Theory of the Two-Impurity Kondo Effect in the Presence of an Impurity-Impurity Exchange Interaction

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We examine the two-impurity Kondo effect by deriving the equation of motion of a set of Green's functions using the two-impurity s-d Hamiltonian with an added exchange term of the form $W(\vec{S}_0 \cdot \vec{S}_1)$, where $\vec{S}_0$ and $\vec{S}_1$ are the spin operators of the two impurities. The resulting Green's functions are truncated and solved for self-consistency, keeping the most divergent terms. Our results show that all the $\ln T$ terms arising in the single-impurity Kondo effect are modified and replaced by $\ln(T^2+W'^2)^{1/2}$, where W' is an energy approximately equal to W. This results in an effective Kondo temperature T_K^E, where $T_K^E = T_K^0[1-(W'/T_K^0)^2]^{1/2}$, and T_K^0 is the single-impurity Kondo temperature. Thus the effective Kondo temperature decreases as the impurity-impurity interaction increases, and when W' is greater than T_K^0 the Kondo divergence is removed by the impurity-impurity interaction. Our results show that the interaction W strongly modifies the spin-compensated state. We also derive expressions for the conduction-electron polarization as a function of W' for high values of W' or high temperatures.

I. INTRODUCTION

In considering the thermodynamic properties of localized magnetic impurities in nonmagnetic metals, one often concentrates on two different aspects of the problem. In one of these, one treats the single magnetic impurity which interacts with the conduction electrons via an s-d interaction and results in the Kondo[1] effect at low temperatures. The other involves the interaction between different magnetic impurities. Since each of these problems is quite complicated by itself, one usually tries to separate the study of the magnetic impurity system into two different regions of temperature T and impurity concentration c: (i) a very-low-concentration region in which the impurities are so widely separated that the interactions between them can, on the average, be neglected, and one can essentially deal with a single-impurity system, and (ii) a region of higher concentration in which impurity-impurity interactions play an important role and Kondo-like effects are unimportant, either because the temperature in question is much above the Kondo temperature, or because the impurity concentration is sufficiently high that Kondo-like effects are suppressed by the impurity-impurity interaction.

The single-impurity effect was originally treated by Kondo,[1] Suhl,[2] Abrikosov,[3] and Nagaoka[4] and is by now reasonably well understood. There are many outstanding works in this area,[5] but we shall only list a few and refer the reader especially to two excellent review articles on the subject, one by Heeger and the other by Kondo.[6]

The works on the more highly concentrated region have so far primarily addressed themselves to the statistical mechanics of the many-impurity system in an effective-field approximation. Such a treatment was originally proposed by Marshall[7] and discussed by Klein and Brout,[8] Friedel,[9] and Liu[10] for low temperatures, and more recently by Klein[11] for all temperatures and all external fields.[12] In calculating the effective molecular field, which is a random variable, one completely neglects the Kondo effect, and for this reason one expects that the calculation will have validity only at temperatures much above the Kondo temperature. Even though this requirement is quite restrictive, there are materials in which the Kondo temperature T_K^0 is sufficiently low (Cu-Mn, for example) that the average impurity-impurity interaction is much greater than T_K^0, and the effective-field calculation is believed to be valid in spite of the fact that the Kondo effect is not considered.

In order to examine how this effective field suppresses the Kondo resistivity, Silverstein[13] and Harrison and Klein[14] (HK) calculated the resistivity in the second Born approximation. The essential result of the HK calculation (Silverstein has not examined the modification of the logarithmic terms by the internal fields) is that $\ln T$ is replaced by $\ln(T^2+H^2)^{1/2}$, where H is the effective internal field. The difficulty with these calculations[13,14] is that since the effective field as well as the Kondo effect arises from the s-d Hamiltonian, discussed by Kasuya[15] and Yosida,[16] it is not clear that the calculation is consistent since both effects should be considered simultaneously. Another difficulty with the effective-field calculation is that the perturbational result (or second Born approximation) is, in general, not valid, since one must consider all orders in the Kondo problem as was discussed by Abrikosov[3] and Hamann.[17] Thus even though the molecular-field calculations are in some cases in

reasonable agreement with experiment, these calculations rest on theoretical foundations whose validity is questionable.

Attempts to do a correct calculation of the many-impurity system using Green's-function techniques have been made by various researchers such as Bresemann and Bailyn,[18] Nagaoka,[19] Kurata,[20] and Blackman and Elliott.[21] Their results can be summarized by the statement that they found no essential change from the single-impurity Kondo temperature and the spin-compensated state. Béal-Monod[22] has treated the resistivity arising from two impurities with an exchange interaction between them, but this calculation was done in the second Born approximation and thus suffers restrictions similar to those of the calculations of Silverstein[13] and Harrison and Klein,[14] in that it is only valid in the region of validity of perturbation theory, i.e., high temperatures.

Recent experiments on low-concentration dilute alloys by Tholence and Tournier[23] and Welsh and Potts[24] indicate that even in the very-low-concentration region two-impurity effects are important. These experiments were done in a temperature regime where the single-impurity Kondo effect gives the major contribution to the magnetic properties and suggest that a better theory than presented up to now is necessary to describe the many-impurity system even at very low concentrations.

Since recent experiments show a strong two-impurity contribution to the single-impurity Kondo effect, one would like to solve self-consistently the two-impurity s-d Hamiltonian in general and obtain the renormalization of the $\ln T$ term by the impurity-impurity interaction. However, a relatively simple argument suggests that solving such a problem by brute force requires the knowledge of at least the five-particle Green's function. This argument goes as follows: The $\ln T$ term arises from the equations of motion of the one- and two-particle Green's functions, and we want the renormalization of the Green's functions by the impurity-impurity interaction (Ruderman–Kittel–Kasuya–Yosida) which involves a summation over two pairs of conduction-electron operators and two impurity spins. Such a term would arise to lowest order from the decoupling of the five-particle Green's function. Thus the complexity of the problem is such that its solution is in practice not feasible. Therefore, in order to find the renormalization of the $\ln T$ term by the impurity-impurity interaction we simulate the interaction by introducing a term $W(R)\vec{S}_0\cdot\vec{S}_1$ into the Hamiltonian. It should be kept in mind that the consistency of such an approach is only justified if $W(R)$ is an interaction which arises from sources other than the s-d interaction.[25] We derive the equations of motion of the relevant Green's functions and decouple into lower-order Green's functions, thereby obtaining a closed set of self-consistent equations. We use the decoupling scheme of Nagaoka[4] and therefore, along with Nagaoka, we treat the most divergent part of the Kondo effect correctly and make an error only in terms which do not contribute to the most divergent part. The essential result of our derivation is that the $\ln T$ arising from the single-impurity Kondo effect is replaced by $\frac{1}{2}\ln(T^2+W'^2)$, where W' is related to W by a simple equation and is approximately proportional to W. Thus we find that the introduction of the second impurity inhibits the formation of the spin-compensated state of the Kondo system. It also indicated that whenever the interaction energy W' is greater than the single-impurity Kondo temperature, the logarithmic terms can be treated using perturbation theory. Similarly, we find that the conduction-electron polarization is appreciably affected by the second impurity.

With an assumed Ruderman–Kittel–Kasuya–Yosida (RKKY) potential,[25,26] we also compare the modification of the $\ln T$ term arising from our method with the modification arising from the Harrison–Klein calculation.[14] For an RKKY interaction the effective Kondo temperature will be concentration and temperature dependent even at low impurity concentrations. This is in qualitative agreement with recent experiments by Loram *et al.*[27] and Souletie and Tournier.[28]

A brief outline of the paper is as follows. In Sec. II and Appendices A and B, we develop the equations of motion of the relevant Green's functions, which we solve in Sec. III. The reader who is not interested in the mathematical formalism may immediately proceed to Secs. IV and V, where the equations obtained are analyzed and the physics of the problem is discussed.

II. MATHEMATICAL DEVELOPMENT

In this section, we derive the equations of motion of the relevant Green's functions using a two-impurity s-d Hamiltonian with an added exchange term between the two impurities. We use the notation of Nagaoka[29] whenever it is convenient.

We assume a Hamiltonian $\mathcal{H}$ of the form discussed by Kasuya[15] and Yosida[16] with an added exchange term of the form

$$\mathcal{H}=\sum_k \epsilon_k c_{k\alpha}^\dagger c_{k\alpha} - \frac{J}{2N}\sum_{kk'}\vec{\sigma}_{\alpha\beta}\cdot(\vec{S}_0+\vec{S}_1 e^{i(\vec{k}-\vec{k}')\cdot\vec{R}})c_{k\alpha}^\dagger c_{k'\beta} - W(R)\vec{S}_0\cdot\vec{S}_1\,, \quad (2.1)$$

where $\vec{S}_0$ and $\vec{S}_1$ are the impurity spins located at sites 0 considered as the origin and 1 at a distance R from it; $c_{k\alpha}^\dagger$ and $c_{k\alpha}$ are the conduction-electron creation and annihilation operators with wave vector $\vec{k}$ and spin α; ϵ_k is the conduction-electron energy measured from the Fermi energy ϵ_F; N is the

total number of atoms in the solid; J is the strength of the exchange interaction between the conduction-electron and impurity spins (assumed to be a constant); $\vec{\sigma}_{\alpha\beta}$ is the matrix element of the Pauli spin operator $\vec{\sigma}$ between the spin states α and β; and $W(R)$ is the exchange energy at a distance $R = |\vec{R}|$ between the two impurity spins discussed in the Introduction. A summation over the spin indices is implied throughout the paper.

The retarded double-time Green's function of the fermion operators A and B is defined by Zubarev[30] to be

$$\langle A|B\rangle_{t-t'} = -i\theta(t-t')\langle [A(t), B(t')]_+\rangle , \tag{2.2}$$

where $\langle\ |\ \rangle_t$ denotes the Green's function, $\langle\ \rangle$ is the average over a grand canonical ensemble, $[A, B]_+$ indicates an anticommutation operation, and $\theta(t-t')$ is the Heaviside unit function which equals 1 for $t > t'$ and zero otherwise. We set $\hbar$ and the Boltzmann constant k_B equal to unity throughout this paper.

We introduce the following retarded double-time Green's functions for the two-impurity problem:

$$G_{kk'} = \tfrac{1}{2}\langle c_{k'\alpha}|c^\dagger_{k\alpha}\rangle_\omega , \tag{2.3}$$

$$\Gamma^n_{kk'} = \tfrac{1}{2}\langle \vec{\sigma}_{\alpha\beta}\cdot\vec{S}_n c_{k'\beta}|c^\dagger_{k\alpha}\rangle_\omega , \tag{2.4}$$

$$V^n_{kll'k'} = \tfrac{1}{2} i\langle \vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{ss'}\times\vec{S}_n c^\dagger_s c_{s'} c_{k'\beta}|c^\dagger_{k\alpha}\rangle_\omega , \tag{2.5}$$

$$U_{kk'} = \tfrac{1}{2} i\langle \vec{\sigma}_{\alpha\beta}\cdot(\vec{S}_0\times\vec{S}_1)c_{k'\beta}|c^\dagger_{k\alpha}\rangle_\omega , \tag{2.6}$$

where n can take values 0 or 1, and $\langle A|B\rangle_\omega$ denotes the Fourier transform of the Green's function of the operators A and B. For convenience, we suppress the suffix ω in $\langle A|B\rangle_\omega$ and the R dependence of $W(R)$.

