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Kondo Resistivity due to a Pair of Interacting Impurities

M. T. Béal-Monod
Laboratoire de Physique des Solides associé au Centre National de la Recherche Scientifique,
Faculté des Sciences, 91 Orsay, France

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The Kondo-type resistivity due to the scattering of conduction electrons by a pair of interacting magnetic impurities of spin $\frac{1}{2}$ dissolved in a nonmagnetic host is calculated as a function of the distance R between the impurities and their coupling W. The Kondo Hamiltonian is used, and the scattering amplitudes are calculated up to third order in energy. For small W/k_BT and large R, the resistivity of the pair reduces to twice the Kondo resistivity of one isolated impurity; for large W/k_BT and small R, the pair acts practically as one single spin, and gives a Kondo resistivity—corresponding to spin of 1, or (depending on the sign of W), no spin-dependent resistivity at all—corresponding to a spin of 0. For intermediate W, one verifies (taking for W the Rudermann-Kittel-Yosida indirect interaction) that the anomalous Kondo resistivity of two correlated impurities increases less rapidly (for decreasing temperature) than the resistivity of two isolated noninteracting impurities; this is in agreement with experiments. Therefore, it is suggested that this simple procedure may be useful to describe the resistivity of dilute alloys of *Cu*Mn type, when the concentration is not sufficiently small to neglect the correlations between the impurities.

I. INTRODUCTION

EXCEPT in the case of extreme dilution one should not, in principle, avoid taking into account the correlations between impurities when describing the Kondo resistivity of dilute alloys like *Cu*Mn. Within the hypothesis of isolated impurities, the scattering of conduction electrons already is a very difficult problem. The situation becomes worse if one wishes to take into account multiple scatterings by coupled impurities. As a very rough attempt in that direction, we present here a calculation of the resistivity due to scattering of conduction electrons by one pair of interacting impurities within the following assumptions, whose limit of validity will be discussed: We perform the calculation of the scattering amplitudes in perturbation theory up to third order; we adopt the *s-d* exchange model of the Kondo[1] Hamiltonian and suppose a well-behaved spin for each impurity which, for the sake of simplicity, we take to be $\frac{1}{2}$; we assume the conduction electrons to be free and the two spins $\mathbf{S}_1$ and $\mathbf{S}_2$ coupled by an interaction W which we will discuss. Our purpose is to obtain information about how the anomalous Kondo behavior $\ln T$ is modified when correlations between impurities cannot be neglected. Experimentally,[2] indeed, the absolute slope of the $\ln T$ term decreases when the impurity concentration increases, i.e., when the correlations become more and more important. It is also interesting to see how this pair resistivity changes from a small-coupling regime (the two impurities very far apart, high temperature) to the large-coupling one (impurities first neighbors, low temperature). The first case is accounted for without any trouble by perturbation theory. As for the second case, one can use the physical analogy between the problem of one impurity in the presence of an external magnetic field H, and the present problem of two impurities with no external field, but where each impurity "feels" the field of the other one. For one impurity in an external field H, More and Suhl[3] have shown that perturbation theory is valid not only for $H \ll k_BT$ above the Kondo temperature T_K, but also for $H \gg k_BT$ below T_K, above a certain critical field H_K. By analogy, we hope here to reach, by means of perturbation theory, a reasonable conclusion in the large-coupling case $W \gg k_BT$, as well as in the small-coupling one $W \ll k_BT$. Actually, the magnetoresistivity problem and the present one, though analogous, exhibit some characteristic differences. In particular, we have shown elsewhere[4] that the $\ln T$ behavior of the resistivity of one impurity in the presence of an external field H switches to a $\ln H$ when one goes from the regime $H \ll k_BT$ to $H \gg k_BT$, because the spin is frozen in the strong field H and can no longer flip with respect to the conduction electron; the spread of the Fermi surface then is no longer in k_BT but in H. Here, too, for a large coupling $W \gg k_BT$, each spin is frozen with respect to the other (and the pair then forms a singlet or a triplet, depending on the sign of W), but the pair, as a whole, can still flip with respect to the conduction electron like one single scatterer. Therefore, one expects that, at variance with the magnetoresistivity, a $\ln T$ behavior still remains in the large coupling case, if the pair is in a triplet state ($|\mathbf{I}| = |\mathbf{S}_1 + \mathbf{S}_2| = 2S$). One finds, of course, no spin-dependent resistivity at all, if the pair is in a singlet state ($|\mathbf{I}| = 0$). Between the two above extreme cases ($W \gg k_BT$ or $\ll k_BT$), we obtain a formula for the resistivity of the pair where the distance R appears in oscillating functions of R describing the interferences between the two scatterings on each impurity, and W/k_BT appears in Boltzmann exponentials describing the state of the pair. For each value of R and W/k_BT, one can

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[1] J. Kondo, Progr. Theoret. Phys. (Kyoto) **32**, 37 (1964).

[2] See for example review papers: M. D. Daybell and W. A. Steyert, Rev. Mod. Phys. **40**, 380 (1968); G. J. van den Berg, *Low Temperature Physics* (Plenum Press, Inc., New York, 1965), p. 955.

[3] R. More and H. Suhl, Phys. Rev. Letters, **20**, 500 (1968).

[4] M. T. Beal-Monod and R. A. Weiner, Phys. Rev. **170**, 552 (1968).

then know the coefficient of the Kondo contribution $\ln T$. In an example given at the end, it is shown that, for physical cases, the absolute slope of the $\ln T$ is decreased by the presence of interactions, which is the behavior observed experimentally.

As far as the hypotheses of the present calculation are concerned, we note the following:

(1) The *s-d* exchange model with two well-defined spins is a basic assumption which has been discussed extensively in the literature for the one-impurity problem. We choose it here only for the sake of simplicity, in order to get a simple explicit formula, keeping in mind that one should, in principle, treat the problem starting from the Anderson Hamiltonian, although the calculations would then be more difficult to handle in an explicit way.

