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Temperature Dependence in the Effective Ruderman-Kittel-Kasuya-Yosida Interaction*

R. H. Bresemann and M. Bailyn
Physics Department, Northwestern University, Evanston, Illinois

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The effective interaction between two magnetic impurities immersed in a simple metal is calculated by means of the method of double-time Green's functions. A Kondo effect is looked for and found, but it is complicated by the existence of effective magnetic fields at the impurity sites. The effect is generally to enhance the magnitude of the interaction as T decreases. We find a continuing temperature dependence at extremely low temperatures even when there are local field energies λ such that $\lambda \gg k_BT$.

1. INTRODUCTION

Great interest has been shown in the *sd* exchange interaction in order to explain some of the properties of dilute magnetic alloys, as evidenced by the large number of recent papers on the subject. One of the most significant of these was Kondo's paper[1] dealing with the problem of the resistance minimum. Kondo showed that in the second Born approximation, a term proportional to $\ln T$ appears in the resistance, which could, in conjunction with other terms, produce a resistance minimum, provided the exchange integral J_0 is negative.

Such a logarithmic term in the scattering cross section gave rise to a divergence at $T=0$, which stimulated Suhl[2] and Nagaoka[3] to look more carefully into the problem for the very low-temperature region. Nagaoka used the method of double-time Green's functions, and obtained the Kondo $\ln T$ term at high temperatures, which however did not persist into the very-low-temperature region. Using a self-consistency argument, he argued that below a critical temperature T_c, the $\ln T$ term disappears, and the resistance saturates at a certain value. Other work on the resistance problem was carried out by Liu[4] and Abrikosov.[5] Abrikosov also considered the effect of a local magnetic field, which we also do here, but no connection with Abrikosov's results will be formulated. Yosida and Okiji[6] considered the corresponding magnetization problem.

In addition to these papers, it has also been shown by Kim[7] that it is possible to have a resistance minimum even if there is no local moment. Kim used the Anderson "mixing" model to show this. Scalapino[8] also used the mixing model to calculate the susceptibility of a dilute alloy, obtaining a resonance type of behavior reminiscent of Yosida and Okiji and Nagaoka. There have been many other papers in this area too numerous to mention.

In the present paper, we turn to the problem of the effective interaction between *two* impurities, known as the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction. From the above-mentioned work, we might expect that a $\ln T$ behavior would exist in say the third power of J_0 terms that would become important at low temperatures. We find in fact a similar behavior. The problem is approached by calculating the average energy of the system by means of Green's functions, keeping in mind the possibility that local magnetic fields may exist at the impurity sites. Our calculation follows fairly closely the method used by Nagaoka.

The paper is organized as follows. In Sec. 2 we set up the Green's functions and the basic equations of motion. In Sec. 3 a chain-breaking method is developed which enables us to calculate some of the more recalcitrant Green's functions. In Sec. 4, the resulting equations are solved algebraically, and in Sec. 5 the effective Heisenberg type of interaction is discussed.

2. THE HAMILTONIAN AND GREEN'S FUNCTIONS

The Hamiltonian for the two-impurity problem on the *sd*-exchange model in a magnetic field $\mathcal{H}_z^{\text{ext}}$ is

$$H'=H-E_FN=\sum \xi(\mathbf{k}\sigma)n_{\mathbf{k}\sigma}-\sum_{j=1}^{2} \mu\mathcal{H}_z^{\text{ext}}S_{jz}$$
$$-(J_0/N)\sum \exp[i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j]2\mathbf{S}_j\cdot\mathbf{S}_{k'k}, \quad (2.1)$$

where we use an abbreviated notation[9]

$$n_{\mathbf{k}'\mathbf{k}\sigma}=a_{\mathbf{k}'\sigma}{}^{\dagger}a_{\mathbf{k}\sigma};\quad n_{\mathbf{k}\sigma}\equiv n_{\mathbf{k}\mathbf{k}\sigma}$$
$$S_{\mathbf{k}'\mathbf{k}\sigma}=a_{\mathbf{k}'\sigma}{}^{\dagger}a_{\mathbf{k},-\sigma};\quad S_{\mathbf{k}'\mathbf{k}z}=2^{-1}(n_{\mathbf{k}'\mathbf{k}+}-n_{\mathbf{k}'\mathbf{k}-})$$
$$2\mathbf{S}_j\cdot\mathbf{S}_{\mathbf{k}'\mathbf{k}}=S_{j+}S_{\mathbf{k}'\mathbf{k}-}+S_{j-}S_{\mathbf{k}'\mathbf{k}+}+S_{jz}(n_{\mathbf{k}'\mathbf{k}+}-n_{\mathbf{k}'\mathbf{k}-}), \quad (2.2)$$

where σ means spin, $a_{\mathbf{k}\sigma}{}^{\dagger}$ and $a_{\mathbf{k}\sigma}$ are electron creation and destruction operators, respectively. The indices $\mathbf{k}$ and $\mathbf{l}$ will always refer to conduction-electron wave vectors, and j refers to the impurities, The energy ξ is written in terms of the unperturbed Bloch energies $E(\mathbf{k})$:

$$\xi(\mathbf{k}\sigma)=E(\mathbf{k})-\tfrac{1}{2}\mu\mathcal{H}_z^{\text{ext}}-E_F\cdots\sigma=+,$$
$$=E(\mathbf{k})+\tfrac{1}{2}\mu\mathcal{H}_z^{\text{ext}}-E_F\cdots\sigma=- \quad (2.3)$$

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

[2] H. Suhl, Phys. Rev. **138**, A515 (1965).

[3] Y. Nagaoka, Phys. Rev. **138**, A1112 (1965).

[4] S. H. Liu, Phys. Rev. **137**, A1209 (1965).

[5] A. A. Abrikosov, Physics **2**, 5 (1965); **2**, 61 (1965).

[6] K. Yosida and A. Okiji, Technical Report of Institute of Solid State Physics, University of Tokyo, Series A, 1965 (unpublished).

[7] D. J. Kim, Phys. Rev. **146**, 455 (1966).

[8] D. J. Scalapino, Phys. Rev. Letters **16**, 937 (1966).

[9] M. Bailyn, Phys. Rev. **137**, A1914 (1965).

containing a magnetic field effect. S_{j+} and S_{j-} are the raising and lowering operators, respectively, for the jth impurity spin. In Eq. (2.1) we have made the approximation $J(\mathbf{k}',\mathbf{k})=J_0$.

Our major interest in this paper is to calculate the average energy

$$E'=\langle H'\rangle=\sum \xi(\mathbf{k}\sigma)\langle n_{\mathbf{k}\sigma}\rangle-\sum \mu\mathcal{H}_z{}^{\mathrm{ext}}\langle S_{jz}\rangle \\ -J_0N^{-1}\sum \exp[i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j]\langle 2S_j\cdot S_{\mathbf{k}'\mathbf{k}}\rangle, \quad (2.4)$$

the angle brackets signifying a grand canonical average. In particular we shall be interested in the part of E that has the form of a Heisenberg interaction between the two impurities

$$E'_{\mathrm{Heis}}=\sum_{jj'=1}^{2} J_{jj'}\langle S_{jz}S_{j'z}\rangle. \quad (2.5)$$

In order to obtain the averaged operators in Eq. (2.4) we shall, following Nagaoka,[3] use retarded Green's functions, the complete theory of which may be found for example in Bonch-Bruevich and Tyablikov[10]:

$$\langle\langle A(\lambda,t)\,|\,B(\lambda',0)\rangle\rangle\equiv -i\langle[A(\lambda t),B(\lambda'0)]_+\rangle\theta(t), \quad (2.6)$$

where

$$\begin{aligned}\theta(t)&=0\cdots t<0\\ &=1\cdots t>0.\end{aligned} \quad (2.7)$$

Here $\hbar$ has been taken as 1, the + subscript means an anticommutator, and $\lambda\lambda'$ refer to a complete set of variables. In equilibrium this Green's function depends only on time through the difference in the two-time indices of the operators A and B. This difference has already been written as $t-0$ for convenience.

The equations of motion are obtained by a time differentiation

$$i\frac{\partial}{\partial t}\langle\langle A(\lambda t)\,|\,B(\lambda'0)\rangle\rangle=\delta(t)\langle[A(\lambda t),B(\lambda'0)]_+\rangle \\ +\langle\langle[A(\lambda t),H]_-\,|\,B(\lambda'0)\rangle\rangle, \quad (2.8)$$

where the − subscript means an ordinary commutator.

The Green's functions just defined and the averages in Eq. (2.4) can be linked together through the energy-Fourier transform of the former:

$$\langle\langle A(\lambda\omega)\,|\,B(\lambda')\rangle\rangle\equiv(2\pi)^{-1}\int_{-\infty}^{\infty} dt\, e^{-i\omega t}\langle\langle A(\lambda t)\,|\,B(\lambda'0)\rangle\rangle. \quad (2.9)$$

Now the theory of Green's functions[10] shows that the thermodynamic average of the product AB is related to the Fourier transform of the retarded Green's function through the formula

$$\langle A(\lambda t)B(\lambda' t)\rangle=2\int_{-\infty}^{\infty} d\omega\, f(\omega)\mathrm{Im}\langle\langle A(\lambda,\,\omega+i0)\,|\,B(\lambda')\rangle\rangle, \quad (2.10)$$

where

$$f(\omega)[\exp(\omega/k_BT)+1]^{-1}. \quad (2.11)$$

The Green's function in Eq. (2.10) has been analytically extended to just above the real axis.