The equation of motion for $G_{kk'}$, $\Gamma^n_{kk'}$, and $U_{kk'}$ are as follows:

$$(\omega-\epsilon_{k'})G_{kk'} = \frac{\delta_{kk'}}{2\pi} - \frac{J}{2N}[\Gamma^0_k + \Gamma^{1R}_k e^{i\vec{k}'\cdot\vec{R}}] , \tag{2.7}$$

$$\begin{aligned}(\omega-\epsilon_{k'})\Gamma^0_{kk'} &= -\frac{J}{2N}\{S(S+1)G_k + \langle\vec{S}_0\cdot\vec{S}_1\rangle e^{i\vec{k}'\cdot\vec{R}}G^R_k - \Gamma^{0}_{k}\} \\ &\quad -\frac{J}{2N}\sum_{ll'} V^0_{kll'k'} - \frac{J}{2N}U^R_k e^{i\vec{k}'\cdot\vec{R}} + WU_{kk'} ,\end{aligned} \tag{2.8}$$

$$\begin{aligned}(\omega-\epsilon_{k'})\Gamma^1_{kk'}e^{i\vec{k}'\cdot\vec{R}} &= -\frac{J}{2N}\{S(S+1)G^R_k + \langle\vec{S}_0\cdot\vec{S}_1\rangle e^{-i\vec{k}'\cdot\vec{R}}G_k - \Gamma^{1R}_k\} \\ &\quad -\frac{J}{2N}\sum_{ll'} V^1_{kll'k'}e^{i(\vec{l}-\vec{l}'-\vec{k}')\cdot\vec{R}} \\ &\quad +\frac{J}{2N}U_k e^{-i\vec{k}'\cdot\vec{R}} - WU_{kk'}e^{-i\vec{k}'\cdot\vec{R}} ,\end{aligned} \tag{2.9}$$

where

$$A_k = \sum_{k'} A_{kk'} , \tag{2.10}$$

$$A^R_k = \sum_{k'} A_{kk'}e^{-i\vec{k}'\cdot\vec{R}} \tag{2.11}$$

for $A_{kk'} = G_{kk'}$, $\Gamma^n_{kk'}$, or $U_{kk'}$. In obtaining Eqs. (2.8) and (2.9), we have decoupled the longitudinal Green's function $\frac{1}{2}\langle\vec{S}_0\cdot\vec{S}_1 c_{k'\alpha}|c^\dagger_{k\alpha}\rangle$ to give $\langle\vec{S}_0\cdot\vec{S}_1\rangle G_{kk'}$.

The term involving $U_{kk'}$ in Eqs. (2.8) and (2.9) introduces quantities involving the exchange interaction W between the two impurities. In order to evaluate U_k and $U_{kk'}$, we obtain the equation of motion of $U_{kk'}$ and later decouple it into lower-order Green's functions. We thus have

$$\begin{aligned}(\omega-\epsilon_{k'})U_{kk'} &= \frac{i}{4\pi}\langle\vec{\sigma}_{\alpha\alpha}\cdot(\vec{S}_0\times\vec{S}_1)\rangle\delta_{kk'} - \frac{iJ}{4N}\sum_{p'}\langle\vec{\sigma}_{\alpha\beta}\cdot(\vec{S}_0\times\vec{S}_1)(\vec{S}_0+\vec{S}_1 e^{i(\vec{k}'-\vec{p}')\cdot\vec{R}})\cdot\vec{\sigma}_{\beta\delta}c_{p'\delta}|c^\dagger_{k\alpha}\rangle \\ &\quad -\frac{J}{4N}\sum_{pp'}\langle(\vec{\sigma}_{\gamma\delta}\times\vec{S}_0)\cdot(\vec{\sigma}_{\alpha p}\times\vec{S}_1)c^\dagger_{p\gamma}c_{p'\delta}c_{k'\beta}|c^\dagger_{k\alpha}\rangle + \frac{J}{4N}\sum_{pp'}\langle(\vec{\sigma}_{\alpha\beta}\times\vec{S}_0)\cdot(\vec{\sigma}_{\gamma\delta}\times\vec{S}_1)c^\dagger_{p\gamma}c_{p'\delta}c_{k'\beta}|c^\dagger_{k\alpha}\rangle e^{i(\vec{p}-\vec{p}')\cdot\vec{R}} \\ &\quad +\frac{W}{2}\langle[(\vec{S}_0\times\vec{S}_1)\cdot(\vec{\sigma}_{\alpha\beta}\times\vec{S}_1)+(\vec{\sigma}_{\alpha\beta}\times\vec{S}_0)\cdot(\vec{S}_0\times\vec{S}_1)]c_{k'\beta}|c^\dagger_{k\alpha}\rangle .\end{aligned} \tag{2.12}$$

We assume that each impurity has spin $\frac{1}{2}$; hence

$$\langle\vec{S}_0\cdot\vec{S}_0\rangle = \langle\vec{S}_1\cdot\vec{S}_1\rangle = S(S+1) = \tfrac{3}{4} . \tag{2.13}$$

For later use, we also define the quantities

$$n_{kk'} = \tfrac{1}{2}\langle c^\dagger_{k\alpha}c_{k'\alpha}\rangle = -2\int_{-\infty}^{+\infty}(\mathrm{Im}G_{kk'})f(\omega)\,d\omega , \tag{2.14}$$

$$m^n_{kk'} = \langle\vec{\sigma}_{\alpha\beta}\cdot\vec{S}_n c^\dagger_{k\alpha}c_{k'\beta}\rangle = -4\int_{-\infty}^{+\infty}(\mathrm{Im}\Gamma^n_{kk'})f(\omega)\,d\omega , \tag{2.15}$$

$$\tilde{u}_{kk'} = i\langle\vec{\sigma}_{\alpha\beta}\cdot\vec{S}_0\times\vec{S}_1 c^\dagger_{k\alpha}c_{k'\beta}\rangle = -4\int_{-\infty}^{\infty}(\mathrm{Im}U_{kk'})f(\omega)\,d\omega , \tag{2.16}$$

where $f(\omega) = (e^{\omega/T}+1)^{-1}$ and Im indicates the imaginary part. Also we define

$$a_k = \sum_{k'} a_{k'k} , \tag{2.17}$$

$$a^R_k = \sum_{k'} a_{k'k}e^{i\vec{k}'\cdot\vec{R}} \tag{2.18}$$

for $a_{kk'} = n_{kk'}$, $m^0_{kk'}$, $m^1_{kk'}$, and $\tilde{u}_{kk'}$.

Note that throughout the whole calculation we use the relationships

$$\begin{aligned}n_{k'} &= \sum_k n_{kk'} = \sum_k n_{kk'}e^{i(\vec{k}-\vec{k}')\cdot\vec{R}} \\ &= \sum_k n_{k'k} = \sum_k n_{k'k}e^{i(\vec{k}'-\vec{k})\cdot\vec{R}} ,\end{aligned} \tag{2.19}$$

$$m_{k'} = \sum_k m^0_{kk'} = \sum_k m^1_{kk'} e^{i(\vec{k}-\vec{k}')\cdot\vec{R}}$$
$$= \sum_k m^0_{k'k} = \sum_k m^1_{k'k} e^{i(\vec{k}'-\vec{k})\cdot\vec{R}} , \quad (2.20)$$

and

$$\tilde{u}_{k'} = \sum_k \tilde{u}_{kk'} = -\sum_k \tilde{u}_{kk'} e^{i(\vec{k}-\vec{k}')\cdot\vec{R}}$$
$$= \sum_k \tilde{u}_{k'k} = -\sum_k \tilde{u}_{k'k} e^{i(\vec{k}'-\vec{k})\cdot\vec{R}} . \quad (2.21)$$

The physical meaning of Eqs. (2.19)–(2.21) is that we assume that the correlation functions defined are position independent in the following sense: The conduction-electron-spin–impurity-spin correlation function $m_{kk'}$ has the same value when S is at $r=0$ and the conduction electrons are created and annihilated at $r=0$ as when S is at $r=R$ and the conduction electrons are created and annihilated at $r=R$. The same assumption is made for $n_{kk'}$ and $\tilde{u}_{kk'}$.[31]

Equations (2.7)–(2.9) have to be solved self-consistently. In order to do so, we decouple our Green's functions into lower-order Green's functions and correlation functions. As mentioned before, we wish to solve the two-impurity Kondo system with the proviso that we keep the most divergent terms, plus the term $U_{kk'}$ which introduces the impurity-impurity interactions. It has been shown by Doniach[32] and Nagaoka[29] that the decoupling of the Green's function $V_{kll'k'}$ given in Eq. (2.5) using the Nagaoka decoupling scheme retains the most divergent logarithmic terms. We thus use a decoupling similar to that of Nagaoka:

$$V^n_{kll'k'} = 2n_{lk'}\Gamma^n_{kl'} - m^n_{lk'}G_{kl'} . \quad (2.22)$$

We decouple the higher-order Green's functions in Eq. (2.12) using the method of cumulant decoupling (Appendix A) discussed by Kubo[33] and Brout and Carruthers.[34] (Note that the Nagaoka decoupling is consistent with the cumulant decoupling scheme.) This decouples the higher-order Green's functions into lower-order functions and gives a closed set of equations, which we then solve.

The decoupling of Eqs. (2.8) and (2.9) is straightforward. Using Eq. (2.22), we get

$$(\omega-\epsilon_{k'})\Gamma^0_{kk'} = \frac{J}{2N}[m_{k'} - S(S+1)]G_k - \frac{J}{N}[n_{k'} - \tfrac{1}{2}]\Gamma^0_k$$
$$- \frac{J}{2N}[\langle \vec{S}_0\cdot\vec{S}_1\rangle G^R_k + U^R_k]e^{i\vec{k}'\cdot\vec{R}} + WU_{kk'} , \quad (2.23)$$

$$(\omega-\epsilon_{k'})\Gamma'_{kk'}e^{-i\vec{k}'\cdot\vec{R}}$$
$$= \frac{J}{2N}[m_{k'} - S(S+1)]G^R_k - \frac{J}{N}[n_{k'} - \tfrac{1}{2}]\Gamma^{1R}_k$$
$$- \frac{J}{2N}[\langle \vec{S}_0\cdot\vec{S}_1\rangle G_k - U_k]e^{-i\vec{k}'\cdot\vec{R}} - WU_{kk'}e^{-i\vec{k}'\cdot\vec{R}} . \quad (2.24)$$

The decoupling of Eq. (2.12) is more complicated and is done in Appendix A; the result is

$$(\omega-\epsilon_{k'})U_{kk'} = \frac{J}{N}\langle \vec{S}_0\cdot\vec{S}_1\rangle[(n_{k'}-\tfrac{1}{2})G_k - (n^R_{k'}-\tfrac{1}{2}e^{i\vec{k}'\cdot\vec{R}})G^R_k]$$
$$+ \frac{J}{3N}[m_{k'} - S(S+1)][\Gamma^{0R}_k e^{i\vec{k}'\cdot\vec{R}} - \Gamma^1_k] - \frac{J}{3N}[m^1_{k'} + \langle \vec{S}_0\cdot\vec{S}_1\rangle][\Gamma^0_k - \Gamma^{1R}_k e^{i\vec{k}'\cdot\vec{R}}]$$
$$- \frac{J}{2N}[n_{k'}U_k + n^R_{k'}U^R_k] + \frac{J}{4N}[\tilde{u}_{k'}G_k + \tilde{u}^R_{k'}G^R_k] + \tfrac{2}{3}\{W[S(S+1) + \langle \vec{S}_0\cdot\vec{S}_1\rangle] + E'\}[\Gamma^0_{kk'} - \Gamma^1_{kk'}] , \quad (2.25)$$

where

$$E' = \frac{J}{2N}\sum_{pp'} m^0_{pp'}e^{i(\vec{p}-\vec{r}')\cdot\vec{R}} = \frac{J}{2N}\sum_{pp'} m^1_{pp'} , \quad (2.26)$$

is the polarization energy at site 0 or site 1. Equations (2.23)–(2.25) together with Eq. (2.7) form a closed set of equations which can be solved self-consistently. It is easy to verify that as $R \to \infty$ all the R-dependent terms vanish, and from Eqs. (2.7) and (2.23) we obtain Nagaoka's[4] single-impurity formulation, as we should, since the impurities are removed an infinite distance from each other.