(2) The interaction W physically represents the indirect interaction[5] between the impurities via the conduction electrons. Therefore, in principle, we should not have to take it for granted by introducing it from the beginning, but we should get it as well as the scattering amplitudes, self-consistently, from the perturbative series. This would be the rigorous way of studying the problem. It is not simple. To make the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction appear in the resistivity in such a way, would imply examining higher orders than the third one in the perturbative series, and self-consistency would probably imply summing the whole series. Work is in progress in that direction. In the present paper, we will speak in terms of a general W (which may as well be any force coupling the two spins) and only at the end give a brief quantitative discussion of the result one obtains when one replaces W by the effective RKKY interaction.

II. CALCULATION OF THE RESISTIVITY OF THE PAIR

We now calculate the relaxation time entering in the calculation of the resistivity within the above hypothesis. The second-order perturbation calculation of this problem has been studied in detail in "pre-Kondo" papers[6] and we start here in exactly the same framework.

The unperturbed Hamiltonian contains the kinetic energy of the free conduction electrons and the coupling between the two impurities:

$$H_0=p^2/2m-W\mathbf{S}_1\cdot\mathbf{S}_2. \tag{1}$$

The eigenvalues of H_0 are

$$E_0=\hbar^2k^2/2m+W_I,\qquad W_I=\tfrac{1}{2}W[\tfrac{3}{2}-I(I+1)], \tag{2}$$

with

$$\mathbf{I}=\mathbf{S}_1+\mathbf{S}_2,\qquad |\mathbf{I}|=0\text{ or }1. \tag{3}$$

The first impurity $\mathbf{S}_1$ is supposed to be located at the origin and the second one $\mathbf{S}_2$ at the distance $\mathbf{R}$. The conduction electron $\mathbf{s}$ is located at $\mathbf{r}$. The perturbation within the *s-d* exchange model contains two spin-independent parts (one on each impurity) and two spin-dependent ones; for N lattice sites in the metal host

$$H_1=1/N\{V(\mathbf{r})+V(\mathbf{r}-\mathbf{R}) -2J(\mathbf{r})\mathbf{s}\cdot\mathbf{S}_1-2J(\mathbf{r}-\mathbf{R})\mathbf{s}\cdot\mathbf{S}_2\}, \tag{4}$$

which, for convenience, we write as follows:

$$H_1=1/N\{V(\mathbf{r})+V(\mathbf{r}-\mathbf{R}) -\{J(\mathbf{r})+J(\mathbf{r}-\mathbf{R})\}s\cdot(\mathbf{S}_1+\mathbf{S}_2) -\{J(\mathbf{r})-J(\mathbf{r}-\mathbf{R})\}\mathbf{s}\cdot(\mathbf{S}_1-\mathbf{S}_2)\}. \tag{5}$$

The $\mathbf{s}\cdot(\mathbf{S}_1+\mathbf{S}_2)$ part will leave the total spin of the pair unchanged, whereas the part $\mathbf{s}\cdot(\mathbf{S}_1-\mathbf{S}_2)$ will allow transition from $|\mathbf{I}|=0$ to $|\mathbf{I}|=1$ and vice versa. As there is no external magnetic field present, the relaxation times τ_+ and τ_- for spin-up and -down electrons are equal. For the same reason, the thermal average of the z component M of $\mathbf{I}$ is zero, but one will need the Boltzmann probabilities for the pair to be in a singlet ($|\mathbf{I}|=0$) or a triplet ($|\mathbf{I}|=1$) state given, respectively, by

$$p_{|\mathbf{I}|=0}=p_0=1/[1+3\exp(W/k_BT)],\qquad p_{|\mathbf{I}|=1}=p_1=\exp(W/k_BT)/[1+3\exp(W/k_BT)],\qquad p_0+3p_1=1. \tag{6}$$

The spatial matrix elements of H_1 between two plane waves of wave vectors $\mathbf{k}$ and $\mathbf{k}'$ lead to the Fourier transforms of $V(\mathbf{r})$ and $J(\mathbf{r})$, for which we adopt the same simplification used by Kondo,[1] assuming

$$V(\mathbf{k}-\mathbf{k}')\simeq\text{const.}=V,\qquad J(\mathbf{k}-\mathbf{k}')\simeq\text{const.}=J. \tag{7}$$

It then remains to take the matrix elements of the Fourier transform of H_1 which is

$$\bar{H}_1=(1+e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}})\{V-J\mathbf{s}\cdot(\mathbf{S}_1+\mathbf{S}_2)\} -(1-e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}})J\mathbf{s}\cdot(\mathbf{S}_1-\mathbf{S}_2). \tag{8}$$

Reading from right to left (with m, equal to the z component of $\mathbf{s}$, having the values $\pm\frac{1}{2}$; and $M=0,\pm1$), the spin matrix elements $\langle m',I',M'|\bar{H}_1|m,I,m\rangle$ involved in the relaxation times, with selection rules taken into

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[5] M. A. Rudermann and C. Kittel, Phys. Rev., **96**, 99 (1954); T. Kasuya, Progr. Theoret. Phys. (Kyoto), **16**, 45 (1956); K. Yosida, Phys. Rev., **106**, 893 (1957); we will henceforth refer to the indirect Rudermann-Kittel-Kasuya-Yosida interaction as the RKKY interaction.