The plan then is to take the Fourier transform of Eq. (2.8), solve, and substitute into Eq. (2.10). To specify just what Green's functions we shall need, we refer to Eq. (2.4) and notice that the following averages are required

$$\begin{gathered}\langle a_{\mathbf{k}\sigma}{}^\dagger a_{\mathbf{k}\sigma}\rangle,\\ \langle m_{j\sigma}a_{\mathbf{k}'\sigma}{}^\dagger a_{\mathbf{k}\sigma}\rangle,\\ \langle S_{j\sigma}a_{\mathbf{k}',-\sigma}{}^\dagger a_{\mathbf{k}\sigma}\rangle,\end{gathered} \quad (2.12)$$

where all the operators refer to the same time, and where for convenience we define

$$\begin{aligned}m_{j\sigma}&\equiv S_{jz}\cdots\sigma=+\\ &\equiv -S_{jz}\cdots\sigma=-.\end{aligned} \quad (2.13)$$

Thus from Eq. (2.10) we need

$$G_\sigma(\mathbf{k}'\mathbf{k}\,|\,t)\equiv\langle\langle a_{\mathbf{k}'\sigma}{}^\dagger(t)\,|\,a_{\mathbf{k}\sigma}(0)\rangle\rangle, \quad (2.14)$$

$$Y_\sigma(j\mathbf{k}'\mathbf{k}\,|\,t)\equiv\langle\langle a_{\mathbf{k}',-\sigma}{}^\dagger(t)S_{j\sigma}(t)\,|\,a_{\mathbf{k}\sigma}(0)\rangle\rangle, \quad (2.15)$$

$$Z_\sigma(j\mathbf{k}'\mathbf{k}\,|\,t)\equiv\langle\langle a_{\mathbf{k}'\sigma}{}^\dagger(t)m_{j\sigma}(t)\,|\,a_{\mathbf{k}\sigma}(0)\rangle\rangle. \quad (2.16)$$

It will be convenient to use also the sum

$$\Gamma\equiv Y+Z. \quad (2.17)$$

The averages in Eq. (2.12) are not needed individually but only in certain groups:

$$\langle n_{\mathbf{k}}\rangle\equiv\langle n_{\mathbf{k}+}+n_{\mathbf{k}-}\rangle \\ =2\sum_\sigma \mathrm{Im}\int f(\omega)G_\sigma(\mathbf{k}\mathbf{k}\,|\,\omega+i0)d\omega, \quad (2.18)$$

$$\langle 2S_j\cdot S_{\mathbf{k}'\mathbf{k}}\rangle=2\sum_\sigma \mathrm{Im}\int f(\omega)\Gamma_\sigma(j\mathbf{k}'\mathbf{k}\,|\,\omega+i0)d\omega. \quad (2.19)$$

Furthermore, we do not need both these groups individually, since they are simply related through use of the G Green's-function's equation of motion. From Eq. (2.22) below, it is easily seen that

$$[\omega-\xi(\mathbf{k}\sigma)]G_\sigma(\mathbf{k}\mathbf{k}\,|\,\omega)=-(2\pi)^{-1}-J_0N^{-1} \\ \times\sum_{\mathbf{k}'j} \exp[i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j]\Gamma_\sigma(j\mathbf{k}'\mathbf{k}\,|\,\omega). \quad (2.20)$$

Going back to Eq. (2.4) we see finally that we need

$$E'=2\sum_\sigma \mathrm{Im}\int d\omega\,\omega f(\omega)\sum_{\mathbf{k}} G_\sigma(\mathbf{k}\mathbf{k}\,|\,\omega+i0) \\ -\sum_{j=1}^{2} \mu\mathcal{H}_z{}^{\mathrm{ext}}\langle S_{jz}\rangle. \quad (2.21)$$

Thus a calculation of the diagonal elements $G_\sigma(\mathbf{k}\mathbf{k}\,|\,\omega)$ of the conduction-electron Green's function is all that

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[10] V. L. Bonch-Bruevich and S. V. Tyablikov, *The Green Function Method in Statistical Mechanics* (North-Holland Publishing Company, Amsterdam, 1962).

is required to determine the average energy of the system. We shall be content to have our results in terms of the averaged $\langle m_{j\sigma}\rangle$'s.

To complete this section we shall write down the basic equations of motion. First we need

$$[\omega-\xi(\mathbf{k}'\sigma)]G_\sigma(\mathbf{k}'\mathbf{k})+J_0N^{-1}\sum_{\mathbf{l}j}\exp[i(\mathbf{k}'-\mathbf{l})\cdot\mathbf{R}_j]\Gamma_\sigma(j\mathbf{l}\mathbf{k})=-(2\pi)^{-1}\delta_{\mathbf{k}',\mathbf{k}}. \tag{2.22}$$

This in turn requires

$$\begin{aligned}&[\omega-\xi(\mathbf{k}'\sigma)]Y_\sigma(j\mathbf{k}'\mathbf{k})+J_0N^{-1}\sum_{\mathbf{l}}\exp[i(\mathbf{k}'-\mathbf{l})\cdot\mathbf{R}_j]\{S_j^2G_\sigma(\mathbf{l}\mathbf{k})\\&\qquad-\langle\langle(m_{j\sigma}^2a_{\mathbf{l}\sigma}^\dagger+S_{j\sigma}m_{j\sigma}a_{\mathbf{l},-\sigma}^\dagger\,|\,a_{\mathbf{k}\sigma}\rangle\rangle-\Gamma_\sigma(j\mathbf{l}\mathbf{k})\}+J_0N^{-1}\sum_{\mathbf{l}}\exp[i(\mathbf{k}'-\mathbf{l})\cdot\mathbf{R}_{j'}]\\&\qquad\times\langle\langle S_{j\sigma}S_{j',-\sigma}a_{\mathbf{l}\sigma}^\dagger-S_{j\sigma}m_{j'\sigma}a_{\mathbf{l},-\sigma}^\dagger\,|\,a_{\mathbf{k}\sigma}\rangle\rangle-J_0N^{-1}\sum_{\mathbf{l}\mathbf{l}'}\exp[i(\mathbf{l}'-\mathbf{l})\cdot\mathbf{R}_j]\\&\qquad\times\langle\langle S_{j\sigma}a_{\mathbf{l}\sigma}^\dagger a_{\mathbf{k}',-\sigma}^\dagger a_{\mathbf{l}'\sigma}-S_{j\sigma}a_{\mathbf{l},-\sigma}^\dagger a_{\mathbf{k}',-\sigma}^\dagger a_{\mathbf{l},-\sigma}-2m_{j\sigma}a_{\mathbf{l}\sigma}^\dagger a_{\mathbf{k}',-\sigma}^\dagger a_{\mathbf{l}',-\sigma}\,|\,a_{\mathbf{k}\sigma}\rangle\rangle=0.\end{aligned} \tag{2.23}$$

$$\begin{aligned}&[\omega-\xi(\mathbf{k}'\sigma)]Z_\sigma(j\mathbf{k}'\mathbf{k})+J_0N^{-1}\sum_{\mathbf{l}}\exp[i(\mathbf{k}'-\mathbf{l})\cdot\mathbf{R}_j]\langle\langle m_{j\sigma}^2a_{\mathbf{l}\sigma}^\dagger+S_{j\sigma}m_{j\sigma}a_{\mathbf{l},-\sigma}^\dagger\,|\,a_{\mathbf{k}\sigma}\rangle\rangle\\&\qquad+J_0N^{-1}\sum_{\mathbf{l}}\exp[i(\mathbf{k}'-\mathbf{l})\cdot\mathbf{R}_{j'}]\langle\langle m_{j\sigma}m_{j'\sigma}a_{\mathbf{l}\sigma}^\dagger+m_{j\sigma}S_{j'\sigma}a_{\mathbf{l},-\sigma}^\dagger\,|\,a_{\mathbf{k}\sigma}\rangle\rangle-J_0N^{-1}\sum_{\mathbf{l}\mathbf{l}'}\exp[i(\mathbf{l}'-\mathbf{l})\cdot\mathbf{R}_{j'}]\\&\qquad\times\langle\langle S_{j,-\sigma}a_{\mathbf{l}\sigma}^\dagger a_{\mathbf{k}'\sigma}^\dagger a_{\mathbf{l}',-\sigma}-S_{j\sigma}a_{\mathbf{l},-\sigma}^\dagger a_{\mathbf{k}'\sigma}^\dagger a_{\mathbf{l}'\sigma}\,|\,a_{\mathbf{k}\sigma}\rangle\rangle=-(2\pi)^{-1}\langle m_{j\sigma}\rangle\delta_{\mathbf{k}',\mathbf{k}}.\end{aligned} \tag{2.24}$$

Here j is one impurity (at $\mathbf{R}_j$) and j' is the other impurity (at $\mathbf{R}_{j'}$). These are rather frightening equations, but as in Nagaoka's paper, after the chain-breaking is managed, only a finite number of unknowns occurs, and the equations can be solved exactly for them. The problem of chain-breaking will be discussed in the next section.

It should be noted that in Eqs. (2.22)–(2.24) and in what follows, the energy dependence of the Green's functions is omitted in notation for convenience, but is always to be understood.

3. CHAIN-BREAKING, AND A THIRD POWER OF J_0 CALCULATION

Equations (2.23) and (2.24) involve Green's functions of higher order for which we must either get new equations of motion, or else chain-break into approximate linear combinations of the basic functions in Eqs. (2.14)–(2.16). Nagaoka followed Zubarev[11] in the manner of chain-breaking, keeping coefficients that conserved the total spin. He verified that the results were exact to terms involving the third power of J_0.

When the operators become more and more complicated, it beomces more and more difficult to know just what linear combination of the basic Green's functions to take. Our approach will be to let the third power of J_0 terms guide from the outset the details of the chain-breaking. The importance of these terms was first demonstrated by Kondo[1] in the scattering problem. He showed that these terms could explain the resistance minimum, and in fact the deluge of papers on this and related problems is a testimonial to the significance of Kondo's paper, and in particular to the importance of the terms of higher power than the second. We shall need G, therefore, accurate to at least three powers of J_0. From Eqs. (2.22)–(2.24) this means that Y and Z are needed to two powers of J_0, and the undecoupled Green's function in the Y and Z equations to one power of J_0. Thus we shall calculate the various equations for the latter to the desired power of J_0 and see if some chain-breaking can be inferred.