III. SOLUTION OF GREEN'S FUNCTIONS

In Sec. II, we derived a closed set of equations for the Green's functions $G_{kk'}$, $\Gamma^n_{kk'}$, and $U_{kk'}$ in terms of their correlation functions $n_{kk'}$, $m^n_{kk'}$, and $\tilde{u}_{kk'}$. In this section, we solve self-consistently for the quantities G_k, G^R_k, Γ^0_k, and Γ^{1R}_k and then substitute these into Eqs. (2.7), (2.23), and (2.24) to obtain $G_{kk'}$, $\Gamma^1_{kk'}e^{i(\vec{k}-\vec{k}')\cdot\vec{R}}$, and $\Gamma^0_{kk'}$.

Before we proceed, it is useful to define the following quantities: Let

$$F(x) = \frac{1}{N}\sum_k \frac{1}{x-\epsilon_k} , \quad (3.1)$$

$$F^R(x) = \frac{1}{N}\sum_k \frac{e^{\pm i\vec{k}\cdot\vec{R}}}{x-\epsilon_k} , \quad (3.2)$$

$$G(x) = \frac{1}{N}\sum_k \frac{n_k - \frac{1}{2}}{x-\epsilon_k} , \quad (3.3)$$

$$\Gamma(x) = \frac{1}{N}\sum_k \frac{m_k - S(S+1)}{x-\epsilon_k} , \quad (3.4)$$

and

$$W'^2=\tfrac{2}{3}W\{W[S(S+1)+\langle\vec{S}_0\cdot\vec{S}_1\rangle]+E'\}\,, \tag{3.5}$$

where E' is given in Eq. (2.26).

From Eq. (2.7) we obtain

$$G_k=\frac{1}{2\pi}\,\frac{1}{\omega-\epsilon_k}-\tfrac{1}{2}J[F(\omega)\Gamma_k^0+F^R(\omega)\Gamma_k^{1R}]\,, \tag{3.6}$$

$$G_k^R=\frac{1}{2\pi}\,\frac{e^{-i\vec{k}\cdot\vec{R}}}{\omega-\epsilon_k}-\tfrac{1}{2}J[F^R(\omega)\Gamma_k^0+F(\omega)\Gamma_k^{1R}]\,. \tag{3.7}$$

Substituting Eq. (2.25) into Eq. (2.23), we obtain

$$\begin{aligned}[(\omega-\epsilon_{k'})-W'^2(\omega-\epsilon_{k'})^{-1}]\Gamma_{kk'}^0 &=\frac{J}{2N}[m_{k'}-S(S+1)]G_k-\frac{J}{N}[n_{k'}-\tfrac{1}{2}]\Gamma_k^0\\ &\quad-\frac{J}{2N}[\langle\vec{S}_0\cdot\vec{S}_1\rangle G_k^R+U_k^R]e^{i\vec{k}\cdot\vec{R}}\\ &\quad+W\sum_i\mathfrak{F}_k^i(\epsilon_{k'})(\omega-\epsilon_{k'})^{-1}\,,\end{aligned} \tag{3.8}$$

where W'^2 was defined in Eq. (3.5), and $\sum_i\mathfrak{F}_k^i(\epsilon_{k'})$ represents a summation over all the terms occurring on the right-hand side of Eq. (2.25), except for $W'^2(\omega-\epsilon_{k'})^{-1}\Gamma_{kk'}^0$, which has been transposed to the left-hand side of Eq. (3.8). Summing Eq. (3.8) over k', we obtain

$$\begin{aligned}[1+JG(\omega\pm W')]\Gamma_k^0&=\tfrac{1}{2}J\Gamma(\omega\pm W')G_k-\tfrac{1}{2}JF^R(\omega\pm W')\\ &\quad\times[\langle\vec{S}_0\cdot\vec{S}_1\rangle G_k^R+U_k^R]\,,\end{aligned} \tag{3.9}$$

where

$$A(\omega\pm W')=\tfrac{1}{2}[A(\omega+W')+A(\omega-W')] \tag{3.10}$$

and A may be any of the quantities defined in Eqs. (3.1)–(3.4). In obtaining Eq. (3.9), we have used the identities

$$\begin{aligned}&[(\omega-\epsilon_{k'})-W'^2(\omega-\epsilon_{k'})^{-1}]^{-1}\\ &\quad=\tfrac{1}{2}[(\omega-\epsilon_{k'}+W')^{-1}+(\omega-\epsilon_{k'}-W')^{-1}]\,,\end{aligned} \tag{3.11a}$$

$$\begin{aligned}&[(\omega-\epsilon_{k'})^2-W'^2]^{-1}\\ &\quad=\frac{1}{2W'}[(\omega-\epsilon_{k'}-W')^{-1}-(\omega-\epsilon_{k'}+W')^{-1}]\,.\end{aligned} \tag{3.11b}$$

Note that we dropped in Eq. (3.9) all the other contributions from $U_{kk'}$, since those contributions carry $[(\omega-\epsilon_{k'})^2-W'^2]^{-1}$ as a factor, and we find after some simple but laborious algebra that all the logarithmically most divergent terms, which are of interest in the Kondo problem, vanish from an expression:

$$\sum_{k'}\mathfrak{F}_k^i(\epsilon_{k'})[(\omega-\epsilon_{k'})^2-W'^2]^{-1}$$

$$=\frac{1}{2W'}[T_k^i(\omega-W')-T_k^i(\omega+W')]\,, \tag{3.12}$$

where $T_k^i(x)=\sum_{k'}\mathfrak{F}_k^i(\epsilon_{k'})(x-\epsilon_{k'})^{-1}$. Solving for Γ_k^{1R} in a similar way, we obtain

$$\begin{aligned}[1+JG(\omega\pm W')]\Gamma_k^{1R}&=\tfrac{1}{2}J\Gamma(\omega\pm W')G_k^R-\tfrac{1}{2}JF^R(\omega\pm W')\\ &\quad\times[\langle\vec{S}_0\cdot\vec{S}_1\rangle G_k-U_k]\,.\end{aligned} \tag{3.13}$$

In order to complete a closed set of equations, we also have to solve for U_k and U_k^R and for Γ_k^{0R} and Γ_k^1, which occur in the equation of motion of U_k and U_k^R. One can thus establish a closed set of simultaneous equations for G_k, G_k^R, Γ_k^0, Γ_k^{1R}, U_k, U_k^R, Γ_k^{0R}, and Γ_k^1, which, in principle, can be solved exactly, but in practice has to be done by an approximation method.

To facilitate our calculations, we make the following observations. To calculate physical quantities such as the resistivity, the specific heat, the conduction-electron polarization, and the magnetic susceptibility, etc., within the context of our present work, one only needs to know the one-particle Green's function $G_{kk'}$, and the two-particle Green's functions $\Gamma_{kk'}^0$ and $\Gamma_{kk'}^1e^{i(\vec{k}-\vec{k}')\cdot\vec{R}}$. It can be shown (Appendix B) that the contributions of U_k^R and $U_ke^{i\vec{k}\cdot\vec{R}}$ to $\Gamma_{kk'}^0$ and $\Gamma_{kk'}^1e^{i(\vec{k}-\vec{k}')\cdot\vec{R}}$ are at most of order $(J\rho/Nk_FR)^2\times$(the differences of two logarithmic contributions), and therefore do not contribute to the most divergent part of the Kondo effect. This allows us, within our approximation, to neglect U_k^R and U_k in Eqs. (3.9) and (3.13). We thus obtain a closed set of simultaneous equations for G_k, G_k^R, Γ_k^0, and Γ_k^{1R} in terms of quantities defined in Eqs. (3.1)–(3.5) and the unperturbed one-particle Green's functions

$$G_k^0=\frac{1}{2\pi}\,\frac{1}{\omega-\epsilon_k} \tag{3.14}$$

and

$$G_k^{0R}=\frac{1}{2\pi}\,\frac{e^{-i\vec{k}\cdot\vec{R}}}{\omega-\epsilon_k}\,. \tag{3.15}$$

Neglecting U_k^R and U_k in Eqs. (3.9) and (3.13), we obtain

$$\begin{aligned}[1+JG(\omega\pm W')]\Gamma_k^0&=\tfrac{1}{2}J\Gamma(\omega\pm W')G_k-\tfrac{1}{2}JF^R(\omega\pm W')\\ &\quad\times\langle\vec{S}_0\cdot\vec{S}_1\rangle G_k^R\,,\end{aligned} \tag{3.16}$$

$$\begin{aligned}[1+JG(\omega\pm W')]\Gamma_k^{1R}&=\tfrac{1}{2}J\Gamma(\omega\pm W')G_k^R-\tfrac{1}{2}JF^R(\omega\pm W')\\ &\quad\times\langle\vec{S}_0\cdot\vec{S}_1\rangle G_k\,.\end{aligned} \tag{3.17}$$

The solution of the four simultaneous equations, Eqs. (3.6), (3.7), (3.16), and (3.17), is straightforward; we have

$$G_k=\frac{1}{2\pi}\,\frac{1}{\omega-\epsilon_k}\,\frac{[1+JG(\omega\pm W')][X-e^{-i\vec{k}\cdot\vec{R}}Y]}{X^2-Y^2}\,, \tag{3.18}$$

$$G_k^R = \frac{1}{2\pi}\,\frac{e^{-i\vec{k}\cdot\vec{R}}}{\omega-\epsilon_k}\,\frac{[1+JG(\omega\pm W')][X-e^{i\vec{k}\cdot\vec{R}}Y]}{X^2-Y^2}\ , \tag{3.19}$$

$$\Gamma_k^0 = \frac{J}{4\pi}\,(\omega-\epsilon_k)^{-1}[X^2-Y^2]^{-1}\{[\Gamma(\omega\pm W')-F^R(\omega\pm W')\langle\vec{S}_0\cdot\vec{S}_1\rangle e^{-i\vec{k}\cdot\vec{R}}]X$$
$$-[\Gamma(\omega\pm W')-F^R(\omega\pm W')\langle\vec{S}_0\cdot\vec{S}_1\rangle e^{i\vec{k}\cdot\vec{R}}]e^{i\vec{k}\cdot\vec{R}}Y\}\ , \tag{3.20}$$

$$\Gamma_k^{1R} = \frac{J}{4\pi}\,\frac{e^{-i\vec{k}\cdot\vec{R}}}{\omega-\epsilon_k}\,[X^2-Y^2]^{-1}\{[\Gamma(\omega\pm W')-F^R(\omega\pm W')\,\langle\vec{S}_0\cdot\vec{S}_1\rangle e^{i\vec{k}\cdot\vec{R}}]X$$
$$-[\Gamma(\omega\pm W')-F^R(\omega\pm W')\langle\vec{S}_0\cdot\vec{S}_1\rangle e^{-i\vec{k}\cdot\vec{R}}]\,e^{i\vec{k}\cdot\vec{R}}Y\}\ , \tag{3.21}$$

where

$$X = 1+JG(\omega\pm W')+\tfrac{1}{4}J^2[F(\omega)\Gamma(\omega\pm W')-F^R(\omega)F^R(\omega\pm W')\langle\vec{S}_0\cdot\vec{S}_1\rangle]\ , \tag{3.22}$$

$$Y = \tfrac{1}{4}J^2[F^R(\omega)\Gamma(\omega\pm W')-F(\omega)F^R(\omega\pm W')\langle\vec{S}_0\cdot\vec{S}_1\rangle]\ . \tag{3.23}$$

