-1}I_{2K_{2}-1}^{2L_{2}-1}+C_{2K_{2}-1;2K_{1}}^{2L_{2}-1}I_{2K_{1}-1}^{2L_{2}-1}\right\}=0,\\ &(\mu H+\varepsilon_{L}+\varepsilon_{L_{1}}+\varepsilon_{L_{2}}-\varepsilon_{K}-\varepsilon_{K_{1}}-\varepsilon_{K_{2}})C_{2K_{2}-1;2K_{1}-1;2K_{1}-1}^{2L_{2}-1}I_{2K_{2}-1}}-\\ &-\left\{C_{2K_{1}-1;2K_{1}-1}^{2L_{2}-1}I_{2K_{2}-1}^{2L_{2}-1}-C_{2K_{1}-1;2K_{2}-1}^{2L_{2}-1}I_{2K_{2}-1}}-C_{2K_{2}-1;2K_{1}-1;2K_{2}-1}^{2L_{2}-1}I_{2K_{2}-1}}\right\}=0,\\ &(\mu H+\varepsilon_{L}+\varepsilon_{L_{1}}+\varepsilon_{L_{2}}-\varepsilon_{K}-\varepsilon_{K_{1}}-\varepsilon_{K_{2}})C_{2K_{2}-1;2K_{1}-1;2K_{1}-1}^{2L_{2}-1}I_{2K_{2}-1}}-\\ &-\left\{C_{2K_{1}-1;2K_{1}-1}^{2L_{2}-1}I_{2K_{2}-1}}-C_{2K_{1}-1;2K_{2}-1}^{2L_{2}-1;2L_{1}-1}I_{2K_{2}-1}}-C_{2K_{1}-1;2K_{1}-1}^{2L_{2}-1}I_{2K_{1}-1}}-C_{2K_{1}-1;2K_{1}-1}^{2L_{2}-1}I_{2K_{1}-1}}-C_{2K_{1}-1;2K_{1}-1}^{2L_{2}-1}I_{2K_{1}-1}}-C_{2K_{1}-1;2K_{1}-1}^{2L_{2}-1}I_{2K_{1}-1}}-C_{2K_{1}-1;2K_{1}-1}^{2L_{2}-1}I_{2K_{1}-1}}-C_{2K_{1}-1;2K_{1}-1}^{2L_{2}-1}I_{2K_{1}-1}}-C_{2K_{1}-1;2K_{1}-1}^{2L_{2}-1}I_{2K_{1}-1}}-C_{2K_{1}-1;2K_{1}-1}^{2L_{2}-1}I_{2K_{1}-1}}-C_{2K_{1}-1;2K_{1}-1}^{2L_{2}-1}I_{2K_{1}-1}}-C_{2K_{1}-1;2K_{1}-1}^{2L_{2}-1}I_{2K_{1}-1}}-C_{2K_{1}-1;2K_{$$

Equations (B.1) can easily be supplemented by scattering terms, and Eqs. (7), (A.1), and (B.1) will still form a complete set. The structure of interaction Hamiltonian (1) is such that scattering leads to connection of the given term only with itself and with two (or one) neighboring

terms. These terms can be obtained from the given one by a change of parity of one of the upper or lower indexes. The relationships among the various terms  $C_{...}$  are presented in Fig. 1.

## APPENDIX C

We are now able to obtain the self-energy parts  $\Sigma_{(K,L)}^{(1)}$  and  $\Sigma_{(K,L)}$  in fourth-order perturbation theory. Straightforward elimination of terms in  $C_{\dots}^{(1)}$  with  $P \ge 2$  from Eqs. (6) using Eqs. (A.2) and (B.1) gives