Before doing this, we should like to demonstrate directly that the third power of J_0 terms are of significance for the Ruderman-Kittel problem. To do this, we have worked out the exact third-power expression G^3 for G, omitting reference to magnetic fields. After a mountainous calculation, we found

$$\begin{aligned}\sum_\sigma G_\sigma^3(\mathbf{k}\mathbf{k}\,|\,\omega)=&-\pi^{-1}[\omega-\xi(\mathbf{k})]^{-1}+J_0N^{-1}[\omega-\xi(\mathbf{k})]^{-2}\\&\times\{\langle S_1^2+S_2^2\rangle[2h(0)(1+2g(0))+4u]+\langle S_{1z}S_{2z}\rangle\\&[4\cos(k\cdot R)h(R)(1+4g(0))\\&-4h(R)(2g(R)+h(R))+8u]\}\,,\end{aligned} \tag{3.1}$$

where

$$h(\mathbf{R})=-J_0N^{-1}\sum_{\mathbf{k}}\exp[i\mathbf{k}\cdot\mathbf{R}][\omega-\xi(\mathbf{k})]^{-1},$$

$$g(\mathbf{R})=-J_0N^{-1}\sum_{\mathbf{k}}\exp[i\mathbf{k}\cdot\mathbf{R}]\times[\omega-\xi(\mathbf{k})]^{-1}[f(\xi(\mathbf{k}))-\tfrac{1}{2}], \tag{3.2}$$

$$u=(J_0/N)^2\sum_{\mathbf{l}\mathbf{l}'}\frac{f(\xi)-f(\xi')}{(\xi-\xi')(\omega-\xi')},\quad \begin{aligned}\xi&=\xi(\mathbf{l})\\ \xi'&=\xi(\mathbf{l}').\end{aligned}$$

$\mathbf{R}$ here is $\mathbf{R}_1-\mathbf{R}_2$.

If one sets $\langle m_{jz}\rangle=0$, and $\langle S_1^2\rangle=\langle S_2^2\rangle=S(S+1)$ in Eq.

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[11] D. N. Zubarev, Usp. Fiz. Nauk **71**, 71 (1960) [English transl.: Soviet Phys.—Usp. **3**, 320 (1960)].

(3.1), the remaining terms give

$$\tau_{\mathbf{k}}^{-1}=\mathrm{Im}G^{-1}(\mathbf{kk})=\frac{3\pi J_0^2S(S+1)c}{E_F}[1+4\ \mathrm{Re}g],\qquad(3.3)$$

where c is the impurity concentration. This expression for the relaxation time (in this case equal to the lifetime) is Kondo's famous result. On the other hand, the first term in the second square bracket of Eq. (3.1) may be inserted into Eq. (2.21) to give a contribution to Eq. (2.5)

$$J_{12}\cong J_{12}^{(0)}\equiv\frac{18\pi J_0^2}{E_F}\frac{x\cos x-\sin x}{x^4},\quad x=2k_FR,\qquad(3.4)$$

which is the standard Ruderman-Kittel-Kasuya-Yosida expression. This method was used by Kim and Nagaoka.[12] The next term in the second square bracket is third power in J_0 and usually neglected, but it looks a good deal like the standard term except for the appearance of the Kondo g factor. This suggests a possible temperature dependence in the effective Heisenberg interaction, and it is this effect that we wish to pursue in greater detail in what follows.

We now return to the problem of chain-breaking Eqs. (2.23) and (2.24). We need for this purpose G, Y, and Z to first power in J_0, as well as certain averages which are to be evaluated by the Green's-function method also. Without the tedious details, we present the results for these quantities, the superscript in parenthesis indicating the power of J_0 up to which these expressions are valid:

$$G_\sigma(\mathbf{k}'\mathbf{k})^{(1)}=[\omega-\xi(\mathbf{k}'\sigma)]^{-1}\left\{-\frac{1}{2\pi}\delta_{\mathbf{k}',\mathbf{k}}+\sum_{j=1}^{2}J_0N^{-1}\langle m_{\sigma j}\rangle\exp[i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}_j][\omega-\xi(\mathbf{k}\sigma)]^{-1}\right\},\qquad(3.5\mathrm{a})$$

$$Z_\sigma(j\mathbf{k}'\mathbf{k})^{(1)}=[\omega-\xi(\mathbf{k}'\sigma)]^{-1}\left\{-\frac{1}{2\pi}\langle m_{\sigma j}\rangle\delta_{\mathbf{k}'\mathbf{k}}+\sum_{j'=1}^{2}J_0N^{-1}\langle m_{\sigma j}m_{\sigma j'}\rangle\exp[i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}_{j'}][\omega-\xi(\mathbf{k}\sigma)]^{-1}\right\},\qquad(3.5\mathrm{b})$$

$$Y_\sigma(j\mathbf{k}'\mathbf{k})^{(1)}=J_0N^{-1}[\omega-\xi(\mathbf{k}'\sigma)]^{-1}[\omega-\xi(\mathbf{k}\sigma)]^{-1}\exp[i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}_j)\{\langle S_{j,-\sigma}S_{j\sigma}\rangle+2f(\xi(\mathbf{k}'\sigma))\langle m_{j\sigma}\rangle\},\qquad(3.5\mathrm{c})$$

$$\langle n_{\mathbf{ll}',\sigma}\rangle^{(1)}=f(\xi(\mathbf{l}\sigma))\delta_{\mathbf{ll}'}+J_0N^{-1}\sum_j\exp[i(\mathbf{l}-\mathbf{l}')\cdot\mathbf{R}_j]\langle m_{\sigma j}\rangle\frac{f(\xi(\mathbf{l}))-f(\xi(\mathbf{l}'))}{\xi(\mathbf{l}')-\xi(\mathbf{l})},\qquad(3.5\mathrm{d})$$

$$\langle m_{\sigma j}n_{\mathbf{ll}',\sigma}\rangle^{(1)}=f(\xi(\mathbf{l}))\langle m_{\sigma j}\rangle\delta_{\mathbf{ll}'}+J_0N^{-1}\sum_{j'}\exp[i(\mathbf{l}-\mathbf{l}')\cdot\mathbf{R}_{j'}]\langle m_{j\sigma}m_{j'\sigma}\rangle\frac{f(\xi(\mathbf{l}))-f(\xi(\mathbf{l}'))}{\xi(\mathbf{l}')-\xi(\mathbf{l})},\qquad(3.5\mathrm{e})$$

$$\langle S_{j\sigma}a_{\mathbf{l},-\sigma}{}^{\dagger}a_{\mathbf{l}',\sigma}\rangle=J_0N^{-1}\exp[i(\mathbf{l}-\mathbf{l}')\cdot\mathbf{R}_j]\left\{\langle S_{j\sigma}S_{j,-\sigma}\rangle\frac{f(\xi(\mathbf{l}))-f(\xi(\mathbf{l}'))}{\xi(\mathbf{l}')-\xi(\mathbf{l})}+2\langle m_{j\sigma}\rangle\frac{f(\xi(\mathbf{l}'))[1-f(\xi(\mathbf{l}))]}{\xi(\mathbf{l}')-\xi(\mathbf{l})}\right\}.\qquad(3.5\mathrm{f})$$

Next, as an example of how the chain-breaking works, consider one of the undecoupled functions in Eq. (2.23) to first order:

$$\langle\langle m_{1\sigma}m_{2\sigma}a_{\mathbf{l}\sigma}{}^{\dagger}|a_{\mathbf{k}\sigma}\rangle\rangle^{(1)}=[\omega-\xi(\mathbf{l}\sigma)]^{-1}\{-\langle m_{1\sigma}m_{2\sigma}\rangle\delta_{\mathbf{lk}}+[\omega-\xi(\mathbf{k}\sigma)]^{-1}J_0N^{-1}\sum_{j'=1}^{2}\exp[i(\mathbf{l}-\mathbf{k})\cdot\mathbf{R}_{j'}]\langle m_{1\sigma}m_{2\sigma}m_{j'\sigma}\rangle\}.\qquad(3.6)$$

But to this order, from Eq. (3.3) we have

$$\langle\langle m_{1\sigma}m_{2\sigma}a_{\mathbf{l}\sigma}{}^{\dagger}|a_{\mathbf{k}\sigma}\rangle\rangle^{(1)}=\langle m_{1\sigma}\rangle Z_\sigma(2\mathbf{lk})^{(1)}+\langle m_{2\sigma}\rangle Z_\sigma(1\mathbf{lk})^{(1)}-\langle m_{1\sigma}m_{2\sigma}\rangle G_\sigma(\mathbf{lk})^{(1)}.\qquad(3.7)$$

The *chain-breaking approximation* consists of assuming that this relation is good to all orders, i.e.,

$$\langle\langle m_{1\sigma}m_{2\sigma}a_{\mathbf{l}\sigma}{}^{\dagger}|a_{\mathbf{k}\sigma}\rangle\rangle\cong\langle m_{1\sigma}\rangle Z_\sigma(2\mathbf{lk})+\langle m_{2\sigma}\rangle Z_\sigma(1\mathbf{lk})-\langle m_{1\sigma}m_{2\sigma}\rangle G_\sigma(\mathbf{lk}).\qquad(3.8\mathrm{a})$$

We have worked this out in detail since it is an important one. Notice the sign before the last term on the right. This decoupling is perhaps not unique, but it is the simplest relation that is satisfied to first power in J_0.[13]