Using Eqs. (3.18)–(3.21) in Eqs. (2.7), (2.23), and (2.24), we obtain

$$G_{kk'} = \frac{1}{2\pi}\,\frac{\delta_{kk'}}{\omega-\epsilon_k}-\frac{J^2}{8\pi N}\,\frac{[X^2-Y^2]^{-1}}{(\omega-\epsilon_k)(\omega-\epsilon_{k'})}$$
$$\times\{[\Gamma(\omega\pm W')(1+e^{i(\vec{k}'-\vec{k})\cdot\vec{R}})-F^R(\omega\pm W')\langle\vec{S}_0\cdot\vec{S}_1\rangle(e^{-i\vec{k}\cdot\vec{R}}+e^{i\vec{k}'\cdot\vec{R}})]X$$
$$-[\Gamma(\omega\pm W')(e^{-i\vec{k}\cdot\vec{R}}+e^{i\vec{k}'\cdot\vec{R}})-F^R(\omega\pm W')\langle\vec{S}_0\cdot\vec{S}_1\rangle(1+e^{i(\vec{k}'-\vec{k})\cdot\vec{R}})]Y\}\ , \tag{3.24}$$

$$\Gamma_{kk'}^0 = \frac{J}{4\pi N}\,\frac{[X^2-Y^2]^{-1}}{(\omega-\epsilon_k)(\omega-\epsilon_{k'}\pm W')}$$
$$\times\Big\{\{[1+JG(\omega\pm W')][m_{k'}-S(S+1)-\langle\vec{S}_0\cdot\vec{S}_1\rangle e^{i(\vec{k}'-\vec{k})\cdot\vec{R}}]-J(n_{k'}-\tfrac{1}{2})[\Gamma(\omega\pm W')-F^R(\omega\pm W')\langle\vec{S}_0\cdot\vec{S}_1\rangle e^{-i\vec{k}\cdot\vec{R}}]\}X$$
$$-\Big([1+JG(\omega\pm W')]\{[m_{k'}-S(S+1)]\,e^{-i\vec{k}\cdot\vec{R}}-\langle\vec{S}_0\cdot\vec{S}_1\rangle e^{i\vec{k}'\cdot\vec{R}}\}$$
$$-J(n_{k'}-\tfrac{1}{2})[\Gamma(\omega\pm W')\,e^{-i\vec{k}\cdot\vec{R}}-F^R(\omega\pm W')\langle\vec{S}_0\cdot\vec{S}_1\rangle]\Big)Y\Big\}\ , \tag{3.25}$$

where

$$(\omega-\epsilon_{k'}\pm W')^{-1} = \tfrac{1}{2}[(\omega-\epsilon_{k'}+W')^{-1}+(\omega-\epsilon_{k'}-W')^{-1}] \tag{3.26}$$

and $\Gamma_{kk'}^1 e^{i(\vec{k}-\vec{k}')\cdot\vec{R}}$ has exactly the same form as $\Gamma_{kk'}^0$, namely,

$$\Gamma_{kk'}^1 e^{i(\vec{k}-\vec{k}')\cdot\vec{R}} = \Gamma_{kk'}^0(\vec{R}\to-\vec{R})\ . \tag{3.27}$$

Equations (3.24), (3.25), and (3.27) are exact (except for the decoupling) and valid for all temperatures. In Sec. IV, we shall analyze these results and obtain the physical quantities of interest from them.

In obtaining these quantities, we confine ourselves to the high-temperature or large-W' limit. Then we are justified in neglecting Y, since $Y \ll X$, and find

$$G_{kk'} = \frac{1}{2\pi}\,\frac{1}{\omega-\epsilon_k}\,\{\delta_{kk'}-\frac{J^2}{4N}\,\frac{X^{-1}}{\omega-\epsilon_{k'}}[\Gamma(\omega\pm W')(1+e^{i(\vec{k}'-\vec{k})\cdot\vec{R}})-F^R(\omega\pm W')\langle\vec{S}_0\cdot\vec{S}_1\rangle(e^{i\vec{k}\cdot\vec{R}}+e^{-i\vec{k}'\cdot\vec{R}})]\}\ , \tag{3.28}$$

$$\Gamma_{kk'}^0 = \frac{J}{4\pi N}\,\frac{X^{-1}}{(\omega-\epsilon_k)(\omega-\epsilon_{k'}\pm W')}\,\{[1+JG(\omega\pm W')][m_{k'}-S(S+1)-\langle\vec{S}_0\cdot\vec{S}_1\rangle e^{i(\vec{k}'-\vec{k})\cdot\vec{R}}]$$
$$-J[n_{k'}-\tfrac{1}{2}][\Gamma(\omega\pm W')-\langle\vec{S}_0\cdot\vec{S}_1\rangle F^R(\omega\pm W')e^{-i\vec{k}\cdot\vec{R}}]\}\ , \tag{3.29}$$

and $\Gamma_{kk'}^1 e^{i(\vec{k}-\vec{k}')\cdot\vec{R}}$ for the high-temperature or large-W' limit can be obtained from Eq. (3.29) using Eq. (3.27).

Equations (3.28) and (3.29) can easily be compared with Nagaoka's single-impurity Green's functions.

IV. ANALYSIS OF TWO-IMPURITY RESULTS

In this section we obtain some useful physical information from Eqs. (3.24), (3.25), and (3.27). We first examine the proper limits of these equations for various cases.

Case 1: $R\to\infty$, $W=0$. In this case, all the R-dependent terms vanish; hence Eqs. (3.24) and (3.25) become

$$G_{kk'}=\frac{1}{2\pi}\,\frac{1}{\omega-\epsilon_{k'}}\left\{\delta_{kk'}-\frac{J^2}{4N}\,\frac{1}{\omega-\epsilon_k}\times\frac{\Gamma(\omega)}{1+JG(\omega)+\frac{1}{4}J^2\Gamma(\omega)F(\omega)}\right\}\,, \tag{4.1}$$

$$\Gamma^0_{kk'}=\frac{J}{4\pi N}\,\frac{1}{(\omega-\epsilon_k)(\omega-\epsilon_{k'})}\times\frac{[1+JG(\omega)][m_{k'}-S(S+1)]-J[n_{k'}-\frac{1}{2}]\Gamma(\omega)}{1+JG(\omega)+\frac{1}{4}J^2\Gamma(\omega)F(\omega)}\,. \tag{4.2}$$

Equations (4.1) and (4.2) are exactly the same as Nagaoka's[4] single-impurity results. Note that Eqs. (3.28) and (3.29) also reduce to a form similar to Eqs. (4.1) and (4.2).

Case 2: $R=0$, $W=0$, *triplet-impurity configuration*. For the case when two impurities each with spin $\frac{1}{2}$ coincide with each other to form a triplet, we have $\vec{S}_0+\vec{S}_1=2\vec{S}$ and $\langle\vec{S}_0\cdot\vec{S}_1\rangle=S^2$, where $|\vec{S}_0|=|\vec{S}_1|=|\vec{S}|=S$; Eq. (3.24) becomes

$$G_{kk'}=\frac{1}{2\pi}\,\frac{1}{\omega-\epsilon_{k'}}\left\{\delta_{kk'}-\frac{J^2}{4N}\,\frac{1}{\omega-\epsilon_k}\times\frac{\Gamma^t(\omega)}{1+JG(\omega)+\frac{1}{4}J^2\Gamma^t(\omega)F(\omega)}\right\} \tag{4.3}$$

and Eqs. (3.25) and (3.27) combine to give

$$\Gamma^t_{kk'}=\frac{J}{4\pi N}\,\frac{[1+JG(\omega)]}{(\omega-\epsilon_k)(\omega-\epsilon_{k'})}\times\frac{[2m_{k'}-2S(2S+1)]-J[n_{k'}-\frac{1}{2}]\Gamma^t(\omega)}{1+JG(\omega)+\frac{1}{4}J^2\Gamma^t(\omega)F(\omega)}\,, \tag{4.4}$$

with

$$\Gamma^t(\omega)=\frac{1}{N}\sum_k\frac{2m_k-2S(2S+1)}{\omega-\epsilon_k} \tag{4.5}$$

and $\Gamma^t_{kk'}=\Gamma^0_{kk'}+\Gamma^1_{kk'}$ evaluated for $R=0$. Equations (4.3) and (4.4) are Nagaoka's single-impurity equations for spin 1.

Case 3: $R=0$, $W=0$, *singlet-impurity configuration*. For the case when two impurities of the same magnitude coincide to form a singlet, we have $\vec{S}_0+\vec{S}_1=0$ and $\langle\vec{S}_0\cdot\vec{S}_1\rangle=-S(S+1)$. For this case,

$$G_{kk'}=\frac{1}{2\pi}\,\frac{\delta_{kk'}}{\omega-\epsilon_{k'}} \tag{4.6}$$

and $\Gamma^s_{kk'}=\Gamma^0_{kk'}+\Gamma^1_{kk}$ evaluated for $R=0$ and $\vec{S}_0+\vec{S}_1=0$ vanishes. This corresponds to the case where there is no localized magnetic moment; thus $G_{kk'}$ is the free-particle Green's function in accordance with physical expectations.

Case 4: *General with R finite and* $W\neq 0$. Before we discuss the general case it is useful to introduce the following new quantities:

$$F(x)=(\pi\rho D/N)(x+iD)^{-1}\,, \tag{4.7}$$

where D is the bandwidth and ρ is the density of states. For $x\ll D$, we have

$$F(x)=-i\pi\rho/N\,, \tag{4.8}$$

$$G(x)=-\frac{\rho}{2N}\ln\left|\frac{x^2+T^2}{D^2}\right|-\frac{i\pi\rho}{N}[f(x)-\tfrac{1}{2}]\,, \tag{4.9}$$

$$F^R(x)=-\frac{\pi\rho}{N}\,\frac{1}{k_FR}\,e^{i[2m^*(x+\epsilon_F)]^{1/2}R}\,, \tag{4.10}$$

where m^* is the effective mass of the conduction electron. For $x\ll\epsilon_F$, we have

$$F^R(x)=-\frac{\pi\rho}{N}\,\frac{1}{k_FR}\,e^{ik_FR}\,. \tag{4.11}$$

Equations (4.7)–(4.9) have been evaluated by Nagaoka[4] and Hamann.[17] Equation (4.10) has been discussed by Koster,[35] Gavan and Doman,[36] Kim,[37] Béal-Monod,[22] and Kurata.[20]

The expressions for this general case are given in Eqs. (3.2)–(3.27) of Sec. III. By observing these equations, we make the following important remark. Because of the impurity-impurity interaction of strength W introduced into the Hamiltonian, Eq. (2.1), all the functions defined in Eqs. (3.1)–(3.4) which arise from the *interacting part* of the Green's functions have their ω dependence replaced by $\omega\pm W'$. This is the central result of our paper and has important physical implications with regard to the Kondo problem. This can be seen most clearly from the expressions for $G_{kk'}$ and $\Gamma^0_{kk'}$ given in Eqs. (3.28) and (3.29).