[6] A. D. Brailsford and A. W. Overhauser, J. Phys. Chem. Solids **15**, 140 (1960); *ibid.*, **21**, 127 (1961); T. Van Peski-Tinbergen and A. J. Dekker, Physica, **29**, 917 (1963); M. T. Beal, Thesis, University of Paris, 1963 (unpublished); J. Phys. Chem. Solids **25**, 543 (1964); M. T. Beal and J. Friedel, Phys. Rev. **135**, A466 (1964).

account, are the following:

$$\begin{aligned}
\langle m,0,0|\bar{H}_1|m,0,0\rangle &= (1+e^{i\mathbf{q}\cdot\mathbf{R}})V, & \epsilon&=0\\
\langle m,1,0|\bar{H}_1|m,0,0\rangle &= -(1-e^{i\mathbf{q}\cdot\mathbf{R}})Jm, & \epsilon&=W\\
\langle m\mp1,\ 1,\ \pm1|\bar{H}_1|m,0,0\rangle &= \pm(1-e^{i\mathbf{q}\cdot\mathbf{R}})J/\sqrt{2}, & \epsilon&=W\\
\langle m,1,M|\bar{H}_1|m,1,M\rangle &= \pm(1+e^{i\mathbf{q}\cdot\mathbf{R}})(V-JmM), & \epsilon&=0\\
\langle m,0,0|\bar{H}_1|m,1,0\rangle &= -(1-e^{i\mathbf{q}\cdot\mathbf{R}})Jm, & \epsilon&=-W\\
\langle m\mp1,\ 1,\ \pm1|\bar{H}_1|m,1,0\rangle &= -(1+e^{i\mathbf{q}\cdot\mathbf{R}})J/\sqrt{2}, & \epsilon&=0\\
\langle m\pm1,\ 1,\ 0|\bar{H}_1|m,1,\ \pm1\rangle &= -(1+e^{i\mathbf{q}\cdot\mathbf{R}})J/\sqrt{2}, & \epsilon&=0\\
\langle m\mp1,\ 0,\ 0|\bar{H}_1|m,\ 1,\mp1\rangle &= \mp(1-e^{i\mathbf{q}\cdot\mathbf{R}})J/\sqrt{2}, & \epsilon&=-W.
\end{aligned}\tag{9}$$

$\mathbf{q}$ is the difference between the wave vectors before and after the transition, and ϵ is the amount of energy absorbed by the conduction electron in each process: It will appear in differences between the energies of the initial and intermediate states of the set {conduction electron+pair}, and in the modification of the transport equations.[6] The calculation of the relaxation time $\tau_+=\tau_-=\tau$ is straightforward, and may be performed as it has been elsewhere,[1,4] taking into account the remark we emphasized in Sec. II.A of Ref. 4. One finds

$$\frac{1}{\tau}=\frac{km\Omega}{2\pi\hbar^3N^2}\int_0^\pi(1-\cos\theta)\,\sin\theta d\theta\frac{1}{4\pi}\int d\Omega_{\mathbf{R}}$$
$$\times\left[aV^2+3bp_0\tfrac{1}{4}J^2\frac{1}{1-f_{\mathbf{k}}(1-e^{-W/k_BT})}+\tfrac{3}{2}J^2ap_1+\tfrac{3}{4}J^2bp_1\frac{1}{1-f_{\mathbf{k}}(1-e^{W/k_BT})}+Z\right],\tag{10}$$

$$Z=\tfrac{3}{4}J^2V(p_0-p_1)\sum_{\mathbf{q}}\left[\left\{\frac{-f_{\mathbf{q}}}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{q}}+W}+\frac{f_{\mathbf{q}}}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{q}}-W}\right\}\{2a-a_1\}\right]$$
$$+\tfrac{3}{4}J^3p_0\sum_{\mathbf{q}}\left[\frac{-f_{\mathbf{q}}}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{q}}+W}\{2b+b_1\}-\frac{f_{\mathbf{q}}}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{q}}}\{2b-b_1\}\right]\frac{1}{1-f_{\mathbf{k}}(1-e^{-W/k_BT})}$$
$$+\tfrac{3}{4}J^3p_1\sum_{\mathbf{q}}\left[\frac{-f_{\mathbf{q}}}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{q}}-W}\{2b+b_1\}-\frac{f_{\mathbf{q}}}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{q}}}\{2b-b_1\}\right]\frac{1}{1-f_{\mathbf{k}}(1-e^{W/k_BT})}$$
$$+\tfrac{3}{4}J^3p_1\sum_{\mathbf{q}}\left[\left\{\frac{-f_{\mathbf{q}}}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{q}}+W}-\frac{f_{\mathbf{q}}}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{q}}-W}\right\}\{2a-a_1\}-\left\{\frac{2f_q}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{q}}}\right\}\{2a+a_1\}\right],\tag{11}$$

where Ω is the total volume of the metal, $(1/4\pi)\int d\Omega_{\mathbf{R}}$ designates an average over all the possible orientations for $\mathbf{R}$, and m is the mass of the electron.

$$\begin{aligned}
a&=(1+e^{i\mathbf{K}\cdot\mathbf{R}})(1+e^{-i\mathbf{K}\cdot\mathbf{R}})=2+(e^{i\mathbf{K}\cdot\mathbf{R}}+e^{-i\mathbf{K}\cdot\mathbf{R}}),\\
b&=(1-e^{i\mathbf{K}\cdot\mathbf{R}})(1-e^{-i\mathbf{K}\cdot\mathbf{R}})=2-(e^{i\mathbf{K}\cdot\mathbf{R}}+e^{-i\mathbf{K}\cdot\mathbf{R}}),
\end{aligned}\tag{12}$$

$$\mathbf{K}=\mathbf{k}'-\mathbf{k},\quad |\mathbf{k}'|\simeq|\mathbf{k}|,\quad |\mathbf{K}|=2k\sin\tfrac{1}{2}\theta,\tag{13}$$

where θ is the scattering angle between $\mathbf{k}$ and $\mathbf{k}'$, and the scatterings can be considered as quasi-elastic. (The error is of order W/ϵ_F, where ϵ_F is the Fermi energy, and can be neglected.)

$$\begin{aligned}
a_1&=\alpha e^{-i\mathbf{q}\cdot\mathbf{R}}+\text{c.c.},\quad b_1=\beta e^{-i\mathbf{q}\cdot\mathbf{R}}+\text{c.c.},\\
\alpha&=2(e^{i\mathbf{k}'\cdot\mathbf{R}}+e^{i\mathbf{k}\cdot\mathbf{R}}),\quad \beta=2(e^{i\mathbf{k}'\cdot\mathbf{R}}-e^{i\mathbf{k}\cdot\mathbf{R}}).
\end{aligned}\tag{14}$$