Another example is the following

$$\begin{aligned}\langle\langle S_{1\sigma}a_{\mathbf{l}-\sigma}{}^{\dagger}a_{\mathbf{k}'\sigma}{}^{\dagger}a_{\mathbf{l}'\sigma}|a_{\mathbf{k}\sigma}\rangle\rangle^{(1)}&=J_0N^{-1}\langle S_{1\sigma}S_{1,-\sigma}\rangle\left\{\exp[i(\mathbf{l}-\mathbf{l}')\cdot\mathbf{R}_1]\frac{f(\xi')-f(\xi)}{\xi'-\xi}\frac{\delta_{\mathbf{k}'\mathbf{k}}}{\omega-\xi(\mathbf{k}'\sigma)}\right.\\&\left.+\exp[i(\mathbf{l}-\mathbf{k})\cdot\mathbf{R}_1]\frac{f(\xi(\mathbf{k}'\sigma))}{\omega-\xi(\mathbf{k}'\sigma)-\xi(\mathbf{k}\sigma)+\xi'}\frac{\delta_{\mathbf{l}'\mathbf{k}'}}{\omega-\xi(\mathbf{k}'\sigma)-\xi+\xi'}\right\}-2J_0N^{-1}\langle m_{1\sigma}\rangle\\&\times\left\{\exp[i(\mathbf{l}-\mathbf{l}')\cdot\mathbf{R}_1]\frac{f(\xi')[1-f(\xi)]}{\xi'-\xi}\frac{\delta_{\mathbf{k}'\mathbf{k}}}{\omega-\xi(\mathbf{k}'\sigma)}+\exp[i(\mathbf{l}-\mathbf{k})\cdot\mathbf{R}_1]\frac{f(\xi(\mathbf{k}'\sigma))[1-f(\xi)]}{\omega-\xi(\mathbf{k}'\sigma)-\xi(\mathbf{k}\sigma)+\xi'}\frac{\delta_{\mathbf{l}'\mathbf{k}'}}{\omega-\xi(\mathbf{k}'\sigma)-\xi+\xi'}\right\}\\&=\langle S_{1\sigma}S_{1\mathbf{l}'-\sigma}\rangle^{(1)}G_\sigma(\mathbf{k}'\mathbf{k})^{(0)}+\langle n_{\mathbf{k}'\mathbf{l}',\sigma}\rangle^{(0)}Y_\sigma(1\mathbf{lk})^{(1)},\end{aligned}$$

where $\xi=\xi(\mathbf{l}\sigma)$ and $\xi'=\xi(\mathbf{l}'\sigma)$. Removal of the superscript (1) gives then the chain-breaking approximation.

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[12] D. J. Kim and Y. Nagaoka, Progr. Theoret. Phys. (Kyoto) **30**, 743 (1963).

[13] This decoupling specifically requires that $\langle m_{j\sigma}\rangle$ be of *zeroth* order. This is a fundamental assumption in the paper.

We now list all the approximations used in the decoupling. The first has already been given in Eq. (3.8a). Then we have

$$\langle\langle m_{1\sigma}S_{2\sigma}a_{1-\sigma}{}^{\dagger}\,|\,a_{\mathbf{k}\sigma}\rangle\rangle,=\langle m_{1\sigma}\rangle Y_{\sigma}(2\mathbf{lk}),\tag{3.8b}$$

$$\langle\langle S_{1\sigma}S_{2,-\sigma}a_{1\sigma}{}^{\dagger}\,|\,a_{\mathbf{k}\sigma}\rangle\rangle=0,\tag{3.8c}$$

$$\langle\langle S_{1\sigma}m_{2\sigma}a_{1,-\sigma}{}^{\dagger}\,|\,a_{\mathbf{k}\sigma}\rangle\rangle=\langle m_{2\sigma}\rangle Y_{\sigma}(1\mathbf{lk}),\tag{3.8d}$$

$$\langle\langle S_{1,-\sigma}a_{1\sigma}{}^{\dagger}a_{\mathbf{k}'\sigma}{}^{\dagger}a_{\mathbf{l}',-\sigma}\,|\,a_{\mathbf{k}\sigma}\rangle\rangle=\langle S_{1,-\sigma}S_{\mathbf{k}'\mathbf{l}'\sigma}\rangle G_{\sigma}(\mathbf{lk})-\langle S_{1,-\sigma}S_{1\mathbf{l}'\sigma}\rangle G_{\sigma}(\mathbf{k}'\mathbf{k})\tag{3.8e}$$

$$\langle\langle S_{1,\sigma}a_{1,-\sigma}{}^{\dagger}a_{\mathbf{k}'\sigma}{}^{\dagger}a_{\mathbf{l}',\sigma}\,|\,a_{\mathbf{k}\sigma}\rangle\rangle=\langle n_{\mathbf{k}'\mathbf{l}'\sigma}\rangle Y_{\sigma}(1\mathbf{lk})-\langle S_{1\sigma}S_{1\mathbf{l}',-\sigma}\rangle G_{\sigma}(\mathbf{k}'\mathbf{k}),\tag{3.8f}$$

$$\langle\langle S_{1\sigma}a_{1\sigma}{}^{\dagger}a_{\mathbf{k}',-\sigma}{}^{\dagger}a_{\mathbf{l}'\sigma}\,|\,a_{\mathbf{k}\sigma}\rangle\rangle=\langle S_{1\sigma}S_{\mathbf{k}'\mathbf{l}',-\sigma}\rangle G_{\sigma}(\mathbf{lk})-\langle n_{1\mathbf{l}'\sigma}\rangle Y_{\sigma}(1\mathbf{k}'\mathbf{k}),\tag{3.8g}$$

$$\langle\langle S_{1\sigma}a_{1,-\sigma}{}^{\dagger}a_{\mathbf{k}',-\sigma}{}^{\dagger}a_{\mathbf{l}',-\sigma}\,|\,a_{\mathbf{k}\sigma}\rangle\rangle=\langle n_{\mathbf{k}'\mathbf{l}',-\sigma}\rangle Y_{\sigma}(1\mathbf{lk})-\langle n_{1\mathbf{l}',-\sigma}\rangle Y_{\sigma}(1\mathbf{k}'\mathbf{k}),\tag{3.8h}$$

$$\langle\langle m_{1\sigma}a_{1\sigma}{}^{\dagger}a_{\mathbf{k}',-\sigma}{}^{\dagger}a_{\mathbf{l}',-\sigma}\,|\,a_{\mathbf{k}\sigma}\rangle\rangle=\tfrac{1}{2}\langle n_{\mathbf{k}'\mathbf{l}'+}+n_{\mathbf{k}'\mathbf{l}'-}\rangle Z_{\sigma}(1\mathbf{lk})-\langle S_{1z}S_{\mathbf{k}'\mathbf{l}'z}\rangle G_{\sigma}(\mathbf{lk}),\tag{3.8i}$$

$$\langle\langle S_{1z}{}^{2}a_{1\sigma}{}^{\dagger}\,|\,a_{\mathbf{k}\sigma}\rangle\rangle=\langle S_{1z}{}^{2}\rangle G_{\sigma}(\mathbf{lk}),\tag{3.8j}$$

$$\langle\langle S_{1\sigma}m_{1\sigma}a_{1,-\sigma}{}^{\dagger}\,|\,a_{\mathbf{k}\sigma}\rangle\rangle=-\tfrac{1}{2}Y_{\sigma}(1\mathbf{lk}).\tag{3.8k}$$

Equation (3.8k) is exact to all orders for $S=\frac{1}{2}$. There seems to be no simple chain-breaking relation for arbitrary spin for this quantity. We therefore shall have in mind a restruction to $S=\frac{1}{2}$ in what follows. Equations (3.8e)–(3.8k) do not differ from what Nagaoka had; however the equations they now satisfy exactly to first order may have terms referring to both impurities. Equations (3.8a)–(3.8d) are new.

Just as we ended the previous section with the equations for G, Y, and Z, we shall end this section with the same three equations, but chain-broken:

$$[\omega-\xi(\mathbf{k}'\sigma)]G_{\sigma}(\mathbf{k}'\mathbf{k})+J_0N^{-1}\sum_{\mathbf{k}''j}\exp[i(\mathbf{k}'-\mathbf{k}'')\cdot\mathbf{R}_j]\Gamma_{\sigma}(j\mathbf{k}''\mathbf{k})=-\delta_{\mathbf{k}',\mathbf{k}}\frac{1}{2\pi},\tag{3.9}$$

$$\begin{aligned}&[\omega-\xi(\mathbf{k}'j\sigma)]Y_{\sigma}(j\mathbf{k}'\mathbf{k})+J_0N^{-1}[\langle S_j{}^2-m_{j\sigma}{}^2\rangle-2\langle S_{\mathbf{k}}{}^{(j)}\cdot S_j\rangle\\&\quad+\langle S_{\mathbf{k}',\sigma}{}^{(j)}S_{j,-\sigma}\rangle]\sum_{\mathbf{k}''}\exp[i(\mathbf{k}'-\mathbf{k}'')\cdot\mathbf{R}_j]G_{\sigma}(\mathbf{k}''\mathbf{k})-J_0N^{-1}\sum_{\mathbf{k}''}\exp[i(\mathbf{k}'-\mathbf{k}'')\cdot\mathbf{R}_j][\langle n_{\mathbf{k}',\sigma}{}^{(j)}-\tfrac{1}{2}\rangle Y_{\sigma}(j\mathbf{k}''\mathbf{k})\\&\qquad-\langle n_{\mathbf{k}'+}{}^{(j)}+n_{\mathbf{k}'-}{}^{(j)}-1\rangle\Gamma_{\sigma}(j\mathbf{k}''\mathbf{k})]-J_0N^{-1}\langle m_{j'\sigma}\rangle\sum_{\mathbf{k}''}\exp[i(\mathbf{k}'-\mathbf{k}'')\cdot\mathbf{R}_{j'}]Y_{\sigma}(j\mathbf{k}''\mathbf{k})=0.\end{aligned}\tag{3.10}$$

$$\begin{aligned}&[\omega-\xi(\mathbf{k}'\sigma)]Z_{\sigma}(j\mathbf{k}'\mathbf{k})+J_0N^{-1}\sum_{\mathbf{k}''}\exp[i(\mathbf{k}'-\mathbf{k}'')\cdot\mathbf{R}_j]\\&\quad\times\{\langle m_{j\sigma}{}^2-S_{\mathbf{k}',-\sigma}{}^{(j)}S_{j\sigma}\rangle G_{\sigma}(\mathbf{k}''\mathbf{k})+\langle n_{\mathbf{k}'\sigma}{}^{(j)}-\tfrac{1}{2}\rangle Y_{\sigma}(j\mathbf{k}''\mathbf{k})\}+J_0N^{-1}\sum_{\mathbf{k}''}\exp[i(\mathbf{k}'-\mathbf{k}'')\cdot\mathbf{R}_{j'}]\{-\langle m_{j\sigma}m_{j'\sigma}\rangle G_{\sigma}(\mathbf{k}''\mathbf{k})\\&\qquad+\langle m_{j'\sigma}\rangle Z_{\sigma}(j\mathbf{k}''\mathbf{k})+\langle m_{j\sigma}\rangle\Gamma_{\sigma}(j'\mathbf{k}''\mathbf{k})\}+P(j\sigma)G_{\sigma}(\mathbf{k}'\mathbf{k})=-\langle m_{j\sigma}\rangle\delta_{\mathbf{k}'\mathbf{k}}(2\pi)^{-1}.\end{aligned}\tag{3.11}$$