Thus in the presence of the interaction W

$$\begin{aligned}&G(\omega)\xrightarrow{W}G(\omega\pm W')\,,\\&\Gamma(\omega)\xrightarrow{W}\Gamma(\omega\pm W')\,,\\&F^R(\omega)\xrightarrow{W}F^R(\omega\pm W')\,.\end{aligned} \tag{4.12}$$

Equation (4.12) is valid for all temperatures.

From Eq. (4.12) we see that all the logarithmically divergent terms (and also some nondivergent ones) arising from the Kondo effect, which without the impurity-impurity interaction W will go like $\ln|T/D|$, are now replaced by $\ln[(T^2+W'^2)/D^2]^{1/2}$. We recall that without the interaction W the spin-compensated state, i.e., Kondo bound state, is formed at about the Kondo temperature:

$$T_K^0\approx De^{-N/|J|\rho}\,. \tag{4.13}$$

In the presence of the interaction W, $\ln|T/D|$ is replaced by $\ln[(T^2+W'^2)/D^2]^{1/2}$. Thus when $W'>T_K^0$, W' strongly inhibits the formation of the spin-compensated state. When $W'<T_K^0$, the formation of the spin-compensated state will be partially inhibited depending upon the ratio of W'/T_K^0. Therefore the single-impurity Kondo effect will only be observed when the average interaction en-

ergy between the impurities is much less than T_K^0.

According to this result, if we assume W to be a long-range interaction of the form of the RKKY interaction, the Kondo effect will disappear at higher impurity concentrations. This is in qualitative agreement with the logarithmic part of the resistivity calculations of Harrison and Klein,[14] which were done in an effective-field approximation using the second Born approximation.

An experimental confirmation of the theoretical predictions that the spin-compensated state is being inhibited by the interaction W is strikingly demonstrated by the experiments of Dreyfus *et al.*,[38] who measured the magnetic susceptibility of Cu-Fe, Cu-Mn, and Au-Fe. These results show that for Cu-Mn, which has presumably a very low Kondo temperature (about 0.05 °K or less), the magnetic susceptibility at low concentrations is approximately independent of the impurity concentration, in agreement with the theoretical predictions of effective-field theories[7-11] without considering the Kondo effect. For Au-Fe, where according to Kitchens,[39] T_K^0 is of the order of 1–2 °K, the susceptibility is again independent of the impurity concentration down to about $c \sim 0.1\%$. When one reduces the concentration even further, the average impurity-impurity interaction becomes less than the Kondo temperature, and spin-compensation effects reduce the magnetic susceptibility. This reduction is inhibited for concentration greater than 0.1% for Au-Fe. Thus one may qualitatively estimate that for Au-Fe, the parameter Δ defined by Eq. (3.4) of Ref. 11 is of the order T_K^0 at $c \sim 0.1\%$, where Δ is the temperature-dependent width of the probability distribution of the internal fields. This would give a Kondo temperature of the order Δ, which is of the order of 2 °K if one uses the relation given for Δ derived from the susceptibility maximum $T_{\max}$ of Table I, of Ref. 11, i.e., $\Delta \approx 2.5 T_{\max}$. The continuous rise of the susceptibility for Cu-Fe in the data of Dreyfus *et al.*[38] is probably caused by a ferromagnetic coupling between the iron impurities at higher concentrations.

It is also expected that the impurity-impurity interaction will inhibit the spin-compensated conduction-electron-spin polarization as measured by a nuclear-magnetic-resonance experiment. This should, at least in some cases, show up in NMR experiments in dilute alloys.

V. CALCULATION OF PHYSICAL QUANTITIES: HIGH-TEMPERATURE OR LARGE-W LIMIT

In this section, we calculate some physical quantities for the two-impurity system for the cases where either the effective impurity-impurity interaction W' is much greater than the single-impurity Kondo temperature T_K^0 or the temperature of the solid is much greater than T_K^0. For both of the above cases, the logarithmic variation of the physical quantities is small. The relationship

$$\left| \frac{J\rho}{2N} \ln\left(\frac{T^2 + W'^2}{D^2}\right) \right| \ll 1 \tag{5.1}$$

holds for any T whenever $W' \gg T_K^0$ and for any W' whenever $T \gg T_K^0$.

A Conduction-Electron-Spin Polarization

The behavior of the conduction-electron-spin polarization around site 0 can be investigated by calculating the quantity

$$\begin{aligned} p(r) &= \sum_{kk'} m^0_{kk'} e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} \\ &= -4 \sum_{kk'} \int_{-\infty}^{\infty} [\mathrm{Im}\Gamma^0_{kk'} e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}] f(\omega)\, d\omega \,, \end{aligned} \tag{5.2}$$

where r is the distance measured from site 0. We examine Eq. (5.2) in the limits given by Eq. (5.1). In this limit $m_{k'}$, as well as terms of order J^2, are neglected from Eq. (3.29); hence

$$\Gamma^0_{kk'} \approx -\frac{J}{4\pi N} \frac{1}{(\omega - \epsilon_k)(\omega - \epsilon_{k'} \pm W')} \times [S(S+1) + \langle \vec{S}_0 \cdot \vec{S}_1 \rangle e^{i(\vec{k}'-\vec{k})\cdot\vec{R}}] \,. \tag{5.3}$$

Using Eq. (5.3) in Eq. (2.15) gives

$$m^0_{kk'} \approx -\frac{J}{2N} \left\{ \frac{f(\epsilon_k) - f(\epsilon_{k'} - W')}{W' + \epsilon_k - \epsilon_{k'}} \; \frac{f(\epsilon_k) - f(\epsilon_{k'} + W')}{\epsilon_k - \epsilon_{k'} - W'} \right\} \times [S(S+1) + \langle \vec{S}_0 \cdot \vec{S}_1 \rangle e^{i(\vec{k}'-\vec{k})\cdot\vec{R}}] \tag{5.4}$$

and

$$p_W(r) \approx -\frac{J}{N} P_{\pm}(r) S(S+1) - \frac{J}{N} P_{\pm}(|\vec{r} - \vec{R}|) \langle \vec{S}_0 \cdot \vec{S}_1 \rangle \,, \tag{5.5}$$

where

$$P_{\pm}(x) = \tfrac{1}{2} \sum_{kk'} \left\{ \frac{f(\epsilon_k) - f(\epsilon_{k'} - W')}{\epsilon_k - \epsilon_{k'} + W'} + \frac{f(\epsilon_k) - f(\epsilon_{k'} + W')}{\epsilon_k - \epsilon_{k'} - W'} \right\} e^{i(\vec{k}-\vec{k}')\cdot\vec{x}} \,. \tag{5.6}$$

Since $W' \ll \epsilon_F$, we may approximate Eqs. (5.4) and (5.5) by

$$m^0_{kk'} \approx -\frac{J}{N} \frac{f(\epsilon_k) - f(\epsilon_{k'})}{\epsilon_k - \epsilon_{k'}} \{S(S+1) + \langle \vec{S}_0 \cdot \vec{S}_1 \rangle e^{i(\vec{k}'-\vec{k})\cdot\vec{R}}\} \,. \tag{5.7}$$

Thus

$$p(r) \approx -\frac{J}{N} P(r) S(S+1) - \frac{J}{N} P(|\vec{r} - \vec{R}|) \langle \vec{S}_0 \cdot \vec{S}_1 \rangle \,, \tag{5.8}$$

where

$$P(x) = \sum_{kk'} \frac{f(\epsilon_k) - f(\epsilon_{k'})}{\epsilon_k - \epsilon_{k'}} e^{i(\vec{k}-\vec{k}')\cdot\vec{x}} \tag{5.9}$$

is the oscillatory part of the RKKY potential. Equations (5.5) and (5.8) thus show how the con-

duction-electron-spin polarization is modified by the RKKY interactions in the high-temperature or large-W limit.

B. RKKY Energy between Impurities

The indirect exchange interaction between two impurity spins can be obtained by isolating the $\langle \vec{S}_0 \cdot \vec{S}_1 \rangle$ part of the energy given by

$$\langle \mathcal{H}' \rangle = -\frac{J}{2N} \sum_{kk'} \{ \langle \vec{\sigma}_{\alpha\beta} \cdot \vec{S}_0 c^\dagger_{k\alpha} c_{k'\beta} \rangle + \langle \vec{\sigma}_{\alpha\beta} \cdot \vec{S}_1 c^\dagger_{k\alpha} c_{k'\beta} \rangle e^{i(\vec{k}-\vec{k}')\cdot\vec{R}} \} . \quad (5.10)$$

Using Eq. (5.7) and the appropriate approximations of Eq. (3.24) in Eq. (5.10) and isolating the $\langle \vec{S}_0 \cdot \vec{S}_1 \rangle$ part, we obtain

$$\langle \mathcal{H} \rangle_{\langle \vec{s}_0 \cdot \vec{s}_1 \rangle} \approx (J^2/N^2) P(R) \langle \vec{S}_0 \cdot \vec{S}_1 \rangle = -E_{RK} \langle \vec{S}_0 \cdot \vec{S}_1 \rangle . \quad (5.11)$$

This expression has been obtained previously by Bresemann and Bailyn[18] and Blackman and Elliott,[21] and is the RKKY energy between the two impurities. Equation (5.11) shows that, starting with the s-d Hamiltonian, we obtain an $\langle \vec{S}_0 \cdot \vec{S}_1 \rangle$ term in energy representing the RKKY interaction. Had we introduced such a term in the original Hamiltonian, we would get this term once more from the conduction-electron polarization. This basically exhibits the mathematical inconsistency of our method when we let $W(R)$ be the RKKY interaction.[25] However, it is physically plausible to examine the case where $W = E_{RK}$. Then from Eq. (3.5) we obtain

$$W'^2 = \tfrac{2}{3} E_{RK} \{ E_{RK} [S(S+1) + \langle \vec{S}_0 \cdot \vec{S}_1 \rangle] + E' \} , \quad (5.12)$$

where

$$E' = \frac{J}{2N} \sum_{kk'} m^0_{kk'} e^{i(\vec{k}-\vec{k}')\cdot\vec{R}} = \tfrac{1}{2} \{ E_{RK} S(S+1) + E^0_{RK} \langle \vec{S}_0 \cdot \vec{S}_1 \rangle \} \quad (5.13)$$

and

$$E^0_{RK} = -\frac{J^2}{N^2} \sum_{kk'} \frac{f(\epsilon_k) - f(\epsilon_{k'})}{\epsilon_k - \epsilon_{k'}} . \quad (5.14)$$

Substituting Eq. (5.13) into (5.12) gives

$$W'^2 = E^2_{RK} S(S+1) + \tfrac{2}{3} \langle \vec{S}_0 \cdot \vec{S}_1 \rangle E_{RK} \{ E_{RK} + \tfrac{1}{2} E^0_{RK} \} . \quad (5.15)$$

This expression of W' will be useful in discussing qualitatively the variation of the effective Kondo temperature in the presence of the RKKY interaction. Note that when the impurities are widely separated and $\langle \vec{S}_0 \cdot \vec{S}_1 \rangle \ll S(S+1)$, we may approximate W' by

$$W' \approx |E_{RK}| [S(S+1)]^{1/2} . \quad (5.16)$$

C. Variation of Effective Kondo Temperature

For a single-impurity system, the Kondo temperature T^0_K is given in Eq. (4.13), where T^0_K is obtained by setting $1 + (|J|\rho/N) \ln T/D = 0$. In our case $\ln|T/D|$ becomes replaced by $\frac{1}{2} \ln|(T^2 + W'^2)/D^2|$. This suggests that in the presence of an interaction W, we define an effective Kondo temperature T^E_K by the relation

$$1 + \frac{|J|\rho}{2N} \ln \left| \frac{(T^E_K)^2 + W'^2}{D^2} \right| = 0 . \quad (5.17)$$

Solving for T^E_K gives

$$T^E_K = T^0_K [1 - (W'/T^0_K)^2]^{1/2} . \quad (5.18)$$

We give Eq. (5.18) the following physical interpretation. For $|W'| > T^0_K$, T^E_K becomes imaginary. This shows that for large effective impurity-impurity interaction $|W'| < T^0_K$, there is no real effective Kondo temperature; i.e., the Kondo spin compensation is mostly suppressed by the impurity-impurity interaction. For $|W'| < T^0_K$, the effective Kondo temperature decreases as W' increases; hence the impurity-impurity interaction tends to inhibit the formation of the spin-compensated d state.