$$\begin{split} \Sigma_{(K,L)}^{(0)} &= \frac{I_{2L_{1}}^{LL_{1}}}{\mu H + \varepsilon_{4}(L,L_{1},K,K_{1}) - |I_{2K_{1}-1}^{2K_{1}}|^{2}/\varepsilon_{6} - |I_{2K_{1}}^{2L_{1}}|^{2}/(\mu H + \varepsilon_{6}) - \delta E} \times \\ &\times \left\{ I_{2K_{1}}^{2L_{1}} - \frac{I_{3K_{1}}^{2K_{1}}}{\mu H + \varepsilon_{4}(L,L_{1},K,K_{1})} \left( I_{2K_{1}}^{2L_{1}} - \frac{I_{2K_{1}}^{2K_{1}}I_{2K_{1}}^{2L_{1}}}{\mu H + \varepsilon_{4}(L,L_{1},K,K_{3})} + \right. \\ &+ \frac{I_{2L_{1}}^{2L_{1}}I_{2K_{1}}^{2L_{1}}}{\mu H + \varepsilon_{4}(L,L_{2},K,K_{2})} - \frac{I_{2K_{1}}^{2K_{1}}I_{2K_{1}-1}^{2L_{1}}}{\varepsilon_{4}(L,L_{1},K,K_{3})} \right) - \frac{I_{2L_{1}}^{2L_{1}}I_{2K_{1}}}{\mu H + \varepsilon_{4}(L,L_{2},K,K_{1})} \times \\ &\times \left( -I_{2K_{1}}^{2K_{1}} + \frac{I_{2K_{1}}^{2K_{1}}I_{2K_{1}}^{2L_{1}}}{\mu H + \varepsilon_{4}(L,L_{2},K,K_{2})} - \frac{I_{2L_{1}}^{2L_{1}}I_{2K_{1}}^{2L_{1}}}{\mu H + \varepsilon_{4}(L,L_{2},K,K_{1})} + \frac{I_{2K_{1}}^{2K_{1}-1}I_{2K_{1}-1}^{2L_{1}}}{\varepsilon_{4}(L,L_{1},K,K_{2})} \right) - \\ &- \frac{I_{2K_{1}}^{2K_{1}-1}}{\varepsilon_{4}(L,L_{1},K,K_{2})} \left( I_{2L_{1}}^{2L_{1}} - \frac{I_{2K_{1}}^{2K_{1}-1}I_{2K_{1}}^{2L_{1}}}{\mu H + \varepsilon_{4}(L,L_{1},K_{1},K_{1})} - \frac{I_{2L_{1}}^{2L_{1}}I_{2K_{1}-1}^{2L_{1}}}{\varepsilon_{4}(L,L_{1},K,K_{2})} - \\ &- \frac{I_{2K_{1}}^{2K_{1}}I_{2K_{1}}^{2L_{1}}}{\mu H + \varepsilon_{4}(L,L_{2},K,K_{1})} + \frac{I_{2K_{1}}^{2L_{1}}I_{2K_{1}-1}^{2L_{1}}}{\mu H + \varepsilon_{4}(L,L_{1},K,K_{2})} - \\ &- \frac{I_{2K_{1}}^{2K_{1}}I_{2K_{1}}^{2L_{1}}}{\mu H + \varepsilon_{4}(L,L_{2},K,K_{1})} + \frac{I_{2L_{1}}^{2K_{1}-1}I_{2K_{1}-1}^{2L_{1}}}{\mu H + \varepsilon_{4}(L,L_{1},K,K_{2})} - \\ &- \frac{I_{2K_{1}}^{2L_{1}}I_{2K_{1}}^{2L_{1}}}{\mu H + \varepsilon_{4}(L,L_{1},K,K_{2})} \right) - \frac{I_{2L_{1}}^{2K_{1}-1}I_{2K_{1}-1}^{2L_{1}}}{\varepsilon_{4}(\mu H + \varepsilon_{4}(L,L_{2},K,K_{1})} \right) + \\ &+ \frac{I_{2L_{1}}^{2L_{1}}I_{2K_{1}-1}^{2L_{1}}}{\mu H + \varepsilon_{4}(L,L_{1},K,K_{2})}} \left( I_{2K_{1}}^{2L_{1}} - \frac{I_{2K_{1}}^{2K_{1}-1}I_{2K_{1}-1}^{2L_{1}}}{\mu H + \varepsilon_{4}(L,L_{1},K,K_{3})} + \\ &+ \frac{I_{2L_{1}}^{2L_{1}}I_{2K_{1}-1}}{\mu H + \varepsilon_{4}(L,L_{1},K,K_{2})}} - \frac{I_{2K_{1}}^{2K_{1}-1}I_{2K_{1}-1}^{2L_{1}}}{\mu H + \varepsilon_{4}(L,L_{1},K,K_{3})} \right) - \frac{I_{2K_{1}}^{2K_{1}-1}I_{2K_{1}-1}}{\varepsilon_{4}(L,L_{1},K,K_{3})}} + \\ &+ \frac{I_{2L_{1}}^{2L_{1}}I_{2K_{1}-1}}{\mu H + \varepsilon_{4}(L,L_{1},K,K_{1})} - \frac{I_{2K_{1}}^{2K_{1}-1}I_{2K_{1}-1}}}{\varepsilon_{4}(L$$