Here j is one impurity, j' the other, and

$$n_{\mathbf{k}'\sigma}{}^{(j)}=\sum_{\mathbf{k}''}\exp[i(\mathbf{k}''-\mathbf{k}')\cdot\mathbf{R}_j]n_{\mathbf{k}'\mathbf{k}''\sigma},\tag{3.12}$$

$$\mathbf{S}_{\mathbf{k}'}{}^{(j)}=\sum_{\mathbf{k}''}\exp[i(\mathbf{k}''-\mathbf{k}')\cdot\mathbf{R}_j]\mathbf{S}_{\mathbf{k}'\mathbf{k}''}.\tag{3.13}$$

The energy denominators in Eqs. (3.9) and (3.11) are defined by Eq. (2.3), and the one in Eq. (3.10) is defined by

$$\xi(\mathbf{k}j\sigma)\equiv\xi(\mathbf{k},\sigma)+E(j\sigma)-E_F,\tag{3.14}$$

where

$$E(j\sigma)=J_0N^{-1}\sum_{\mathbf{k}}\langle n_{\mathbf{k}\sigma}{}^{(j)}-n_{\mathbf{k},-\sigma}{}^{(j)}\rangle.\tag{3.15}$$

The expression on the right in Eq. (3.15) can be shown (see Appendix B) to contain the Ruderman-Kittel formula, to terms of second power in J_0, plus a self-energy term. Finally, in Eq. (3.11)

$$p(j\sigma)=J_0N^{-1}\sum_{\mathbf{k}}[\langle S_{j,-\sigma}S_{\mathbf{k}\sigma}{}^{(j)}\rangle-\langle S_{j\sigma}S_{\mathbf{k},-\sigma}{}^{(j)}\rangle].\tag{3.16}$$

Equations (3.9)–(3.11) are still rather frightful, but at least only G's, Y's, and Z's appear as unknowns.

4. SOLVING THE EQUATIONS

In order to solve Eqs. (3.9)–(3.11) we must introduce certain sums:

$$\begin{aligned}G_{\sigma}(j'\mathbf{l})&\equiv\sum\exp[-i\mathbf{k}'\cdot\mathbf{R}_{j'}]G_{\sigma}(\mathbf{k}'\mathbf{k}),\\Y_{\sigma}(jj'\mathbf{l})&\equiv\sum\exp[-i\mathbf{k}'\cdot\mathbf{R}_{j'}]Y_{\sigma}(j\mathbf{k}'\mathbf{l}),\\Z_{\sigma}(jj'\mathbf{l})&\equiv\sum\exp[-i\mathbf{k}'\cdot\mathbf{R}_{j'}]Z_{\sigma}(j\mathbf{k}'\mathbf{l}).\end{aligned}\tag{4.1}$$

We also need

$$\bar{G}_\sigma(j\mathbf{l})=\sum_{\mathbf{k}'}\exp[-i\mathbf{k}'\cdot\mathbf{R}_j][\omega-\xi(\mathbf{k}'\sigma)]^{-1}G_\sigma(\mathbf{k}'\mathbf{k})\,. \tag{4.2}$$

Now by multiplying Eqs. (3.9)–(3.11) by $\exp(-i\mathbf{k}'\cdot\mathbf{R}_1)$ and summing over $\mathbf{k}'$, we get equations depending only on the set of functions in Eqs. (4.1)–(4.2). Similarly we multiply by $\exp(-i\mathbf{k}'\cdot\mathbf{R}_2)$ and sum. The resulting set of equations involves then a finite (and small) number of unknowns, which can be solved for without approximation. The equations obtained in this way are the following:

$$G_\sigma(1\mathbf{k})=\alpha_\sigma(1\mathbf{k})+h_\sigma(0)\Gamma_\sigma(11\mathbf{k})+h_\sigma(\mathbf{R})\Gamma_\sigma(22\mathbf{k})\,, \tag{4.3}$$

$$\begin{aligned}Y_\sigma(11\mathbf{k})=[g'_{+,1\sigma}(0)+g'_{-,1\sigma}(0)]\Gamma_\sigma(11\mathbf{k})\\ -g'_{\sigma,1\sigma}(0)Y_\sigma(11\mathbf{k})-\langle m_{2\sigma}\rangle h_{1\sigma}(\mathbf{R})Y_\sigma(12\mathbf{k})\\ +K_{1\sigma}(1|0)G_\sigma(1\mathbf{k})\,,\end{aligned} \tag{4.4}$$

$$\begin{aligned}Y_\sigma(12\mathbf{k})=[g'_{+,1\sigma}(\mathbf{R})+g'_{-,1\sigma}(\mathbf{R})]\Gamma_\sigma(11\mathbf{k})\\ -g'_{\sigma,1\sigma}(\mathbf{R})Y_\sigma(11\mathbf{k})-\langle m_{2\sigma}\rangle h_{1\sigma}(0)Y_\sigma(12\mathbf{k})\\ +K_{1\sigma}(1|\mathbf{R})G_\sigma(1\mathbf{k})\,,\end{aligned} \tag{4.5}$$

$$\begin{aligned}Z_\sigma(11\mathbf{k})=\langle m_{1\sigma}\rangle\alpha_\sigma(1\mathbf{k})+g'_{\sigma,\sigma}(0)Y_\sigma(11\mathbf{k})\\ +L_\sigma(1|0)G_\sigma(1\mathbf{k})+\langle m_{1\sigma}\rangle h_\sigma(\mathbf{R})\Gamma_\sigma(22\mathbf{k})\\ +\langle m_{2\sigma}\rangle h_\sigma(\mathbf{R})Z_\sigma(12\mathbf{k})\\ -\langle m_{1\sigma}m_{2\sigma}\rangle h_\sigma(\mathbf{R})G_\sigma(2\mathbf{k})+p(1\sigma)\bar{G}_\sigma(1\mathbf{k})\,,\end{aligned} \tag{4.6}$$

$$\begin{aligned}Z_\sigma(12\mathbf{k})=\langle m_{1\sigma}\rangle\alpha_\sigma(2\mathbf{k})+g'_{\sigma,\sigma}(\mathbf{R})Y_\sigma(11\mathbf{k})\\ +L_\sigma(1|\mathbf{R})G_\sigma(1\mathbf{k})+\langle m_{1\sigma}\rangle h_\sigma(0)\Gamma_\sigma(22\mathbf{k})\\ +\langle m_{g\sigma}\rangle h_\sigma(0)Z_\sigma(12\mathbf{k})-\langle m_{1\sigma}m_{2\sigma}\rangle h_\sigma(0)G_\sigma(2\mathbf{k})\\ +p(1\sigma)\bar{G}_\sigma(2\mathbf{k})\,.\end{aligned} \tag{4.7}$$

In these equations, a large number of abbreviations have been used, which will now be enumerated. First there are the α's, K's, and L's:

$$\alpha_\sigma(1\mathbf{k})=(2\pi)^{-1}\exp[-i\mathbf{R}_1\cdot\mathbf{k}][\omega-\xi(\mathbf{k}\sigma)]^{-1}, \tag{4.8}$$

$$\begin{aligned}K_{1\sigma}(1|\mathbf{R})=\langle S_1{}^2-m_{1\sigma}{}^2\rangle h_{\sigma 1}(\mathbf{R})\\ -2\gamma'_{1\sigma}(1|\mathbf{R})+\gamma'_{-\sigma,1\sigma}(1|\mathbf{R})\,,\end{aligned} \tag{4.9}$$

$$L_\sigma(1|\mathbf{R})=\langle m_{1\sigma}{}^2\rangle h_\sigma(\mathbf{R})-\gamma'_{-\sigma,\sigma}(1|\mathbf{R})\,. \tag{4.10}$$

These are abbreviations used simply to shorten the other equations.