The conductivity is then given by

$$\sigma=-\frac{e^2}{3\pi^2m}\int k^3\tau\frac{\partial f}{\partial\epsilon_{\mathbf{k}}}d\epsilon_{\mathbf{k}}.\tag{15}$$

The resistivity $\rho=\sigma^{-1}$ can be calculated explicitly, for any value of W/k_BT, only in the case $J\ll V$. Let us separate:

$$\int_0^\pi(1-\cos\theta)\,\sin\theta d\theta\frac{1}{4\pi}\int d\Omega_{\mathbf{R}}\frac{Z}{N}=\bar{Z}_0+\bar{Z}_1,\tag{16}$$

where $\bar{Z}_0$ contains terms in a and b, and $\bar{Z}_1$ contains terms in a_1 and b_1. According to formulas already used in Ref. (4), which we summarize in Appendix A, one finds

$$\begin{aligned}\bar{Z}_0=&\tfrac{3}{2}J^2V(p_0-p_1)\bar{a}(3z/2\epsilon_F)\{-\tfrac{1}{2}J^-(W/k_BT)+\tfrac{1}{2}J^+(W/k_BT)\}\\&+\tfrac{3}{2}J^3p_0\bar{b}[1-f_{\mathbf{k}}(1-e^{-W/k_BT})]^{-1}\{2+\ln|k_BT/2\epsilon_F|-\tfrac{1}{2}J^-(W/k_BT)-\tfrac{1}{2}J(0)\}\\&+\tfrac{3}{2}J^3p_1\bar{b}[1-f_{\mathbf{k}}(1-e^{W/k_BT})]^{-1}\{2+\ln|k_BT/2\epsilon_F|-\tfrac{1}{2}J^+(W/k_BT)-\tfrac{1}{2}J(0)\}\\&+\tfrac{3}{2}J^3p_1\bar{a}\{4+2\ln|k_BT/2\epsilon_F|-\tfrac{1}{2}J^+(W/k_BT)-\tfrac{1}{2}J^-(W/k_BT)-J(0)\},\end{aligned}\tag{17}$$

where z is the number of conduction electrons per atom.

$$\begin{aligned}\bar{a}&=\int_0^\pi(1-\cos\theta)\sin\theta d\theta\frac{1}{4\pi}\int d\Omega_{\mathbf{R}}a=4+16/(2kR)^4[2(2kR)\sin(2kR)-(\{2kR\}^2-2)\cos(2kR)-2],\\\bar{b}&=\int_0^\pi(1-\cos\theta)\sin\theta d\theta\frac{1}{4\pi}\int d\Omega_{\mathbf{R}}b=4-16/(2kR)^4[2(2kR)\sin(2kR)-(\{2kR\}^2-2)\cos(2kR)-2],\end{aligned}\tag{18}$$

$$\int-\frac{\partial f}{\partial\epsilon_{\mathbf{k}}}d\epsilon_{\mathbf{k}}\bar{Z}_0=\tfrac{3}{2}J^3\frac{3z}{2\epsilon_F}\left[\bar{b}p_1\mu\left\{4+2\ln\left|\frac{k_BT}{2\epsilon_F}\right|+2I_2\left(\frac{W}{k_BT}\right)\right\}+\bar{a}p_1\left\{4+2\ln\left|\frac{k_BT}{2\epsilon_F}\right|+I_1\left(\frac{W}{k_BT}\right)+I_1(0)\right\}\right].\tag{19}$$

The functions I_1 and I_2 are also reviewed in Appendix A.

$$\mu=\frac{W/k_BT}{e^{W/k_BT}-1}\tag{20}$$

p_1 is given by (6).

$$\begin{aligned}\bar{Z}_1=&\tfrac{3}{2}J^2V(p_0-p_1)(A^+-A^-)\bar{\alpha}+\tfrac{3}{2}J^3p_0/[1-f_{\mathbf{k}}(1-e^{-W/k_BT})](-A^++A^-)\bar{\beta}\\&+\tfrac{3}{2}J^3p_1/[1-f_{\mathbf{k}}(1-e^{W/k_BT})](-A^++A^-)\bar{\beta}+\tfrac{3}{2}J^3-p_1(A^++A^--2A^0)\bar{\alpha},\end{aligned}\tag{21}$$

$$\begin{aligned}\bar{\alpha}&=\int_0^\pi(1-\cos\theta)\sin\theta d\theta\frac{1}{4\pi}\int d\Omega_{\mathbf{R}}\alpha=\frac{8\sin kR}{kR}\\\bar{\beta}&=\int_0^\pi(1-\cos\theta)\sin\theta d\theta\frac{1}{4\pi}\int d\Omega_{\mathbf{R}}\beta=0\end{aligned}\tag{22}$$

$$\int-\frac{\partial f}{\partial\epsilon_{\mathbf{k}}}d\epsilon_{\mathbf{k}}\bar{Z}_1=\tfrac{3}{4}J^3p_1\frac{16\sin^2(k_FR)}{(k_FR)^2}\frac{3z}{2_F}\left[I_1(0)-I_1\left(\frac{W}{k_BT}\right)\right],\tag{23}$$

and then the resistivity is given by

$$\begin{aligned}\rho=&\frac{3\pi}{2\epsilon_F}\frac{m}{e^2h}\frac{v_0}{N}\frac{1}{2}\left[\bar{a}_FV^2+\tfrac{3}{2}J^2\bar{a}_Fp_1+6J^2p_1\mu+\frac{9J^3z}{\epsilon_F}\left[\tfrac{1}{2}\bar{b}_Fp_1\mu\left(1.568+\ln\left|\frac{k_BT}{2\epsilon_F}\right|+I_2\left(\frac{W}{k_BT}\right)-I_1(0)\right)\right.\right.\\&\left.\left.+\tfrac{1}{2}\bar{a}_Fp_1\left[1.568+\ln\left|\frac{k_BT}{2_F}\right|+\tfrac{1}{2}\left(I_1\left(\frac{W}{k_BT}\right)-I_1(0)\right)\right]+4p_1\frac{1-\cos(2k_FR)}{(2k_FR)^2}\left(I_1(0)-I_1\left(\frac{W}{k_BT}\right)\right)\right]\right],\end{aligned}\tag{24}$$

$\bar{a}_F$ and $\bar{b}_F$ are the value of $\bar{a}$ and $\bar{b}$ for $k=k_F$; and v_0 is the atomic volume of the metal.