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$$\begin{split} &- \frac{I_{2K_{1}}^{2K_{1}-1}I_{2K_{1}-1}^{2L_{1}-1}}{\varepsilon_{4}(L,L_{1},K,K_{3})} - \frac{I_{2K_{1}}^{2K_{1}-1}}{\varepsilon_{4}(L,L_{1},K,K_{3})} \left( I_{2K_{1}-1}^{2L_{1}-1} - \frac{I_{2K_{1}-1}^{2K_{1}}I_{2K_{1}-1}^{2L_{1}-1}}{\mu H + \varepsilon_{4}(L,L_{1},K,K_{3})} + \\ &+ \frac{I_{2L_{2}-1}^{2L_{1}-1}I_{2K_{2}-1}^{2L_{2}-1}}{\varepsilon_{4}(L,L_{2},K,K_{2})} - \frac{I_{2K_{1}-1}^{2K_{1}-1}I_{2K_{1}-1}}{\varepsilon_{4}(L,L_{1},K,K_{3})} \right) + \frac{I_{2L_{1}-1}^{2L_{1}-1}I_{2L_{1}-1}^{2L_{2}-1}I_{2K_{1}-1}^{2L_{2}-1}}{\varepsilon_{4}(L,L_{2},K,K_{1})(\mu H + \varepsilon_{4}(L,L_{3},K,K_{1}))} - \\ &- \frac{I_{2L_{2}}^{2K_{1}}I_{2K_{1}}^{2L_{1}}I_{2K_{2}-1}^{2L_{1}}}{(\mu H + \varepsilon_{6})(\mu H + \varepsilon_{4}(L,L_{1},K,K_{2}))} \right\} + \\ &+ \frac{I_{2L_{1}-1}^{2K_{1}-1}}{\varepsilon_{4}(L,L_{1},K,K_{1}) - |I_{2L_{2}-1}^{2K_{1}-1}|^{2}/(\mu H + \varepsilon_{6}) - |I_{2L_{2}-1}^{2K_{2}-1}|^{2}/\varepsilon_{6} - \delta E} \times \\ &\times \left\{ I_{2K_{1}-1}^{2L_{1}-1} - \frac{I_{2K_{1}-1}^{2K_{1}-1}}{\mu H + \varepsilon_{4}(L,L_{1},K,K_{2})} \left( I_{2K_{1}-1}^{2L_{1}-1} - \frac{I_{2K_{1}}^{2K_{1}}I_{2K_{1}-1}^{2L_{1}-1}}{\mu H + \varepsilon_{4}(L,L_{1},K,K_{3})} - \\ &- \frac{I_{2K_{1}-1}^{2K_{1}-1}I_{2K_{1}-1}^{2L_{1}-1}}{\mu H + \varepsilon_{4}(L,L_{1},K,K_{2})} \left( I_{2K_{1}-1}^{2L_{1}-1} - \frac{I_{2K_{1}}^{2K_{1}}I_{2K_{1}-1}^{2L_{1}-1}}{\omega H + \varepsilon_{4}(L,L_{1},K,K_{3})} - \\ &- \frac{I_{2K_{1}-1}^{2K_{1}-1}I_{2K_{1}-1}^{2L_{1}-1}}{\varepsilon_{4}(L,L_{1},K,K_{3})} - \frac{I_{2K_{1}-1}^{2L_{1}-1}I_{2K_{1}-1}^{2L_{1}-1}}{\varepsilon_{4}(L,L_{1},K,K_{3})} - \\ &- \frac{I_{2K_{1}-1}^{2K_{1}-1}I_{2K_{1}-1}}{\varepsilon_{4}(L,L_{1},K,K_{3})} + \frac{I_{2L_{1}-1}^{2L_{1}-1}I_{2K_{1}-1}}{\varepsilon_{4}(L,L_{2},K,K_{2})} - \frac{I_{2K_{1}-1}^{2K_{1}-1}I_{2K_{1}-1}}}{\varepsilon_{4}(L,L_{1},K,K_{3})} \right) + \\ &+ \frac{I_{2L_{2}-1}^{2L_{1}-1}I_{2K_{1}-1}}}{\varepsilon_{4}(L,L_{2},K,K_{1})} \left( I_{2K_{1}-1}^{2L_{2}-1}I_{2K_{1}-1}} - \frac{I_{2K_{1}-1}^{2L_{2}-1}}{\varepsilon_{4}(L,L_{2},K,K_{2})} + \\ &+ \frac{I_{2L_{1}-1}^{2L_{1}-1}I_{2K_{1}-1}}}{\varepsilon_{4}(L,L_{2},K,K_{1})} - \frac{I_{2K_{1}-1}^{2L_{2}-1}}{\varepsilon_{4}(L,L_{2},K,K_{2})} + \\ &+ \frac{I_{2L_{2}-1}^{2L_{2}-1}I_{2K_{2}-1}}{\varepsilon_{4}(L,L_{2},K,K_{1})} - \frac{I_{2K_{1}-1}^{2L_{2}-1}}{\varepsilon_{4}(L,L_{2},K,K_{2})} - \\ &- \frac{I_{2K_{1}-1}^{2L_{2}-1}I_{2K_{2}-1}}}{\varepsilon_{4}(L,L_{2},K,K_{1})}} - \frac{I_{2K_{1}-1}^{2L_{2}-1}}{\varepsilon_$$