Next there are the g's, h's, and γ's. These are sums defined as follows:

$$\begin{aligned}g'_{\sigma',1\sigma}(\mathbf{R})=-J_0N^{-1}\sum_{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{R})\\ \times\langle n_{\mathbf{k}\sigma'}{}^{(1)}-\tfrac{1}{2}\rangle[\omega-\xi(\mathbf{k}1\sigma)]^{-1},\end{aligned} \tag{4.11}$$

$$\begin{aligned}h_{1\sigma}(\mathbf{R})=-J_0N^{-1}\sum_{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{R})\\ \times[\omega-\xi(\mathbf{k}1\sigma)]^{-1},\end{aligned} \tag{4.12}$$

$$\begin{aligned}\gamma'_{\sigma',1\sigma}(1|\mathbf{R})=-J_0N^{-1}\sum_{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{R})\\ \times\langle S_{\mathbf{k}\sigma'}{}^{(1)}\cdot S_{1,-\sigma'}\rangle[\omega-\xi(\mathbf{k}1\sigma)]^{-1},\end{aligned} \tag{4.13}$$

using Eqs. (3.12) and (3.13) .The subscripts and superscripts on these quantities are not altogether randomly placed; they mean the following. The superscript on g and γ refers to the superscript on the n and $S_{\mathbf{k}}$ that appear in their summands. Similarly the first spin index σ' on g and γ, refers to the spin index on the n and $S_{\mathbf{k}}$. The second subscripts on g and γ, and the only subscript on h refer to the $\xi(\mathbf{k}1\sigma)$ in the energy denominator. If instead of the subscript 1σ we had simply σ, then the energy denominator would be simply $\omega-\xi(\mathbf{k}\sigma)$. Thus

$$\begin{aligned}g'_{\sigma',\sigma}(\mathbf{R})=-J_0N^{-1}\sum_{\mathbf{k}}\exp[i\mathbf{k}\cdot\mathbf{R}]\\ \times\langle n_{\mathbf{k}\sigma'}{}^{(1)}-\tfrac{1}{2}\rangle[\omega-\xi(\mathbf{k}\sigma)]^{-1}.\end{aligned} \tag{4.14}$$

As regards the first spin subscript on g and γ, we shall adopt the convention that if it does not appear at all, then the following sums are meant:

$$g'_{,1\sigma}(\mathbf{R})=\tfrac{1}{2}\sum_{\sigma'}g'_{\sigma',1\sigma}(\mathbf{R})\,, \tag{4.15}$$

$$\begin{aligned}\gamma'_{,1\sigma}(1|\mathbf{R})=-J_0N^{-1}\sum\exp(i\mathbf{k}\cdot\mathbf{R})\\ \times\langle S_{\mathbf{k}}{}^{(1)}\cdot S_1\rangle[\omega-\xi(\mathbf{k}1\sigma)]^{-1}.\end{aligned} \tag{4.16}$$

This completes the definitions of the functions that appear in Eqs. (4.3)–(4.7). If one of the g, h, or γ appear as a function of 0 rather than of $\mathbf{R}$, then they are obtained from the above formulas by setting $\mathbf{R}=0$.

The g function is related to Kondo's similarly notated function (but containing an extra $\frac{1}{2}$ in the numerator of the summand) and gives rise to the log-T dependence in the resistivity, if we replace $\langle n_{\mathbf{k}}\rangle$ by a step function, and neglect local field effects at the impurity. If the latter are taken into account, then at very low temperatures g becomes temperature-independent. In Appendix A we derive these two expressions, and infer an interpolation formula. In any case it is clear that we must be careful to take into account situations where a local field occurs, especially since in the Heisenberg interaction, we are dealing with these very fields.

Before proceeding, notice the various orders of smallness indicated by the three types of sums g, h, and γ. Because of the log-T behavior, g must be taken to zeroth order in smallness even though the factor J_0 appears in it. (As is well known the real part of $1+2g$ is actually set equal to zero in defining the resonance temperature.[3])

However h is always of the order of J_0n_c, where n_c is the density of states at the energy E. The important E's are near the Fermi surface, and in that case J_0n_c is quite small. We therefore treat h as of first order in smallness.

Finally, γ will also be treated as first order. It looks as if it might be second order, since it contains one factor of J_0 in its definition, and another factor in the lowest order terms of its summand. The latter we regard as a true first-order effect, but the sum over k gives rise to a logarithmic term that may nullify the effect of the

the other factor J_0. Thus we conclude that γ is of first order.

While we are on this topic of orders, notice that the p and $E(j\sigma)$ of Eqs. (3.15) and (3.16) are of second order.

In what follows and in fact in what preceded we make a distinction between powers of J_0 and orders of n_cJ_0. The chain-breaking approximations referred only to the powers of J_0, but not necessarily to the orders of J_0n_c.

We are now faced with solving Eqs. (4.3)–(4.7). This is an algebraic problem of no unusual difficulty, although it becomes enormously tedious. We shall write the answer down directly for G without going through any of the intermediate steps. We mention, however, that it is somewhat simpler if one solves first for Γ and then for G. The answer is

$$G_\sigma(\mathbf{k}'\mathbf{k})=-\delta_{\mathbf{k}',\mathbf{k}}\frac{1}{2\pi}\frac{1}{\omega-\xi(\mathbf{k}'\sigma)}-\frac{J_0N^{-1}}{\omega-\xi(\mathbf{k}'\sigma)}\frac{1}{D_\sigma}\times\sum_{j=1}^{2}\exp(i\mathbf{k}'\cdot\mathbf{R}_j)\{C_\sigma(j'\mathbf{k})A_\sigma(jj')+C_\sigma(j\mathbf{k})[1+A_\sigma(j'j')]\}. \tag{4.17}$$

Here the denominator D is symmetric in j and j' (j' is always the impurity that is not j here)

$$D_\sigma=D_\sigma(jj')=[1+A_\sigma(jj)][1+A_\sigma(j'j')]-A_\sigma(jj')A_\sigma(j'j). \tag{4.18}$$

The expression for C is

$$C_\sigma(j\mathbf{k})=\alpha_\sigma(j\mathbf{k})[\langle m_{j\sigma}\rangle+B_\sigma(j)]+p(j\sigma)[\omega-\xi(\mathbf{k}\sigma)]^{-2}(2\pi)^{-1}\{\exp(-i\mathbf{k}\cdot\mathbf{R}_j)+\exp(-i\mathbf{k}\cdot\mathbf{R}_{j'})h_\sigma(\mathbf{R})\langle m_{j'\sigma}{}^{(-)}\rangle\} \tag{4.19}$$

in terms of a B to be defined below; and $A(j'j)$ is

$$A_\sigma(jj')=2\pi\sum_{\mathbf{k}}\exp(i\mathbf{R}_{j'}\cdot\mathbf{k})C_\sigma(j\mathbf{k})=-h_\sigma(\mathbf{R})[\langle m_{j\sigma}\rangle+B_\sigma(j)]+p(j\sigma)\times\left[\frac{dh_\sigma(\mathbf{R})}{d\omega}+h_\sigma(\mathbf{R})\frac{dh_\sigma(0)}{d\omega}\langle m_{j'\sigma}{}^{(-)}\rangle\right]. \tag{4.20}$$

The quantity $A(jj)$ splits up into two parts

$$A_\sigma(jj)=2\langle m_{j'\sigma}{}^{+}\rangle h_{j\sigma}(\mathbf{R})g_{,j\sigma}{}^{j}(\mathbf{R})+A_\sigma'(j), \tag{4.21}$$

A' being also in terms of B

$$A_\sigma'(j)=-2g^{j}{}_{,j\sigma}(0)-[g^{j}{}_{\sigma,\sigma}(0)-g^{j}{}_{\sigma,j\sigma}(0)+\epsilon_1]\times\frac{2g^{j}{}_{,j\sigma}(0)+\epsilon_2}{1+g^{j}{}_{\sigma,j\sigma}(0)+\epsilon_3}-h_\sigma(0)B_\sigma(j)+[h_\sigma(\mathbf{R})]^2\times\langle m_{j\sigma}m_{j'\sigma}{}^{(-)}\rangle+p(j\sigma)\left\{\frac{d}{dE}[h_\sigma(0)]+h_\sigma(\mathbf{R})\frac{d}{dE}[h_\sigma(\mathbf{R})]\langle m_{j'\sigma}{}^{(-)}\rangle\right\}. \tag{4.22}$$

Also

$$\langle m_{j'\sigma}{}^{(\pm)}\rangle=\frac{\langle m_{j'\sigma}\rangle}{1\pm h_\sigma(0)\langle m_{j'\sigma}\rangle}. \tag{4.23}$$

There have been used here a number of quantities which ultimately will play no role and will eventually be neglected. Thus B is a first-order quantity:

$$B_\sigma(j)=-\langle S_j{}^2\rangle h_{j\sigma}(0)+2\gamma^{j}{}_{,j\sigma}(j|0)+\langle m_{j\sigma}{}^2\rangle\times[h_\sigma(0)-h_{j\sigma}(0)]+\gamma^{j}{}_{-\sigma,j\sigma}(j|0)-\gamma^{j}{}_{-\sigma,\sigma}(j|0)+\epsilon_4+[g^{j}{}_{\sigma,\sigma}(0)-g^{j}{}_{\sigma,j\sigma}(0)+\epsilon_1]\frac{K_{j\sigma}(j|0)+\epsilon_5}{1+g^{j}{}_{\sigma,j\sigma}(0)+\epsilon_3} \tag{4.24}$$

and a series of ϵ's have been defined that are always of higher order than other terms that appear in the same bracket:

$$\begin{aligned}\epsilon_1&=h_{j\sigma}(\mathbf{R})[g_{\sigma,j\sigma}{}^{j}(\mathbf{R})\langle m_{j'\sigma}{}^{+}\rangle]+h_\sigma(\mathbf{R})[g^{j}{}_{\sigma,\sigma}(\mathbf{R})\langle m_{j'\sigma}{}^{-}\rangle],\\ \epsilon_2&=-2\langle m_{j'\sigma}{}^{(+)}\rangle h_{j\sigma}(\mathbf{R})g^{j}{}_{,j\sigma}(\mathbf{R}),\\ \epsilon_3&=-\langle m_{j'\sigma}{}^{(+)}\rangle h_{j\sigma}(\mathbf{R})g^{j}{}_{\sigma,j\sigma}(\mathbf{R}),\\ \epsilon_4&=-\langle m_{j'\sigma}{}^{(+)}\rangle h_{j\sigma}(\mathbf{R})K_\sigma(j\mathbf{R})+\langle m_{j'\sigma}{}^{(-)}\rangle h_\sigma(\mathbf{R})L_\sigma(j|\mathbf{R}),\\ \epsilon_5&=-\langle m_{j'\sigma}{}^{(+)}\rangle h_{j\sigma}(\mathbf{R})K_{j\sigma}(j|\mathbf{R}).\end{aligned} \tag{4.25}$$

Notice that all the ϵ's are proportional to $\langle m_{j'\sigma}\rangle$ and disappear in the one impurity problem.