Now we can compare our result with previous random-molecular-field calculation on the many-impurity system. In an effective-field calculation like the one made by Harrison and Klein,[14] it was found that

$$\ln T \to \tfrac{1}{2} \ln(T^2 + H^2) ,$$

where H is the effective internal field, whereas in our calculation we find that

$$\ln T \to \tfrac{1}{2} \ln(T^2 + W'^2) .$$

There are thus some important difference between the two. The major difference is that the effective internal field H depends on $\langle \vec{S}_n \rangle$ and vanishes at high temperatures, whereas W'^2 depends on $\langle \vec{S}_n \cdot \vec{S}_{n'} \rangle$, and also has a temperature-independent part at high temperatures when W is independent of temperature. Thus in our case there is a possible modification of the effective Kondo temperature even at very high temperatures.

Under the conditions given in Eqs. (5.16) and (5.18), the effective Kondo temperature becomes

$$T^E_K \approx T^0_K [1 - (E_{RK}/T^0_K)^2]^{1/2} \quad (5.19)$$

when the impurity spins interact via the RKKY interaction. We may generalize Eq. (5.19) to a system of finite concentration of impurity spins by assuming E_{RK} to be a concentration-dependent random variable. Thus one expects that at higher concentrations the logarithmic variation of Kondo-like effect will be suppressed. Such a detailed examination will be given elsewhere.

Note added in proof. Throughout this paper it is assumed that the impurity concentration is sufficiently low and the impurity-impurity interaction is sufficiently weak that the single-impurity treatment is still a good starting approximation to the problem. Thus, the thermal averages of $\vec{S}^2_i$ are replaced by $S(S+1)$. This assumes that on the average, only a weak coupling exists between the impurities. This physical approximation distinguishes our approach from that of K. Matho and M. T. Béal-Monod [Phys. Rev. B 5, 1899 (1972)] who put the treatment of the two impurities on equal footing.

APPENDIX A: EQUATION OF MOTION OF $U_{kk'}$

In this appendix, we decouple the Green's functions entering in the equation of motion of $U_{kk'}$. From Eq. (2.12) we have

$$(\omega-\epsilon_{k'})U_{kk'}=\frac{\delta_{kk'}}{4\pi}\,i\langle\vec{\sigma}_{\alpha\alpha}\cdot(\vec{S}_0\times\vec{S}_1)\rangle-\frac{iJ}{4N}\sum_{p'}\langle\vec{\sigma}_{\alpha\beta}\cdot(\vec{S}_0\times\vec{S}_1)(\vec{S}_0+\vec{S}_1\,e^{i(\vec{k}'-\vec{p}')\cdot\vec{R}})\cdot\vec{\sigma}_{\beta\delta}c_{p'\delta}\,|\,c^\dagger_{k\alpha}\rangle$$

$$-\frac{J}{4N}\sum_{pp'}\langle(\vec{\sigma}_{\gamma\delta}\times\vec{S}_0)\cdot(\vec{\sigma}_{\alpha\beta}\times\vec{S}_1)\,c^\dagger_{p\gamma}c_{p'\delta}c_{k'\beta}\,|\,c^\dagger_{k\alpha}\rangle+\frac{J}{4N}\sum_{pp'}\langle(\vec{\sigma}_{\alpha\beta}\times\vec{S}_0)\cdot(\vec{\sigma}_{\gamma\delta}\times\vec{S}_1)c^\dagger_{p\gamma}c_{p'\delta}c_{k'\beta}\,|\,c^\dagger_{k\alpha}\rangle\,e^{i(\vec{p}-\vec{p}')\cdot\vec{R}}$$

$$+\tfrac{1}{2}W\langle[(\vec{S}_0\times\vec{S}_1)\cdot(\vec{\sigma}_{\alpha\beta}\times\vec{S}_1)+(\vec{\sigma}_{\alpha\beta}\times\vec{S}_0)\cdot(\vec{S}_0\times\vec{S}_1)]\,c_{k'\beta}\,|\,c^\dagger_{k\alpha}\rangle\,. \quad \text{(A1)}$$

We denote the first, second, third, fourth, fifth, and sixth terms on the right-hand side of Eq. (A1) by U_1, U_2, U_3, U_4, U_5, and U_6, respectively.

Then

$$U_1=\langle\vec{\sigma}_{\alpha\alpha}\cdot(\vec{S}_0\times\vec{S}_1)\rangle=0\,. \quad \text{(A2)}$$

After summing over the index β we obtain

$$U_2=-\frac{J}{4N}\sum_{p'}\langle(\vec{S}_0\cdot\vec{S}_1)\,c_{p'\alpha}\,|\,c^\dagger_{k\alpha}\rangle(1-e^{i(\vec{k}'-\vec{p})\cdot\vec{R}})+\frac{J}{4N}\sum_{p'}\langle[(\vec{S}_0\cdot\vec{S}_0)(\vec{\sigma}_{\alpha\delta}\cdot\vec{S}_1)-(\vec{S}_0\cdot\vec{S}_1)(\vec{\sigma}_{\alpha\delta}\cdot\vec{S}_0)]\,c_{p'\delta}\,|\,c^\dagger_{k\alpha}\rangle$$

$$-\frac{J}{4N}\sum_{p'}\langle[(\vec{S}_1\cdot\vec{S}_1)(\vec{\sigma}_{\alpha\delta}\cdot\vec{S}_0)-(\vec{S}_0\cdot\vec{S}_1)(\vec{\sigma}_{\alpha\delta}\cdot\vec{S}_1)]\,c_{p'\delta}\,|\,c^\dagger_{k\alpha}\rangle\,e^{i(\vec{k}'-\vec{p}')\cdot\vec{R}}\,. \quad \text{(A3)}$$

In obtaining Eq. (A3), we have used the following identities:

$$\sum_\beta(\vec{\sigma}_{\alpha\beta}\cdot\vec{S}_A)(\vec{\sigma}_{\beta\delta}\cdot\vec{S}_B)=\delta_{\alpha\delta}\vec{S}_A\cdot\vec{S}_B+i\vec{\sigma}_{\alpha\delta}\cdot\vec{S}_A\times\vec{S}_B\,, \quad \text{(A4a)}$$

$$(\vec{A}\times\vec{B})\cdot(\vec{C}\times\vec{D})=(\vec{A}\cdot\vec{C})(\vec{B}\cdot\vec{D})-(\vec{B}\cdot\vec{C})(\vec{A}\cdot\vec{D})\,, \quad \text{(A4b)}$$

We may decouple the first, second, and third terms on the right-hand side of Eq. (A3) as follows. Let $U_2\equiv U_2^1+U_2^2+U_2^3$; then

$$U_2^1=-\frac{J}{2N}\langle\vec{S}_0\cdot\vec{S}_1\rangle G_k+\frac{J}{2N}\langle\vec{S}_0\cdot\vec{S}_1\rangle e^{i\vec{k}'\cdot\vec{R}}G_k^R\,, \quad \text{(A5)}$$

$$U_2^2=\frac{J}{4N}\sum_{p'}\sum_{i,j}\langle(S_0^iS_0^i\sigma^j_{\alpha\delta}S_1^j-S_0^iS_1^i\sigma^j_{\alpha\delta}S_0^j)c_{p'\delta}\,|\,c^\dagger_{k\alpha}\rangle$$

$$=\frac{J}{4N}\sum_{p'}\sum_{i\neq j}\langle(S_0^iS_0^i\sigma^j_{\alpha\delta}S_1^j-S_0^iS_1^i\sigma^j_{\alpha\delta}S_0^j)c_{p'\delta}\,|\,c^\dagger_{k\alpha}\rangle\,, \quad \text{(A6)}$$

where $i,j=x,y,z$. The second part of Eqs. (A6) was obtained by noting that for $i=j$, $U_2^2=0$. When $i\neq j$ we obtain

$$\sum_{i\neq j}\langle S_0^iS_0^i\sigma^j_{\alpha\delta}S_1^jc_{p'\delta}\,|\,c^\dagger_{k\alpha}\rangle=\tfrac{2}{3}\langle\vec{S}_0\cdot\vec{S}_0\rangle\langle\vec{\sigma}_{\alpha\delta}\cdot\vec{S}_1c_{p'\delta}\,|\,c^\dagger_{k\alpha}\rangle \quad \text{(A7a)}$$

and

$$\sum_{i\neq j}\langle S_0^iS_1^i\sigma^j_{\alpha\delta}S_0^jc_{p'\delta}\,|\,c^\dagger_{k\alpha}\rangle=\tfrac{2}{3}\langle\vec{S}_0\cdot\vec{S}_1\rangle\langle\vec{\sigma}_{\alpha\delta}\cdot\vec{S}_0c_{p'\delta}\,|\,c^\dagger_{k\alpha}\rangle. \quad \text{(A7b)}$$

Equations (A7a) and (A7b) are the only two surviving terms of U_2^2; the others vanish because for $i\neq j$; $\langle S_0^iS_0^j\rangle=0$, $\langle\sigma^i_{\alpha\delta}S_0^jc_{p'\delta}\,|\,c^\dagger_{k\alpha}\rangle=0$, and $\langle\vec{S}_i\rangle=0$. Combining Eqs. (A7a) and (A7b) gives

$$U_2^2=\frac{J}{3N}[\langle\vec{S}_0\cdot\vec{S}_0\rangle\Gamma_k^1-\langle\vec{S}_0\cdot\vec{S}_1\rangle\Gamma_k^0]\,. \quad \text{(A8)}$$

Similarly, we have

$$U_2^3=-\frac{J}{3N}[\langle\vec{S}_1\cdot\vec{S}_1\rangle\Gamma_k^{0R}-\langle\vec{S}_0\cdot\vec{S}_1\rangle\Gamma_k^{1R}]\,e^{i\vec{k}'\cdot\vec{R}}\,. \quad \text{(A9)}$$