III. QUALITATIVE DISCUSSION

Let us first examine some special cases:

(a) $W/k_BT\to 0$, $R\to\infty$; i.e., practically noninteracting impurities, very far apart from each other. One expects the resistivity of this pair to reduce to the sum of two Kondo resistivities on isolated impurities. And, indeed, (24) leads, then, to

$$\rho=\frac{3\pi}{2\epsilon_F}\frac{m}{e^2h}v_0\frac{2}{N}\times\left[V^2+\tfrac{3}{4}J^2\left\{1+\frac{3Jz}{\epsilon_F}\left(1.568+\ln\left|\frac{k_BT}{2_F}\right|\right)\right\}\right].\tag{25}$$

Let us recall that the usual Kondo resistivity on one spin S is

$$\rho_{\mathrm{Kondo}}=\frac{3\pi}{2\epsilon_F}\frac{m}{e^2\hbar}v_0\frac{1}{N}\bigg[V^2+J^2S(S+1)\times\left\{1+\frac{3Jz}{\epsilon_F}\left(1.568+\ln\left|\frac{k_BT}{2\epsilon_F}\right|\right)\right\}\bigg].$$

Here $S=\frac{1}{2}$, so $S(S+1)=\frac{3}{4}$.

(b) $W/k_BT\rightarrow 0$, R finite; i.e., two impurities at a distance R from each other, uncorrelated. One gets from (24)

$$\rho=\frac{3\pi}{2\epsilon_F}\frac{m}{e^2\hbar}\frac{v_0}{N}\frac{1}{2}\bigg[\bar{a}_FV^2+\tfrac{3}{8}J^2\bar{a}_F+\tfrac{3}{2}J^2+\frac{9J^3z}{\epsilon_F}\left(1.568+\ln\left|\frac{k_BT}{2\epsilon_F}\right|\right)\bigg]. \tag{26}$$

[This is the formula we should have found instead of (24) if we had not introduced W in (1).] Whereas oscillating interference terms appear in second order through a_F, there is no interference in the third-order contribution. This is quite understandable: cf. the fact that, in optics, two incoherent sources of light cannot give rise to any interference; here, the coherence which existed between the scattered parts of the conduction-electron plane wave on the two spins in second order vanishes in third order if there is no coupling between the two spins, because, after the intermediate processes on each spin, there is no more coherence between the two outgoing waves.

(c) $W/k_BT\rightarrow +\infty$, $R\rightarrow 0$; i.e., the two spins come into contact (of course, in a metal this extreme case cannot happen, $R_{\min}$ is equal to the first neighbor distance), and they are ferromagnetically coupled, so they form a triplet of total spin $I=1$ and a spin-independent potential equal to $2V$. So a Kondo resistivity due to a spin of 1 is expected. And indeed (24) gives

$$\rho=\frac{3\pi}{2\epsilon_F}\frac{m}{e^2\hbar}\frac{v_0}{N}\times\bigg[(2V)^2+2J^2\left\{1+\frac{3Jz}{\epsilon_F}\left(1.568+\ln\left|\frac{k_BT}{2\epsilon_F}\right|\right)\right\}\bigg]. \tag{27}$$

$$[J^2I(I+1)=2J^2 \text{ for } I=1].$$

(d) $W/k_BT>10$, R finite; i.e., two strongly ferromagnetically coupled spins but separated by the distance R. At variance with the magnetoresistivity problem[4] for $H/k_BT>10$, according to the discussion in the Introduction and in agreement with the preceding case, the resistivity is still temperature dependent; writing $\ln|W/2k_BT|=\ln|W/4\epsilon_F|-\ln|k_BT/2\epsilon_F|$, one expects a contribution $\ln|k_BT/2\epsilon_F|$ to remain. One, in fact, finds

$$\rho=\frac{3\pi}{2\epsilon_F}\frac{m}{e^2\hbar}\frac{v_0}{N}\frac{1}{2}\bigg[\bar{a}_FV^2+\bar{a}_F\tfrac{1}{2}J^2+\frac{9J^3z}{\epsilon_F}\times\left\{\left(1.568+\ln\left|\frac{k_BT}{2\epsilon_F}\right|\right)\left(\tfrac{1}{12}\bar{a}_F+\frac{4}{3}\frac{1-\cos(2k_FR)}{(2k_FR)^2}\right)+\left(2+\ln\left|\frac{W}{4\epsilon_F}\right|\right)\left(\tfrac{1}{12}\bar{a}_F-\frac{4}{3}\frac{1-\cos(2k_FR)}{(2k_FR)^2}\right)\right\}\bigg]. \tag{28}$$

Thus (28) has a purely Kondo-like temperature dependence, through $\ln|k_BT/2\epsilon_F|$, but with a coefficient different from the Kondo resistivity (25) by a ratio $\frac{1}{12}\bar{a}_F+\frac{4}{3}[1-\cos(2k_FR)]/(2k_FR)^2$.