The result in Eq. (4.17) is exact subject to the chain-breaking approximations. It is however limited to $S=\frac{1}{2}$. It is clear that if we remove all terms involving $\mathbf{R}$ and $m_{j'}$ we should get the corresponding solution for the one impurity problem. It is easily seen that in this case

$$G_\sigma(\mathbf{k}',\mathbf{k})=-\delta_{\mathbf{k}',\mathbf{k}}\frac{1}{2\pi}\frac{1}{\omega-\xi(\mathbf{k}'\sigma)}-\frac{J_0N^{-1}}{\omega-\xi(\mathbf{k}'\sigma)}\times\frac{\alpha_\sigma(j\mathbf{k})[\langle m_{j\sigma}\rangle+B_\sigma(j)]+p(j\sigma)[2\pi(\omega-\xi(\mathbf{k}\sigma))^2]^{-1}}{1-2g^{j}{}_{,j\sigma}(0)\dfrac{1+g^{j}{}_{\sigma,\sigma}(0)}{1+g^{j}{}_{\sigma,j\sigma}(0)}-h_\sigma(0)B_\sigma(j)+p(j\sigma)\dfrac{d}{dE}h_\sigma(0)}. \tag{4.26}$$

Here B is still quite complicated. This result differs from Nagaoka's by containing all the local field effects. If these are now eliminated (so that $\langle m_{j\sigma}\rangle=0$, $j=1$, 2) we get

$$G_\sigma(\mathbf{k}',\mathbf{k})=-\delta_{\mathbf{k}',\mathbf{k}}\frac{1}{2\pi}\frac{1}{\omega-\xi(\mathbf{k}')}-\frac{J_0N^{-1}}{\omega-\xi(\mathbf{k}')}\frac{\alpha_\sigma(j\mathbf{k})B_\sigma(j)}{1+2g^{j}(0)-h(0)B_\sigma(j)}, \tag{4.27}$$

where now B simplifies to

$$B_\sigma(j) = -\langle S_j^2\rangle h(0) + 2\gamma^j(j|0)\,. \tag{4.28}$$

5. THE EFFECTIVE HEISENBERG INTERACTION

It is clear from the preceding section that the solution in Eq. (4.17) is quite formidable. Fortunately for what we seek, most of the complications disappear to lowest order, and it is therefore in this approximation that we wish to continue the calculation. We are after terms proportional to $\langle m_{j\sigma} m_{j'\sigma}\rangle$, and the lowest order of such terms is second. Remember that a factor of g does not raise the order.

A first simplification to note is that the terms containing p in the A's and C's are generally of third order, and will be neglected. Second, the $A(jj')A(j'j)$ term in D, Eq. (4.18), is second order, and it can be seen that it can never produce a Heisenberg term in second order, if the denominator can be expanded. Such an expansion is valid only if $1+A$ does not go to zero. We shall assume that this restriction is permitted. The result of these approximations is that

$$\begin{aligned} G_\sigma(\mathbf{k}'\mathbf{k}) \cong{} & -\delta_{\mathbf{k}'\mathbf{k}} \frac{1}{2\pi} \frac{1}{\omega - \xi(\mathbf{k}'\sigma)} \\ & - \frac{J_0 N^{-1}}{\omega - \xi(\mathbf{k}'\sigma)} \sum_{j=1}^{2} \exp(i\mathbf{k}'\cdot\mathbf{R}_j) \\ & \times \{ -\alpha_\sigma(j'\mathbf{k}) h_\sigma(\mathbf{R}) X_\sigma(j) X_\sigma(j') + \alpha_\sigma(j\mathbf{k}) X_\sigma(j) \}\,, \end{aligned} \tag{5.1}$$

where

$$\begin{aligned} X_\sigma(j) = \frac{\langle m_{j\sigma}\rangle + B_\sigma(j)}{1 + A_\sigma(j)} \cong \frac{\langle m_{j\sigma}\rangle + B_\sigma(j)}{1 + A_\sigma'(j)} & \\ \times \left[1 - \frac{2\langle m_{j'\sigma}{}^{(+)}\rangle h_{j\sigma}(\mathbf{R}) g^j{}_{,j\sigma}(\mathbf{R})}{1 + A_\sigma'(j)} + \cdots \right]. & \end{aligned} \tag{5.2}$$

Once again we assume an expansion is possible, so that $1+A'$ must not go to zero. The expansion of X utilizes the separation of A in Eq. (4.21). This was the reason for the separation. Glancing at Eq. (5.1) and Eq. (2.21), we see that a Heisenberg type of term in the energy can come about through an X linearly, or quadratically. And in fact from Eq. (5.2) we see that X does have a second-order Heisenberg contribution

$$X_\sigma(j)|_{\mathrm{Heis}} = -2 \frac{\langle m_{j\sigma} m_{j'\sigma}\rangle}{\{1 + A_\sigma'(j)\}^2} h_{j\sigma}(\mathbf{R}) g^j{}_{,j\sigma}(\mathbf{R}) \tag{5.3}$$

and so does the quadratic term. Summing up, and placing in Eq. (2.5) we find

$$E'_{\mathrm{Heis}} = \sum J_{jj'} \langle S_{jz} S_{j'z}\rangle\,, \tag{5.4}$$

where

$$\begin{aligned} J_{jj'} = \frac{1}{2\pi} \sum_\sigma \mathrm{Im} \int_{-\infty}^{\infty} d\omega\, f(\omega)\omega \Bigg\{ - \left[\frac{d}{d\omega} h_\sigma(\mathbf{R})^2 \right] & \\ \times [1 + A_\sigma'(j)]^{-1} [1 + A_\sigma'(j')]^{-1} + 2 \sum_{j''} \left[\frac{d}{d\omega} h_\sigma(0) \right] & \\ \times h_{j''\sigma}(\mathbf{R}) g^{j''}{}_{,j''\sigma}(\mathbf{R}) [1 + A_\sigma'(j'')]^{-2} \Bigg\}\,. & \end{aligned} \tag{5.5}$$

This completes the derivation of the basic expression for the effective Heisenberg interaction to second order.

It should be noted that this is considerably simplified from the rather monstrous expressions at the end of Secs. 2 and 3. We can get a further simplification by integrating by parts the first term in curly brackets. The integrated out part will vanish at the limits, and the term proportional to $\omega df/d\omega$ will give zero also since $df/d\omega$ acts as a delta function (at $\omega = 0$). The result is then

$$\begin{aligned} J_{jj'} \equiv J(\mathbf{R}) = \mathrm{Im} \int_{-\infty}^{\infty} d\omega\, f(\omega) & \\ \times \Bigg\{ \sum_\sigma [h_\sigma(\mathbf{R})]^2 \left[\beta_{1,\sigma}{}^{(\omega)} + \omega \frac{d}{d\omega} \beta_{1,\sigma}{}^{(\omega)} \right] & \\ + \sum_{j''=1}^{2} \sum_\sigma h_{j''\sigma}(\mathbf{R}) g^{j''}{}_{,j''\sigma}(\mathbf{R}) \omega \beta_{2,j''\sigma}(\omega) \Bigg\}\,, & \end{aligned} \tag{5.6}$$

where we have isolated the R-dependent factors, the others abbreviated by

$$\beta_{1,\sigma} = \frac{1}{2\pi} [1 + A_\sigma'(1)]^{-1} [1 + A_\sigma'(2)]^{-1}\,, \tag{5.7}$$

$$\beta_{2,j''\sigma} = \frac{1}{2\pi} \frac{dh_\sigma(0)}{d\omega} [1 + A_\sigma'(j'')]^{-2}\,. \tag{5.8}$$

Up to now all the approximations have been made with powers of J_0 or orders of $J_0 n_c$ in mind. Equation (5.6) must be regarded as a first term in an expansion of powers of $J_0 n_c$ for example. In the next step, we shall appeal to another kind of approximation, namely that stemming from R being large. This is the typical situation envisaged: a very dilute alloy, with indirect interactions having nevertheless a surprising and significant effect. For very large R, one can employ asymptotic expansions for the integrals in Eq. (5.6) and a further simplification ensues. Namely terms containing the factors $\omega f(\omega)$ will provide higher order (in the sense of higher powers of $1/R$) effects than terms containing just $f(\omega)$ by itself. We shall not derive a complete defense of this statement; it can be verified by appeal to the methods described by Lighthill[14] for example. A plausi-

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[14] M. J. Lighthill, *Introduction to Fourier Analysis and Generalized Functions* (Cambridge University Press, New York, 1958).

bility argument can easily be made however. The factor $h(\mathbf{R})$ in the free-electron approximation is a swiftly oscillating function of $\omega^{1/2}R$, and $f(\omega)$ at low temperatures can be regarded as a function with a discontinuity at $\omega=0$. An integral containing a product of these factors will, for large R, "oscillate away" over most of the region of integration, the region right near the discontinuity being the exception. Thus the rest of the integrand can be (approximately) removed at the value $\omega=0$. But in the terms referred to above, the rest of the integrand contains a factor ω, and hence when removed at $\omega=0$ gives just 0. This means of course, zero to lowest order in powers of $1/R$. A term like the one containing $\beta_1(\omega)$ in Eq. (5.6) will not however disappear in lowest order when that is done, and hence the asymptotic expansion of Eq. (5.6) starts off as follows:

$$J(R)\sim \operatorname{Im}\sum \beta_{1,\sigma}(0)\int_{-\infty}^{\infty} d\omega\, f(\omega)[h_\sigma(R)]^2. \quad (5.9)$$

If we set $\beta_1=1$, we get exactly Kim and Nagaoka's[12] expression for the standard Ruderman-Kittel-Kasuya-Yosida expression [containing however a magnetic field effect which we neglect since it provides corrections of order $(\mu\mathcal{H}_z^{\text{ext}}/E_F)^{1/2}$]:

$$J(\mathbf{R})\sim J(\mathbf{R})^{(0)}\tfrac{1}{2}\sum_\sigma \operatorname{Re}[1+A_\sigma'(1)]^{-1}[1+A_\sigma'(2)]^{-1}, \quad (5.10)$$

where [see Eq. (3.4)]

$$J(\mathbf{R})^{(0)}=\frac{18\pi J_0^2}{E_F}\frac{\cos 2k_FR}{(2k_FR)^3}. \quad (5.11)$$

In obtaining this result, we have considered only the real part of β_1 to be significant, the imaginary part being of higher order in J_0n_c (at least until the resonance appears).