From Eqs. (6) and (A.2), the quantities  $C_{2K}^{2L-1}$  and  $C_{2K-1}^{2L-1}$  can easily be obtained in the third order of perturbation theory. We do not give these expressions here because only one statement is essential for us: direct comparison of the quantities  $\delta E$  (Eq. (4)) and self-energy  $\Sigma_{K,L}$  (Eq. (C.2)) shows that

$$\delta E + \Sigma_{K,L} \Big|_{\varepsilon_K = \varepsilon_L = \varepsilon_F} = 0. \tag{C.3}$$

Equation (C.3) is valid for arbitrary spectrum  $\varepsilon_K, \varepsilon_L$  and arbitrary transition matrix elements  $I_{\dots}^{\dots}$ . Our conjecture is that Eq. (C.3) holds in all orders of perturbation theory, and hence we can put

$$\delta E + \Sigma_{K,L} \Big|_{\varepsilon_K = \varepsilon_L = \varepsilon_F} = -\Delta, \tag{C.4}$$

where  $\Delta$  is exponentially small and can be considered as an order parameter. We also obtain from Eqs. (C.1) and (C.2) that self-energies  $\Sigma_{KL}^{(1)}$  and  $\Sigma_{KL}$  coincide only in the second order of perturbation theory. They start to be different in the third order of perturbation theory. In the fourth order of perturbation theory, we obtain from Eqs. (C.1) and (C.2)

$$\begin{split} \Sigma^{(0)}_{(K,L)} &- \Sigma_{(K,L)} = I_{2L_{1}}^{2K_{1}} I_{2L_{2}}^{2L_{1}} \left( \frac{1}{(\mu H + \varepsilon_{4}(L,L_{1},K,K_{1})(\mu H + \varepsilon_{4}(L,L_{2},K,K_{1}))} - I_{\varepsilon_{4}(L,L_{1},K,K_{1})\varepsilon_{4}(L,L_{2},K,K_{1})} \right) - I_{2K_{1}}^{2K_{1}} I_{2L_{1}}^{2L_{1}} I_{2K_{1}}^{2L_{1}} I_{2K_$$

where

$$\varepsilon_4(L, L_1, K, K_1) \equiv \varepsilon_L + \varepsilon_{L_1} - \varepsilon_K - \varepsilon_{K_1} ,$$
  

$$\varepsilon_6 \equiv \varepsilon_L + \varepsilon_{L_1} + \varepsilon_{L_2} - \varepsilon_K - \varepsilon_{K_2} - \varepsilon_{K_2} .$$
(C.6)

Straightforward calculation of the integrals in Eq. (C.5) leads to Eqs. (40) and (41). Both Eqs. (40) and (41) are proved in two orders of perturbation theory. Our conjecture is that Eq. (41) is exact.

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# APPENDIX D

In this Appendix we consider the role of the right-hand side of Eqs. (7) for a negative value of the coupling constant, g < 0. In the first order of perturbation theory, we obtain from (A.2)