(e) $W/k_BT\rightarrow -\infty$, $R\rightarrow 0$: One has two interacting spins with a total spin 0 (antiferromagnetic coupling); then no spin-dependent resistivity at all is expected:

$$\rho=\frac{3\pi}{2\epsilon_F}\frac{m}{e^2\hbar}\frac{v_0}{N}4V^2. \tag{29}$$

(f) $W/k_BT<-10$, R finite; two strongly antiferromagnetically coupled spins at distance R give no temperature-dependent resistivity

$$\rho=\frac{3\pi}{2\epsilon_F}\frac{m}{e^3\hbar}\frac{v_0}{N}\tfrac{1}{2}\bar{a}_FV^2. \tag{30}$$

In the general case, let us compare (24) with what is known experimentally.[2] The experimental situation is the following: when the impurity concentration increases, i.e., when the correlations between impurities can no longer be neglected, one observes a maximum in the complete $\rho-T$ curve. This maximum corresponds to some spin "ordering" (see, for example, the fourth and fifth of Ref. 6 or last section of Ref. 4). Below the maximum, the resistivity is better described in terms of an average molecular field. We are interested here in the part of this curve above the maximum. Above the maximum, experimentally,

(4) The coefficient of $\ln|k_BT/2\epsilon_F|$, constant for extreme dilution, then becomes *temperature-dependent:* the straight line obtained by plotting ρ versus $\ln T$ becomes curved.

(2) This coefficient remains *negative,* as it was for extreme dilution, but its absolute value *decreases;* the "slope" of $\ln T$ becomes less steep.

We can conclude here from (24) that

(1) the coefficient λ of $\ln|k_BT/2\epsilon_F|$, which is

$$\lambda=\frac{9J^3z}{2\epsilon_F}\{\tfrac{1}{2}\bar{b}_Fp_1\mu+\tfrac{1}{2}\bar{a}_Fp_1\} \tag{31}$$

is indeed *temperature-dependent* through $p_1(T)$ and $\mu(T)$, except for extreme dilution, i.e., for very weak coupling and a large distance between impurities ($W/k_BT \rightarrow 0$, $R \rightarrow \infty$), where

$$\lambda \rightarrow \lambda_\infty = 9J^3z/2\epsilon_F\,, \tag{32}$$

which is the coefficient of $\ln T$ in the Kondo resistivity for isolated impurities [cf. (25)].

(2) λ is indeed *negative* because J is negative and the bracket in (31) is positive: p_1 and μ are positive for all values of W/k_BT; and $\bar{a}_F$ and $\bar{b}_F$ take on positive values very close to 4, whatever the value of R.

(3) Moreover, the absolute value of λ is smaller than the absolute value of λ_∞:

$$\tfrac{1}{8}\bar{b}_F p_1 \mu + \tfrac{1}{8}\bar{a}_F p_1 < 1\,. \tag{33}$$

We have verified that (33) is true for all values, positive or negative of W/k_BT, and for R up to sixth neighbor distance. So the absolute value of λ *decreases* from its value λ_∞.

Therefore, the expansion (24) seems in good qualitative agreement with the experimental observation. In Sec. IV we will examine (24) quantitatively.

IV. NUMERICAL EXAMPLE

The interesting point is now to examine the temperature variation of resistivity (24) and, more specifically, the coefficient λ of the $\ln T$ contribution. This implies the use of an explicit W. When W is due to the indirect exchange via the conduction electrons, which leads to the RKKY interaction,[5] keeping in mind the last remark of the introduction, one should in principle use in (4) not the bare J and V but some J' and V' "dressed" by the polarization contained in (1) in W. In the absence of any information on J' and V', we present here a numerical result with the bare J and V, simply to give an example of what the pair resistivity looks like. It has been shown[7] that if J is used in the resistivity, $(2l+1)J$ should replace J in the RKKY interaction to take into account the orbital degeneracy l:

$$W = -\tfrac{9}{2}\pi \frac{(2l+1)^2 J^2 z^2}{\epsilon_F} \times \frac{(2k_FR_n)\cos(2k_FR_n) - \sin(2k_FR_n)}{(2k_FR_n)^4}\,. \tag{34}$$

R_n is the distance between the two spins of the pair in position of nth neighbors. Typically (in Cu-Mn, for example), $J \simeq -0.3$ eV, $(2l+1)J \sim -1.5$ eV, $\epsilon_F \sim 7.1$ eV, $z=1$. As we are merely trying to present a simple numerical example, we neglect the temperature dependence of the RKKY interaction, which should be taken into account in a self-consistent study.

Let us write the pair resistivity (24) as

$$\rho_{\text{pair}} = \frac{3\pi}{2\epsilon_F} \frac{m}{e^2\hbar} \frac{v_0}{N} \{R + \Delta R\}\,, \tag{35}$$

where we separate the second-order contribution R and the third-order contribution ΔR:

$$R = \tfrac{1}{2}\bar{a}_F V^2 + \tfrac{3}{4}J^2 \bar{a}_F p_1 + 3J^2 p_1 \mu\,, \tag{36}$$

$$\begin{aligned}\Delta R = \frac{9J^3z}{2\epsilon_F} \bigg\{ & \tfrac{1}{2}\bar{b}_F p_1 \mu \left(1.568 + \ln\left|\frac{k_BT}{2\epsilon_F}\right| + I_2\left(\frac{W}{k_BT}\right) - I_1(0)\right) \\ & + \tfrac{1}{2}\bar{a}_F p_1 \left[1.568 + \ln\left|\frac{k_BT}{2\epsilon_F}\right| + \tfrac{1}{2}I_1\left(\frac{W}{k_BT}\right) - \tfrac{1}{2}I_1(0)\right] \\ & + 4p_1 \frac{1-\cos(2k_FR)}{(2k_FR)^2}\left[I_1(0) - I_1\left(\frac{W}{k_BT}\right)\right]\bigg\}\,. \end{aligned} \tag{37}$$

The contribution R has been studied elsewhere.[6] On Fig. 1 we have only plotted ΔR versus T (on semilog plot) for six different distances R_n between the two spins of the pair: $n=1$ corresponds to first neighbors, curve A; $n=2$ corresponds to second neighbors, curve B; etc; $n=6$ corresponds to sixth neighbors, curve F. The corresponding values of the interaction W are

$$\begin{array}{rll} W = & -113.4°\text{K}, & \text{for } R_n = R_1 \\ & +\ 51°\text{K}, & R_2 \\ & -\ 28°\text{K}, & R_3 \\ & -\ 3.5°\text{K}, & R_4 \\ & +\ 14.25°\text{K}, & R_5 \\ & +\ 2.25°\text{K}, & R_6\,. \end{array} \tag{38}$$