Equation (5.10) is then our corrected effective Heisenberg interaction. To zeroth order we have [see Eq. (4.22)]

$$A_\sigma'(j)=-2g^j{}_{,j\sigma}(0)\frac{1+g^j{}_{\sigma,\sigma}}{1+g^j{}_{\sigma,j\sigma}(0)}. \quad (5.12)$$

We remember that the subscript $j\sigma$ means that the energy denominator contains reference to the effective field at the site of the jth impurity. Thus the numerator of the fraction in Eq. (5.12) does *not* contain this effective field effect (it does however contain reference to an external magnetic field if there is one). The difference between these two cases is significant because, as shown in Appendix A, at low temperatures, if there is no local field, then g is approximately,

$$g_\sigma(0)=-J_0n_c\ln(E_F/k_BT),\quad \omega=0 \quad (5.13)$$

and if there is a local field it saturates to a value

$$g_{,j\sigma}(0)=-J_0n_c\ln[E_F/|\lambda_j|],\quad \omega=0, \quad (5.14)$$

where λ_j is the magnetic field energy. An interpolation formula (Appendix A) is then

$$\begin{aligned} g_{,j\sigma}(0)&\cong -J_0n_c\ln[E_F/(k_BT+|\lambda_j|)],\quad \omega=0 \quad (5.15)\\ &\equiv -J_0n_c\ln[b_j(T)]. \end{aligned}$$

Referring to Eq. (5.12), we see that if there is no effective field, then

$$A_\sigma'(j)=-2g(0)\cong 2J_0n_c\ln(E_F/k_BT),\quad \omega=0 \quad (5.16)$$

and if there is, then

$$A_\sigma'(j)=-a_{,j\sigma}[1-J_0n_c\ln(E_F/k_BT)],\quad \omega=0, \quad (5.17)$$

where

$$a_{,j\sigma}=\frac{-2J_0n_c\ln[b_j(T)]}{1-J_0n_c\ln[b_j(T)]}. \quad (5.18)$$

Here $b_j(T)$ as T gets lower and lower depends less and less on T and approaches a certain finite value. We shall assume that the denominator in Eq. (5.18) does not vanish. However, we envisage the possibility that $J_0n_c\ln b_j$ could become of the order of magnitude 1, so that $a_{,j\sigma}$ could be of order of magnitude 1. It could be smaller, but we shall treat it as not a negligible quantity.

By analyzing the various cases and temperature dependences of the quantities involved, we have reached the following conclusions on the basis of the results just obtained.

(1) If no local molecular fields exist, then Eq. (5.16) inserted into Eq. (5.10) shows that a logarithmic temperature dependence will occur that is quite similar to what arises in the resistivity. Our results indicate a resonance (we have left out the imaginary parts and hence the resonance width, but it is there) at a critical temperature

$$1+2J_0n_c\ln[E_F/k_BT_c]=0 \quad (5.19)$$

just the same as for the resistivity. Below this resonance it is not clear that our evaluation of the g's is correct, since some self-consistency correction is probably necessary.[3] This effect will be to raise the magnitude of the RKKY interaction if J_0 is negative, and to lower the magnitude if J_0 is positive. If J_0 is negative, then as T_c is reached the effect is much larger than could ever occur if J_0 is positive.

(2) If a local molecular field exists, then no matter what the sign of J_0 is, a critical temperature signaling a resonance will occur at T_c':

$$1-a_{,j\sigma}-\frac{2(J_0n_c)^2}{1-J_0n_c\ln b_j(T_c')}\ln[E_F/k_BT_c']=0. \quad (5.20)$$

We assume here that the denominator $1-J_0n_c\ln b_j$ is positive, however.

Let us consider the temperature effect for J_0 negative and a local field existing. At large T, $J(\mathbf{R})$ equals $J(\mathbf{R})^{(0)}$. As T drops, J gradually increases (both because of the linear and the quadratic terms in J_0 in A') until a maximum is reached, after which it falls. The maximum would not be infinite because of the resonant widths left out of our expressions.

Consider now the case where J_0 is positive, and a local field exists. Again at large T, $J(\mathbf{R})$ equals $J(\mathbf{R})^{(0)}$. As T decreases, we imagine that at first the terms linear in J_0 will have the largest effect, and these terms will *decrease* J. However, eventually these terms reach a final value given by Eq. (5.14), and then the explicitly T-dependent term in Eq. (5.17) takes over. The effect of this term will be to raise $J(\mathbf{R})$, so that as T decreases, first J decreases and then it increases to a maximum value, after which it finally decreases again.

These consitute the conclusions of the paper. There are two further comments we wish to make. The local field itself is usually thought to contain the RKKY term in it. For just two impurities, we could then formulate a self-consistency condition, and try to determine J as a function of m_j treating the local field energy λ as a known function of the unknown J. The temperature dependence might alter significantly because of this new place for the unknown. A calculation of this sort is deferred to a later paper.

Finally, a remark about accuracy. In the local-field-dependent expressions, the important T-dependent term in Eq. (5.17) contains two powers of J_0. If we expand the denominator containing A', this T-dependent term will occur in J only in fourth power of J_0 or higher. Since our approximations were valid exactly only to third power of J_0, could it not be the case that this local field effect is spurious? We see no convincing answer to this criticism. What we have obtained is an estimate of the powers of J_0 effects higher than the third, but we can not assume that the estimate is rigorous. We should have to perform the chain-breaking at one higher power of J_0 in order to be absolutely certain. Such a calculation seems almost prohibitive in complexity, but the indications are that the very low-temperature behavior might require it for the future.

APPENDIX A: EVALUATION OF g

We consider g at $\omega=0$ containing a local field energy λ in general in the denominator. We shall estimate on the basis of approximating $n_{\mathbf{k}}$ as a step function. We have then to evaluate

$$g=-J_0N^{-1}\sum_{\mathbf{k}} f_0[E(\mathbf{k})][E_F+\lambda-E(\mathbf{k})]^{-1}$$

$$=J_0\int dE\, n_c(E)f_0(E)(E-E_F-\lambda)^{-1}, \quad \text{(A1)}$$

where f_0 is the Fermi function relative to the Fermi energy E_F. Integration by parts gives

$$g=I_1+I_2, \quad \text{(A2)}$$

where

$$I_1=-J_0\int dE\frac{dn_c}{dE}f_0\ln\left|\frac{E-E_F-\lambda}{E_F}\right|, \quad \text{(A3)}$$

$$I_2=-J_0\int dE\, n_c\frac{df_0}{dE}\ln\left|\frac{E-E_F-\lambda}{E_F}\right|. \quad \text{(A4)}$$

Using a free-electron model

$$I_1=-\frac{3J_0}{2E_F}[x_+\ln x_+-x_-\ln x_-], \quad \text{(A5)}$$

where

$$x_\pm\equiv\left[\frac{E_F+\lambda}{E_F}\right]^{1/2}\pm1. \quad \text{(A6)}$$

I_1 is therefore of order J_0n_c and is neglected.

The other integral becomes on simple manipulations

$$I_2=-J_0n_c(E_F)[I_3+\ln(E_F/k_BT)], \quad \text{(A7)}$$

where

$$I_3=\int_{-\infty}^{\infty}d\epsilon\left[\frac{d}{d\epsilon}\frac{1}{e^\epsilon+1}\right]\ln|\epsilon-\lambda|k_BT|$$

$$=-\ln|\lambda/k_BT|, \quad \lambda\gg k_BT$$

$$=O(1), \qquad \lambda\rightarrow0. \quad \text{(A8)}$$

Since for $\lambda\rightarrow0$ we neglect this integral anyway, we infer an interpolation formula

$$I_3\cong-\ln[1+|\lambda/k_BT|], \quad \text{(A9)}$$

whence

$$g\cong-J_0n_c(E_F)\ln\left[\frac{E_F}{k_BT+|\lambda|}\right]. \quad \text{(A10)}$$

APPENDIX B: THE EVALUATION OF $E(j\sigma)$

From the definition in Eq. (3.15), and the relation in Eq. (3.5d) we have to second order

$$E(j\sigma)=2(J_0/N)^2\Bigg\{\langle m_{j'\sigma}\rangle \times\sum_{\mathbf{l}\mathbf{l}'}\exp[i(\mathbf{l}-\mathbf{l}')\cdot\mathbf{R}]\frac{f(\xi(\mathbf{l}))-f(\xi(\mathbf{l}'))}{\xi(\mathbf{l}')-\xi(\mathbf{l})} +m_{j\sigma}\sum_{\mathbf{l}\mathbf{l}'}\frac{f(\xi(\mathbf{l}))-f(\xi(\mathbf{l}'))}{\xi(\mathbf{l}')-\xi(\mathbf{l})}\Bigg\} \quad \text{(B1)}$$

The first term is the Ruderman-Kittel effective field from impurity j', and the second term is the effective field from that part of the conduction electron polarization caused by the jth impurity itself.