$$C_{2K_{1};2K}^{2L_{1};2L-1} = \frac{1}{\mu \tilde{H} + \varepsilon_{4}(L, L_{1}, K, K_{1}) + \Delta} \times \left[ C_{2K_{1}}^{2L-1} I_{2K}^{2L_{1}} - C_{2K}^{2L-1} I_{2K_{1}}^{2L_{1}} + C_{2K}^{2L_{1}} I_{2K_{1}}^{2L-1} - C_{2K_{1}}^{2L_{1}} I_{2K}^{2L-1} \right], \\ C_{2K_{1}-1;2K}^{2L_{1};2L-1} = \frac{1}{\varepsilon_{4}(L, L_{1}, K, K_{1}) + \Delta} \left[ I_{2K_{1}-1}^{2L_{1}} C_{2K}^{2L-1} - C_{2K}^{2L_{1}} I_{2K_{1}-1}^{2L-1} \right],$$
(D.1)  
$$C_{2K_{1};2K-1}^{2L_{1}-1;2L-1} = \frac{1}{\mu \tilde{H} + \varepsilon_{4}(L, L_{1}, K, K_{1}) + \Delta} \left[ C_{2K_{1}-1}^{2L_{1}-1} I_{2K_{1}}^{2L-1} - C_{2K_{1}-1}^{2L_{1}-1} I_{2K_{1}}^{2L_{1}-1} \right], \\ C_{2K_{1}-1;2K-1}^{2L_{1}-1} = \frac{1}{\varepsilon_{4}(L, L_{1}, K, K_{1}) + \Delta} \times \left[ I_{2K_{1}-1}^{2L_{1}-1} C_{2K_{1}-1}^{2L_{1}-1} - C_{2K_{1}-1}^{2L_{1}-1} I_{2K_{1}-1}^{2L_{1}-1} \right].$$

Inserting (D.1) into (6), we obtain

$$A_{1}\left(C_{2K}^{2L-1}; C_{2K-1}^{2L-1}, C_{2K}^{2L}\right) = -\sum \frac{I_{2L_{1}}^{2K_{1}}\left(C_{2K_{1}}^{2L-1}I_{2K}^{2L_{1}} + C_{2K}^{2L_{1}}I_{2K_{1}}^{2L-1} - C_{2K_{1}}^{2L_{1}}I_{2K}^{2L-1}\right)}{\mu\tilde{H} + \varepsilon_{4}(L, L_{1}, K, K_{1}) + \Delta} - \sum \frac{I_{2L_{1}}^{2K_{1}-1}I_{2K_{1}-1}^{2L-1}C_{2K}^{2L_{1}}}{\varepsilon_{4}(L, L_{1}, K, K_{1}) + \Delta},$$
(D.2)

$$\begin{split} A_2 \Big( C_{2K}^{2L-1}; C_{2K+1}^{2L-1}, C_{2K}^{2L} \Big) &= \\ &= -\sum \frac{I_{2L_1-1}^{2K_1-1} \Big( C_{2K_1-1}^{2L-1} I_{2K-1}^{2L_1-1} - C_{2K_1-1}^{2L_1-1} I_{2K-1}^{2L-1} + C_{2K-1}^{2L_1-1} I_{2K_1-1}^{2L-1} \Big)}{\varepsilon_4 (L, L_1, K, K_1) + \Delta} - \\ &- \sum \frac{I_{2L_1-1}^{2K_1} I_{2K_1}^{2L-1} C_{2K-1}^{2L_1-1}}{\mu \tilde{H} + \varepsilon_4 (L, L_1, K, K_1) + \Delta} \,, \end{split}$$

$$A_{3}\left(C_{2K}^{2L-1}; C_{2K-1}^{2L-1}, C_{2K}^{2L}\right) = \sum \frac{I_{2L_{1}-1}^{2K_{1}}\left(C_{2K_{1}}^{2L_{1}-1}I_{2K}^{2L} - C_{2K}^{2L_{1}-1}I_{2K_{1}}^{2L} - C_{2K_{1}}^{2L_{1}}I_{2K}^{2L_{1}-1}\right)}{\mu \tilde{H} + \varepsilon_{4}(L, L_{1}, K, K_{1}) + \Delta} - \sum \frac{I_{2L_{1}-1}^{2K_{1}-1}I_{2K_{1}-1}^{2L}C_{2K}^{2L_{1}-1}}{\varepsilon_{4}(L, L_{1}, K, K_{1}) + \Delta}.$$

The quantities  $\varepsilon_4$ ,  $\varepsilon_6$  here are the same as in Eq. (C.6).