Therefore, curves A, C, and D correspond to antiferromagnetic pairs and B, E, and F to ferromagnetic ones. For $T \ll |W|$, curves A, C, and D correspond to the resistivities of singlets of spin 0 studied in III (f), so $\Delta R = 0$ [cf. Eq. (30)]; whereas curves B, E, and F correspond to triplets acting as isolated spins $I=1$, as was explained in III (d). For these last cases the corresponding low-temperature straight lines depend on the distances R_n; their slopes

$$\frac{9J^3z}{2\epsilon_F}\left(\tfrac{1}{12}\bar{a}_F + \frac{4}{3}\frac{1-\cos(2k_FR_n)}{(2k_FR_n)^2}\right)$$

are actually very close to the asymptotic value $\frac{1}{3}(9J^3z/2\epsilon_F)$ (as even $2k_FR_2$ is already much bigger than 1), so the three lines appear parallel on the figure. The straight line on the right-hand side of the figure is the Kondo resistivity of two isolated impurities given by Eq. (25); it represents the common limit of all the curves A to F when $T \gg |W|$. In between, all these curves present a maximum at a temperature T equal to the corresponding coupling (38) $T=W$.

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[7] See, for example, A. Blandin, J. Appl. Phys. **39**, 1285 (1968).

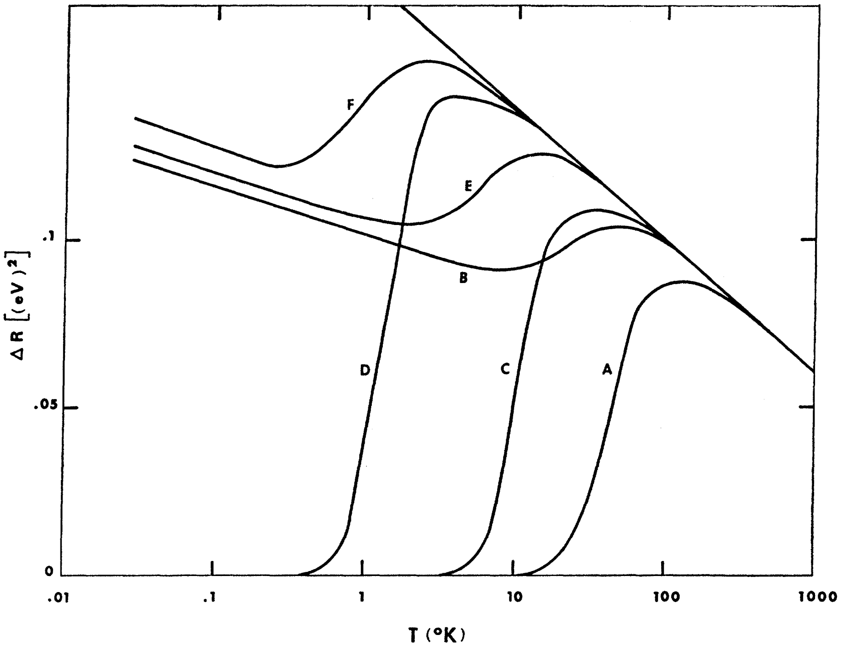

FIG. 1. Third-order contribution ΔR to the pair resistivity (35), in units of $(\mathrm{eV})^2$ versus $\ln T(°\mathrm{K})$. The six curves A–F represent the contribution of six pairs at increasing distances: A corresponds to the resistivity of a pair of two first neighbor impurities, B to the second neighbors, $\cdots$, F to sixth neighbors. The straight line, envelope of these curves, at high temperature, is just the usual Kondo $\ln T$ term for two independent spins, uncorrelated.

The behavior of these curves is quite encouraging, and indicates that it might be worth while to refine this approach in order to describe the resistivity of a real dilute alloy, when correlations become important. One must, of course, keep in mind that to the temperature dependence of ΔR must be added the temperature dependence of R, the second-order term, which has not been included in Fig. 1. The description of a real dilute alloy by a power expansion in C (the atomic impurity concentration) up to C^2 involves:

(1) a generalization of the above calculation to an arbitrary spin S;

(2) an average of the contributions of all possible pairs, taken so that each pair contributes only if it is isolated from other impurities. The first part could be done easily, and may also include an external magnetic field; the second is more difficult to do rigorously. Finally, the problem of self-consistency, pointed out in the introduction, is more important but much more difficult.

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APPENDIX A

We review here some formulas studied in Ref. 4, which are useful in the present calculation:

$$\frac{1}{N}\sum_{\mathbf{q}}\frac{-f_q}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{q}}\pm W}=\frac{3z}{2\epsilon_F}\left[1+\tfrac{1}{2}\ln\left|\frac{k_BT}{2\epsilon_F}\right|-\tfrac{1}{2}J^{\mp}\left(\frac{W}{k_BT}\right)\right], \tag{A1}$$

$$\int k^3\left(-\frac{\partial f}{\partial\epsilon_{\mathbf{k}}}\right)d\epsilon_{\mathbf{k}}\left(-\tfrac{1}{2}J(0)\right)=\tfrac{1}{2}k_F{}^3I_1(0), \tag{A2}$$

$$\int k^3\left(-\frac{\partial f}{\partial\epsilon_{\mathbf{k}}}\right)d\epsilon_{\mathbf{k}}\left(-\tfrac{1}{2}J^{\mp}\left(\frac{W}{k_BT}\right)\right)=\tfrac{1}{2}k_F{}^3I_1\left(\frac{W}{k_BT}\right), \tag{A3}$$