Using Eqs. (A5), (A8), and (A9) in Eq. (A3) gives

$$U_2=-\frac{J}{2N}\langle\vec{S}_0\cdot\vec{S}_1\rangle[G_k-G_k^Re^{i\vec{k}'\cdot\vec{R}}]$$

$$+\frac{J}{3N}S(S+1)[\Gamma_k^1-\Gamma_k^{0R}e^{i\vec{k}'\cdot\vec{R}}]$$

$$+\frac{J}{3N}\langle\vec{S}_0\cdot\vec{S}_1\rangle[\Gamma_k^{1R}e^{i\vec{k}'\cdot\vec{R}}-\Gamma_k^0]\,, \quad \text{(A10)}$$

where $\langle\vec{S}_0\cdot\vec{S}_0\rangle=\langle\vec{S}_1\cdot\vec{S}_1\rangle=S(S+1)$. Using Eq. (A4b) in the expressions for U_5 and U_6 and decoupling gives

$$U_5=\tfrac{2}{3}W[S(S+1)\Gamma^0_{kk'}-\langle\vec{S}_0\cdot\vec{S}_1\rangle\Gamma^1_{kk'}]\,, \quad \text{(A11)}$$

$$U_6=\tfrac{2}{3}W[\langle\vec{S}_0\cdot\vec{S}_1\rangle\Gamma^0_{kk'}-S(S+1)\Gamma^1_{kk'}]\,. \quad \text{(A12)}$$

Combining Eqs. (A11) and (A12) gives

$$U_5+U_6=\tfrac{2}{3}W[S(S+1)+\langle\vec{S}_0\cdot\vec{S}_1\rangle][\Gamma^0_{kk'}-\Gamma^1_{kk'}]\,. \quad \text{(A13)}$$

Next we decouple the four-particle Green's functions U_3 and U_4. We use the method of cumulant expansions, which will be described in detail in what follows. (For a discussion of the cumulant expansion, the reader may refer to Kubo[33] and Brout and Carruthers.[34]) The cumulant expansion of a correlation function which involves six quantum-mechanical operators $\langle x^6\rangle_c$ is given by

$$\langle x^6\rangle_c = \langle x^6\rangle - 6\langle x\rangle\langle x^5\rangle - 15\langle x^2\rangle\langle x^4\rangle - 10\langle x^3\rangle\langle x^3\rangle + 30\langle x\rangle^2\langle x^4\rangle + 120\langle x\rangle\langle x^2\rangle\langle x^3\rangle + 30\langle x^2\rangle^3 - 270\langle x\rangle^2\langle x^2\rangle^2 - 120\langle x\rangle^3\langle x^3\rangle + 360\langle x\rangle^4\langle x^2\rangle - 120\langle x\rangle^6 , \quad \text{(A14)}$$

where $\langle x^n\rangle_c$ and $\langle x^n\rangle$ denote the cumulant and thermal averages of the n-operator correlation function, respectively. Let

$$\langle x^6\rangle = -\langle(\vec{\sigma}_{\gamma\delta}\times\vec{S}_0)\cdot(\vec{\sigma}_{\alpha\beta}\times\vec{S}_1)c^\dagger_{p'\gamma}c_{p'\delta}c_{k'\beta}\,|\,c^\dagger_{k\alpha}\rangle . \quad \text{(A15)}$$

We assume that the cumulant average of the six-operator Green's function U_3 vanishes; thus

$$\langle x^6\rangle = 15\langle x^2\rangle\langle x^4\rangle + 10\langle x^3\rangle\langle x^3\rangle - 2\times 15\langle x^2\rangle^3 . \quad \text{(A16)}$$

Equation (A16) is obtained by letting the right-hand side of Eq. (A14) be zero. Note that all the terms which contain $\langle x\rangle$ have been omitted, since $\langle x\rangle = 0$, where $\langle x\rangle$ is any one of the operators $x_1 = S_0$, $x_2 = S_1$, $x_3 = c^\dagger_{p'\gamma}$, $x_4 = c_{p'\delta}$, $x_5 = c_{k'\beta}$, and $x_6 = c_{k\alpha}$. The numbers 15 and 10 in Eq. (A16) represent the possible ways to factor the decoupled terms, while 2 is a coefficient arising from the expansion. Using Eq. (A16), the nonvanishing terms in our expansion are

$$\langle x^6\rangle = \langle x_1x_2x_3x_4x_5x_6\rangle = [\langle x_1x_2\rangle\langle x_3x_4x_5x_6\rangle + \langle x_3x_5\rangle\langle x_1x_2x_4x_6\rangle + \langle x_4x_6\rangle\langle x_1x_2x_3x_5\rangle] + [\langle x_1x_3x_4\rangle\langle x_2x_5x_6\rangle + \langle x_2x_3x_4\rangle\langle x_1x_5x_6\rangle + \langle x_1x_3x_5\rangle\langle x_2x_4x_6\rangle + \langle x_2x_3x_5\rangle\langle x_1x_4x_6\rangle] - 2\langle x_1x_2\rangle\langle x_3x_5\rangle\langle x_4x_6\rangle . \quad \text{(A17)}$$

As seen from Eq. (A17) only 3 of the 15 $\langle x^2\rangle\langle x^4\rangle$ terms, and 4 of the 10 $\langle x^3\rangle\langle x^3\rangle$ terms, and 1 of the 15 $\langle x^2\rangle^3$ terms survive. Equation (A17) is subject to a certain constraint; for example,

$$\langle x_1x_2\rangle = \langle S^i_0S^j_1\rangle\delta_{ij} = \langle\vec{S}_0\cdot\vec{S}_1\rangle , \quad \text{(A17a)}$$

$$\langle x_3x_5\rangle = \langle c^\dagger_{p\gamma}c_{k'\beta}\rangle\delta_{\gamma\beta} = 2n_{pk'} , \quad \text{(A17b)}$$

$$\langle x_4x_6\rangle = \langle c_{p'\delta}\,|\,c^\dagger_{k\alpha}\rangle\delta_{\alpha\delta} = 2G_{kp'} , \quad \text{(A17c)}$$

$$\langle x_1x_3x_4\rangle = \langle S^+_0c^\dagger_{p'\uparrow}c_{p'\downarrow}\rangle = \tfrac{1}{3}m^0_{pp'} , \quad \text{(A17d)}$$

$$\langle x_2x_5x_6\rangle = \langle S^-_1c_{k'\downarrow}\,|\,c^\dagger_{k\uparrow}\rangle = \tfrac{2}{3}\Gamma^1_{kk'} , \quad \text{(A17e)}$$

etc. Using the conditions in (A17a)–(A17e), etc., we have

$$\langle x_1x_2\rangle\langle x_3x_4x_5x_6\rangle = -\tfrac{2}{3}\langle\vec{S}_0\cdot\vec{S}_1\rangle\langle\vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{\gamma\delta}c^\dagger_{p\gamma}c_{p'\delta}c_{k'\beta}\,|\,c^\dagger_{k\alpha}\rangle , \quad \text{(A18)}$$

$$\langle x_3x_5\rangle\langle x_1x_2x_4x_6\rangle = 2n_{pk'}\langle\vec{S}_0\cdot\vec{S}_1\,c_{p'\alpha}\,|\,c^\dagger_{k\alpha}\rangle - 2n_{pk'}U_{kp'} , \quad \text{(A19)}$$

$$\langle x_4x_6\rangle\langle x_1x_2x_3x_5\rangle = 2\langle\vec{S}_0\cdot\vec{S}_1c^\dagger_{p\gamma}c_{k'\gamma}\rangle G_{kp'} + \tilde{u}_{kp'} , \quad \text{(A20)}$$

$$-2\langle x_1x_2\rangle\langle x_3x_5\rangle\langle x_4x_6\rangle = -8\langle\vec{S}_0\cdot\vec{S}_1\rangle n_{pk'}G_{kp'} , \quad \text{(A21)}$$

$$\langle x_1x_3x_4\rangle\langle x_2x_5x_6\rangle = \tfrac{2}{3}[m^0_{pp'}\Gamma^1_{kk'} - m^0_{pp'}\Gamma^1_{kk'}] = 0 , \quad \text{(A22)}$$

$$\langle x_2x_3x_4\rangle\langle x_1x_5x_6\rangle = \tfrac{4}{3}m^1_{pp'}\Gamma^0_{kk'} , \quad \text{(A23)}$$

$$\langle x_1x_3x_5\rangle\langle x_2x_4x_6\rangle = -\tfrac{4}{3}m^0_{pk'}\Gamma^1_{kp'} , \quad \text{(A24)}$$

$$\langle x_2x_3x_5\rangle\langle x_1x_4x_6\rangle = -\tfrac{4}{3}m^1_{pk'}\Gamma^0_{kp'} . \quad \text{(A25)}$$

To express Eq. (A1) in terms of n, G, m, Γ, and $\tilde{u}$, U, we further decouple Eq. (A18) and the first terms of (A19) and (A20) to give

$$\langle\vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{\gamma\delta}\,c^\dagger_{p\gamma}c_{p'\delta}c_{k'\beta}\,|\,c^\dagger_{k\alpha}\rangle = -6n_{pk'}G_{kp'} , \quad \text{(A26)}$$

$$\langle\vec{S}_0\cdot\vec{S}_1\,c_{p'\alpha}\,|\,c^\dagger_{k\alpha}\rangle = 2\langle\vec{S}_0\cdot\vec{S}_1\rangle G_{kp'} . \quad \text{(A27)}$$

Summing Eqs. (A18)–(A25) using Eqs. (A26) and (A27) gives

$$U_3 = \frac{J}{N}\langle\vec{S}_0\cdot\vec{S}_1\rangle n_{k'}G_k + \frac{J}{4N}\tilde{u}_{k'}G_k - \frac{J}{2N}n_{k'}U_k - \frac{J}{3N}m^0_{k'}\Gamma^1_k - \frac{J}{3N}m^1_{k'}\Gamma^0_k + \frac{J}{3N}\sum_{pp'}m^1_{pp'}\Gamma^0_{kk'} . \quad \text{(A28)}$$

Similarly

$$U_4 = -\frac{J}{N}\langle\vec{S}_0\cdot\vec{S}_1\rangle n^R_{k'}G^R_k + \frac{J}{4N}\tilde{u}^R_{k'}G^R_k - \frac{J}{2N}n^R_{k'}U^R_k + \frac{J}{3N}m^{1R}_{k'}\Gamma^{0R}_k e^{i\vec{k}'\cdot\vec{R}} + \frac{J}{3N}m^{0R}_{k'}\Gamma^{1R}_k e^{i\vec{k}'\cdot\vec{R}} - \frac{J}{3N}\sum_{pp'}m^0_{pp'}e^{i(\vec{p}-\vec{p}')\cdot\vec{R}}\Gamma^1_{kk'} . \quad \text{(A29)}$$

Let

$$E' = \frac{J}{2N}\sum_{pp'}m^1_{pp'} = \frac{J}{2N}\sum_{pp'}m^0_{pp'}e^{i(\vec{p}-\vec{p}')\cdot\vec{R}} . \quad \text{(A30)}$$

Substituting Eqs. (A2), (A10), (A13), (A28), and (A29) into Eq. (A1) gives Eq. (2.25).