As before, only convolutions  $Z_L, Y_L$  are large for g < 0. Furthermore,

$$|Z_L + Y_L| \sim g^2 |Z_L - Y_L|.$$
 (D.3)

As the result, Eqs. (7) can be reduced to just one equation:

$$\begin{pmatrix} Z_L - Y_L \end{pmatrix} \left[ 1 + g \ln \frac{\varepsilon_F}{y + \Delta} + g \ln \frac{\varepsilon_F}{\mu \tilde{H} + y + \Delta} + \frac{g^3}{2} \left( \frac{I_1}{g \ln[\varepsilon_F / (\mu \tilde{H} + y + \Delta)]} + \frac{I_2}{g \ln[\varepsilon_F / (y + \Delta)]} \right) \right] = Ig \left( \ln \frac{\varepsilon_f}{\mu \tilde{H} + y + \Delta} + \ln \frac{\varepsilon_F}{y + \Delta} \right) + g \int dx \left( \frac{X_K}{\mu \tilde{H} + y + x + \Delta} - \frac{Y_K}{y + x + \Delta} \right),$$
(D.4)

where

$$I_{1} = \int \frac{dx \, dy \, dx_{1}}{(\mu \tilde{H} + y + x + \Delta)(\mu \tilde{H} + y + x_{1} + \Delta)(\mu \tilde{H} + y + x + y_{1} + x_{1} + \Delta)},$$

$$I_{2} = \int \frac{dx \, dy \, dx_{1}}{(y + x + \Delta)(y + x_{1} + \Delta)(y + x + y_{1} + x_{1} + \Delta)}.$$
(D.5)

A simple calculation of the integrals (D.5) gives

$$I_{1} = \frac{1}{3} \ln^{3} \left( \frac{\varepsilon_{F}}{\mu \tilde{H} + y + \Delta} \right) , \qquad (D.6)$$
$$I_{2} = \frac{1}{3} \ln^{3} \left( \frac{\varepsilon_{F}}{y + \Delta} \right) .$$

Now we can define the Kondo temperature  $T_c$  to be

$$g|\ln\frac{\varepsilon_F}{T_c} = z,\tag{D.7}$$

where z is a root of the quadratic equation

$$1 - 2z + \frac{z^2}{3} = 0, \qquad z = 3 - \sqrt{6} \approx 0.5505.$$
 (D.8)

From Eq. (D.4) we obtain

$$Z_L - Y_L = -\frac{I\tilde{\beta}}{|g|(1 - z/3)\ln((\mu \tilde{H} + y + \Delta)(y + \Delta)/T_c^2)},$$
 (D.9)

where  $\tilde{\beta}$  is a number of order 1. Instead of Eqs. (41) and (42) we have now

$$\mu \tilde{H} = \mu H - \delta \Sigma; \qquad \delta \Sigma = -\mu H z (-1/2 + \langle S_z \rangle). \tag{D.10}$$

As before, the average spin  $\langle S_z \rangle$  is given by Eq. (27) with the replacement  $\mu H \rightarrow \mu \tilde{H}$ :

$$\langle S_z \rangle = \frac{\mu \tilde{H}}{4 (T_c^2 + (\mu \tilde{H}/2)^2)^{1/2}}.$$
 (D.11)

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Fig. 2. Magnetic field dependence of the average spin  $\langle S_z \rangle$ . Dots are experimental of Ref. [4]

The magnetic field dependence of the average spin  $\langle S_z \rangle$  (Eqs. (D.10) and (D.11)) is given in Fig. 2. Dots are the experimental results of Ref. [4].

## References

- 1. A. A. Abrikosov and A. A. Migdal, J. of Low Temp. Phys. 3, 519 (1970).
- 2. A. M. Tsvelick and P. B. Wigmann, Adv. in Phys. 32, 453 (1983).
- 3. N. Andrei, K. Furuya, and J. H. Lowenstein, Rev. Mod. Phys. 55, 331 (1983).
- 4. W. Felsch, Z. Phys. B 29, 212 (1978).
- 5. S. D. Bader, N. E. Phillips, M. B. Haple, and C. A. Luengo, Sol. St. Commun. 16, 1263 (1975).
- 6. Yu. N. Ovchinnikov, A. M. Dyugaev, P. Fulde, and V. Z. Kresin, JETP Lett. 66, 184 (1997).
- 7. P. Nozieres and T.C. de Dominicis, Phys. Rev. 178, 1097 (1969).
- 8. K. Yosida, Phys. Rev. 147, 223 (1966).
- 9. Hiroumi Ishii, Prog. Theor. Phys. 40, 201 (1968).
- 10. Hiroumi Ishii, Prog. Theor. Phys. 43, 578 (1970).
- 11. M. Fowler and A. Zawadowskii, Solid St. Comm. 9, 471 (1971).