$$\int k^3\left(-\frac{\partial f}{\partial\epsilon_{\mathbf{k}}}\right)d\epsilon_{\mathbf{k}}\frac{1}{1-f_{\mathbf{k}}(1-e^{\mp W/k_BT})}=k_F{}^3\frac{W}{2k_BT}\,\frac{e^{\pm W/2k_BT}}{Sh(W/2k_BT)}, \tag{A4}$$

$$\begin{aligned}\int k^3\left(-\frac{\partial f}{\partial\epsilon_{\mathbf{k}}}\right)d\epsilon_{\mathbf{k}}\left(-\tfrac{1}{2}J(0)\right)\frac{1}{1-f_{\mathbf{k}}(1-e^{\mp W/k_BT})}&=\int k^3\left(-\frac{\partial f}{\partial\epsilon_{\mathbf{k}}}\right)d\epsilon_{\mathbf{k}}\left(-\tfrac{1}{2}J^{\mp}\left(\frac{W}{k_BT}\right)\right)\frac{1}{1-f_{\mathbf{k}}(1-e^{\mp W/k_BT})}\\&=\tfrac{1}{2}k_F{}^3e^{\pm W/2k_BT}\frac{W}{2k_BT}\,\frac{I_2(W/k_BT)}{Sh(W/2k_BT)}.\end{aligned} \tag{A5}$$

For $|x|<2$

$$\begin{aligned}I_1(x)&\simeq-0.432+0.091x^2,\\I_2(x)&\simeq-0.432+0.030x^2.\end{aligned} \tag{A6}$$

For $|x|>|0$

$$I_1(x)\simeq\ln|\tfrac{1}{2}x|-\frac{3.27}{x^2},$$
$$I_2(x)\simeq\ln|\tfrac{1}{2}x|-1+\frac{3.27}{x^2}. \tag{A7}$$

The functions $I_1(x)$ and $I_2(x)$ are drawn in Ref. 4 for all values of x.

APPENDIX B

We want to calculate the sum

$$A^{\pm}=\frac{1}{N}\sum_q \frac{f(q)e^{i\mathbf{q}\cdot\mathbf{R}}}{\epsilon_\kappa-\epsilon_{\mathbf{q}}} \tag{B1}$$

$$=\frac{v_0}{8\pi^3}\int d^3q f(q)\frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{\epsilon_\kappa-\epsilon_{\mathbf{q}}}, \tag{B2}$$

where v_0 is the atomic volume. The angular integrals give

$$A=\frac{v_0}{\pi^2}\frac{1}{R}\int_0^\infty \frac{q\sin(qR)f(q)}{\kappa^2-q^2}, \tag{B3}$$

where $\epsilon_\kappa=\epsilon_k\pm W=\frac{1}{2}k^2\pm W$ and $\epsilon_{\mathbf{q}}=q^2/2$ in units $m=\hbar=e=1$.

Let us first study

$$g(q)=\int_0^q \frac{x\sin(Rx)dx}{\kappa^2-x^2}, \tag{B4}$$

which is given by tables of integrals.[8]

$$g(q)=-\tfrac{1}{2}\pi\cos(\kappa R)-\tfrac{1}{2}\cos(\kappa R)$$
$$\times\{si\{R(\kappa+q)\}+si\{R(q-\kappa)\}\}$$
$$+\tfrac{1}{2}\sin(\kappa R)\{ci\{R(\kappa+q)\}-ci\{R(q-\kappa)\}\}, \tag{B5}$$

where

$$si(u)=-\int_u^\infty \frac{\sin t}{t}dt,$$
$$ci(u)=-\int_u^\infty \frac{\cos t}{t}dt, \tag{B6}$$
$$ci(u)\simeq 0.577+\ln u,\quad \text{for}\quad u\to 0$$
$$si(u)\simeq-\tfrac{1}{2}\pi+u.$$

Upon integrating (B3) by parts one is left with

$$A=\frac{-v_0}{\pi^2}\frac{1}{R}\int_0^\infty g(q)\frac{\partial f(q)}{\partial q}dq. \tag{B7}$$

One will need

$$B=\int\frac{\partial f}{\partial k}A dk=+\frac{v_0}{\pi^2}\frac{1}{R}\int\frac{-\partial f}{\partial k}\frac{\partial f}{\partial q}dkdq\, g(q). \tag{B8}$$

With writing in the neighborhood of the Fermi level

$$q-\kappa=\frac{q^2-\kappa^2}{q+\kappa}\simeq\frac{q^2-\kappa^2}{2k_F}=\frac{\epsilon_q-\epsilon_\kappa}{k_F}, \tag{B9}$$

and

$$\epsilon_q-\epsilon_k=2kTV, \tag{B10}$$

so

$$\epsilon_q-\epsilon_\kappa=2kTV\mp W,$$

$$B\simeq\frac{v_0}{\pi^2R}\bigg\{\frac{\pi}{4}\cos(k_FR)+\tfrac{1}{2}\cos(k_FR)si(2k_FR)$$
$$-\tfrac{1}{2}\sin(k_FR)ci(2k_FR)+\tfrac{1}{2}\sin k_FR$$
$$\times\left\{0.577+\ln\left(2k_FR\frac{k_BT}{2\epsilon_F}\right)+I_1\left(\frac{W}{kT}\right)\right\}\bigg\}, \tag{B11}$$

$$\frac{v_0}{\pi^2R}=\frac{3z}{2\epsilon_F}\frac{1}{k_FR}.$$

The function $I_1(W/k_BT)$ is studied in Ref. 4 and reviewed in this appendix. One notes that for very large $R\simeq\epsilon_F/k_Fk_BT$ the divergent term in (B11) $\ln(2k_FRk_BT/2\epsilon_F)$ vanishes, which is physically reasonable, as impurities that are very far apart can no longer act as a whole to give a Kondo divergence, but act separately as isolated impurities, each giving rise to a Kondo divergent contribution.

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[8] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals Series and Products* (Academic Press Inc., New York, 1965).