APPENDIX B: EVALUATION OF U_k AND U^R_k

In this appendix we evaluate the Green's function U_k by summing Eq. (2.25) over k'. This appendix clearly shows that all correlation functions, which without the interaction W would be dependent upon ω, become now dependent on $\omega \pm W'$. Summing Eq. (2.25) over k' gives

$$U_k = J\langle\vec{S}_0\cdot\vec{S}_1\rangle[G(\omega)G_k - G^R(\omega)G^R_k] + \tfrac{1}{3}J[\Gamma^R(\omega)\Gamma^{0R}_k - \Gamma(\omega)\Gamma^1_k] - \tfrac{1}{2}J[g(\omega)U_k + g^R(\omega)U^R_k]$$

$$-\tfrac{1}{3}J[\tilde{\Gamma}(\omega)\Gamma_k^0-\tilde{\Gamma}^R(\omega)\Gamma_k^{1R}]+\tfrac{1}{4}J[\tilde{U}(\omega)G_k+\tilde{U}^R(\omega)G_k^R]+\frac{W'^2}{W}\sum_k[\Gamma_{kk'}^0-\Gamma_{kk'}^1](\omega-\epsilon_{k'})^{-1}\,, \quad \text{(B1)}$$

where

$$G^R(x)=N^{-1}\sum_k[n_k^R-\tfrac{1}{2}e^{i\vec{k}\cdot\vec{R}}](x-\epsilon_k)^{-1}\,, \quad \text{(B2a)}$$

$$g(x)=G(x)+\tfrac{1}{2}F(x)\,,\quad g^R(x)=G^R(x)+\tfrac{1}{2}F^R(x)\,, \quad \text{(B2b)}$$

$$\Gamma^R(x)=N^{-1}\sum_k[m_k-S(S+1)]\,e^{i\vec{k}\cdot\vec{R}}(x-\epsilon_k)^{-1}\,, \quad \text{(B2c)}$$

$$\tilde{U}(x)=N^{-1}\sum_k\tilde{u}_k(x-\epsilon_k)^{-1}\,,\quad \tilde{U}^R(x)=N^{-1}\sum_k\tilde{u}^R(x-\epsilon_k)^{-1}\,, \quad \text{(B2d)}$$

$$\tilde{\Gamma}(x)=N^{-1}\sum_k[m_k^1+\langle\vec{S}_0\cdot\vec{S}_1\rangle](x-\epsilon_k)^{-1}\,,\quad \tilde{\Gamma}^R(x)=N^{-1}\sum_k[m_k^1+\langle\vec{S}_0\cdot\vec{S}_1\rangle]\frac{e^{i\vec{k}\cdot\vec{R}}}{x-\epsilon_k}\,. \quad \text{(B2e)}$$

It is useful to point out here that for nonzero W' in Eq. (B1), only the terms $g(\omega)$ and $g^R(\omega)$ diverge logarithmically in the limit as $T\to 0$. We will, however, find that when the values of $\Gamma_{kk'}^0$ given in Eq. (3.8) are substituted into Eq. (B1), all the terms which go like $g(\omega)$ or $g^R(\omega)$ cancel out. Thus we will be left only with terms which depend on $\omega\pm W'$.

We evaluate the quantity $\sum_{k'}(\omega-\epsilon_{k'})^{-1}\Gamma_{kk'}^0$ in Eq. (B1). Using Eq. (3.3), we obtain

$$\sum_{k'}\Gamma_{kk'}^0(\omega-\epsilon_{k'})^{-1}=\frac{J}{N}\sum_{k'}[(\omega-\epsilon_{k'})^2-W'^2]^{-1}\{\tfrac{1}{2}[m_{k'}-S(S+1)]\,G_k-[n_{k'}-\tfrac{1}{2}]\,\Gamma_k^0-\tfrac{1}{2}\langle\vec{S}_0\cdot\vec{S}_1\rangle\,e^{i\vec{k}'\cdot\vec{R}}\,G_k^R-\tfrac{1}{2}e^{i\vec{k}'\cdot\vec{R}}U_k^R\}$$
$$+\sum_{k'}\sum_i\mathcal{F}_k^i(\epsilon_{k'})\,(\omega-\epsilon_{k'})^{-1}[(\omega-\epsilon_{k'})^2-W'^2]^{-1}\,. \quad \text{(B3)}$$

Substituting Eq. (3.11b) and the relationship

$$(\omega-\epsilon_{k'})^{-1}[(\omega-\epsilon_{k'})^2-W'^2]^{-1}=\frac{1}{2W'^2}[(\omega-\epsilon_{k'}-W')^{-1}+(\omega-\epsilon_{k'}+W')^{-1}-2(\omega-\epsilon_{k'})^{-1}] \quad \text{(B4)}$$

into the right-hand side of Eq. (B3) and summing over k' gives

$$\begin{aligned}\sum_{k'}\Gamma_{kk'}^0(\omega-\epsilon_{k'})^{-1}=\frac{J}{W'}\{&\tfrac{1}{4}[\Gamma(\omega-W')-\Gamma(\omega+W')]\,G_k-\tfrac{1}{2}[G(\omega-W')-G(\omega+W')]\,\Gamma_k^0\\&-\tfrac{1}{4}[F^R(\omega-W')-F^R(\omega+W')][\langle\vec{S}_0\cdot\vec{S}_1\rangle\,G_k^R+U_k^R]\}\\&+\frac{JW}{W'^2}\{\langle\vec{S}_0\cdot\vec{S}_1\rangle[G(\omega\pm W')-G(\omega)]\,G_k-\langle\vec{S}_0\cdot\vec{S}_1\rangle[G^R(\omega\pm W')-G^R(\omega)]\,G_k^R\\&+\tfrac{1}{3}[\Gamma^R(\omega\pm W')-\Gamma^R(\omega)]\,\Gamma_k^{0R}-\tfrac{1}{3}[\Gamma(\omega\pm W')-\Gamma(\omega)]\,\Gamma_k^1-\tfrac{1}{2}[g(\omega\pm W')-g(\omega)]\,U_k\\&-\tfrac{1}{2}[g^R(\omega\pm W')-g^R(\omega)]G_k^R+\tfrac{1}{4}[\tilde{u}(\omega\pm W')+\tilde{u}(\omega)]\,G_k+\tfrac{1}{4}[\tilde{u}^R(\omega\pm W')-\tilde{u}^R(\omega)]\,G_k^R\\&-\tfrac{1}{3}[\tilde{\Gamma}(\omega\pm W')-\tilde{\Gamma}(\omega)]\,\Gamma_k^0+\tfrac{1}{3}[\tilde{\Gamma}^R(\omega\pm W')-\tilde{\Gamma}^R(\omega)]\,\Gamma_k^{1R}\}\\&-\tfrac{1}{2}\sum_{k'}\Gamma_{kk'}^1[(\omega-\epsilon_{k'}+W')^{-1}+(\omega-\epsilon_{k'}-W')^{-1}-2(\omega-\epsilon_{k'})^{-1}]\,. \quad \text{(B5)}\end{aligned}$$

Note that all the terms which have a coefficient J/W' in Eq. (B5) vanish as $\omega\to 0$ from the expression given in Eq. (3.12). Substituting Eq. (B5) into Eq. (B1) gives

$$\begin{aligned}U_k=&J\langle\vec{S}_0\cdot\vec{S}_1\rangle[G(\omega\pm W')G_k-G_k^R(\omega\pm W')G_k^R]+\tfrac{1}{3}J[\Gamma^R(\omega\pm W')\Gamma_k^{0R}-\Gamma(\omega\pm W')\Gamma_k^1]\\&-\tfrac{1}{3}J[\tilde{\Gamma}(\omega\pm W')\Gamma_k^0-\tilde{\Gamma}^R(\omega\pm W')\Gamma_k^{1R}]-\tfrac{1}{2}J[g(\omega\pm W')U_k+g^R(\omega\pm W')U_k^R]\\&+\tfrac{1}{4}J[\tilde{u}(\omega\pm W')G_k+\tilde{u}^R(\omega\pm W')G_k^R]-\frac{W'^2}{W}\sum_{k'}\Gamma_{kk'}^1(\omega-\epsilon_{k'}\pm W')^{-1}\,. \quad \text{(B6)}\end{aligned}$$

The modified equation of motion of U_k^R can be evaluated in a similar fashion. We have

$$\begin{aligned}U_k^R=&J\langle\vec{S}_0\cdot\vec{S}_1\rangle[G^R(\omega\pm W')G_k-G(\omega\pm W')G_k^R]+\tfrac{1}{3}J[\Gamma(\omega\pm W')\Gamma_k^{0R}-\Gamma^R(\omega\pm W')\Gamma_k^1]\\&-\tfrac{1}{3}J[\tilde{\Gamma}^R(\omega\pm W')\Gamma_k^0-\tilde{\Gamma}(\omega\pm W')\Gamma_k^{1R}]-\tfrac{1}{2}J[g^R(\omega\pm W')U_k+g(\omega\pm W')U_k^R]\\&-\tfrac{1}{4}J[\tilde{u}^R(\omega\pm W')G_k+\tilde{u}(\omega\pm W')G_k^R]-\frac{W'^2}{W}\sum_{k'}\frac{\Gamma_{kk'}^1e^{-i\vec{k}'\cdot\vec{R}}}{\omega-\epsilon_{k'}\pm W'}\,. \quad \text{(B7)}\end{aligned}$$

It can further be shown that the last expressions on the right-hand side of Eqs. (B6) and (B7) are of higher orders and have no logarithmic divergency, and hence can be neglected.

Next, we examine the contributions of U_k^R and $U_k e^{+i\vec{k}\cdot\vec{R}}$ to $\Gamma_{kk'}^0$ and $\Gamma_{kk'}^1 e^{i(\vec{k}-\vec{k}')\cdot\vec{R}}$. The leading logarithmically divergent terms in Eqs. (B6) and (B7) are

$$\mathrm{Re}g(0\pm W') = \mathrm{Re}G(0\pm W') = -\frac{\rho}{2N}\ln\left(\frac{T^2+W'^2}{D^2}\right) \tag{B8}$$

and

$$\mathrm{Re}g^R(0\pm W') = \mathrm{Re}G(0\pm W') = -\frac{\rho}{2N}\frac{\sin k_F R}{k_F R}\ln\left(\frac{T^2+W'^2}{D^2}\right), \tag{B9}$$

where Re denotes the real part, and Eq. (B9) has been discussed by Gavan and Doman[36] for $1 \ll k_F R \ll 2\epsilon_F/\pi T$. Using Eqs. (B8) and (B9) and noting that $e^{\pm i\vec{k}\cdot\vec{R}} = \sin(k_F R)/k_F R$ when averaged over all angles of $\vec{k}\cdot\vec{R}$ near the Fermi surface, we find that the contributions of U_k^R and $U_k e^{+i\vec{k}\cdot\vec{R}}$ to $\Gamma_{kk'}^0$ and $\Gamma_{kk'}^1 e^{i(\vec{k}-\vec{k}')\cdot\vec{R}}$ have the form $[J\rho\sin(k_F R)/Nk_F R]^2$ × (the difference of two logarithmic contributions). This justifies the approximation made by Blackman and Elliott,[21] who neglected the contributions of the transverse Green's functions U_k and U_k^R.

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[25]The results derived in this paper are consistent and valid when $W(R)$ is a direct exchange interaction between magnetic impurities. In this case the mathematical treatment is properly justified, but to postulate such a direct interaction is physically not very reasonable for the magnetic alloy problem. On the other hand, it is physically plausible to assume that $W(R)$ arises from the Ruderman–Kittel interaction (Ref. 26) but then the mathematical consistency of our solutions is not justified. This is a major dilemma in our theory, which we posed but have not resolved in this paper. We suggest that if one worked out the consistent behavior of the s-d interaction using higher-order Green's function, the result would be, qualitatively at least, not very different from what one obtains from the effective Hamiltonian with $W(R)\,\vec{S}_0\cdot\vec{S}_1$ used in this paper. It is therefore of real interest to do a detailed comparison of the results presented in this paper with experiments on dilute alloys. This, however, will be delegated to a future work on the subject.

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