Kondo Effect in the Ruderman-Kittel-Kasuya-Yosida Interaction*

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Thei ndirect interaction between two impurity spins in a dilute magnetic alloy is studied in the temperature region where the Kondo effect is operative, using an extension of the Nagaoka approach. It is found that above the Kondo temperature there is no appreciable alteration in the standard Ruderman-Kittel-Kasuya-Yosida expression (RKKY) for the effective coefficient of interaction, contrary to the results of our previous paper, which predicted that a logarithmic temperature dependence occurs in this temperature region. But, in general, it is found that an additional term E' occurs in the effective interactions, which may be expressed in terms of the single-impurity t matrix. E' is calculated using both (a) the Nagaoka simple-pole expression for $t(\xi)$ and (b) the Bloomfield-Hamann solution. We find in case (a) that a ferromagnetic (nonoscillatory) supplement to the standard RKKY interaction arises for $T \ll T_K$, but that for case (b), this same interaction term E' is very much smaller than that found in case (a).

1. INTRODUCTION

IN a previous paper[1] (referred to as I in what follows), we have considered an extension of the single-impurity problem for dilute magnetic alloys to systems where two impurity spins interact simultaneously with the conduction electrons. This was done in order to investigate the effects of the anomalous Kondo terms[2] on the indirect impurity interactions of the Ruderman-Kittel-Kasuya-Yosida (RKKY) type at low temperatures. In I, a major assumption was that the statistical average of the spins, $\langle S_{jz} \rangle$, on the impurities was of zeroth order (orders being measured relative to powers of J_0/E_F, where J_0 is the exchange integral and E_F is the Fermi energy). A general formula for the effective RKKY-interaction term was obtained on this basis, subject to a certain decoupling of the Green's-function hierarchy of equations, and an attempt was made to evaluate the result for temperatures T greater than the Kondo temperature T_K. Unfortunately, it was pointed out to us[3] that the evaluation of a certain integral in this result was incorrect, and the general conclusion that a measureable, and in particular a logarithmic, temperature dependence in the RKKY interaction was not a true consequence of our general result. In fact, for $T > T_K$, our expression gives results identical to Suhl's. But it has been conjectured by a number of people that below T_K an enhanced RKKY interaction of a ferromagnetic type should occur on the Nagaoka Green's-function approach.[4] In the present paper, we investigate the problem to see if this conjecture is borne out by a detailed estimate of the energy expression below T_K. In this regard we generalize the results of I so as not to be restricted to $\langle S_{jz} \rangle$ of zeroth order, and we search for a solution for $T < T_K$.

Our results for the interaction terms between two impurities are given in terms of the one-impurity t matrix, so that a variety of special cases can be discussed, in principle, depending on which approximations go into the expressions to be used for the solution of the one-impurity problem. When the simple-pole approximation of Nagaoka is used, we find that, indeed, a ferromagnetic supplement to the ordinary RKKY interaction occurs below T_K, which is definitely ferromagnetic and corresponds precisely to Nagaoka's correlation result.[4] But using the more accurate expression for the t matrix derived by Bloomfield and Hamann[5] (BH), we find that the corresponding term is small compared to the standard RKKY term.

We have organized the paper as follows. In Sec. 2, we introduce the Hamiltonian containing two impurity spins interacting with the conduction electrons, and we set up the equations of motion for the Green's functions needed to calculate the average value of this Hamiltonian. In Sec. 3, we introduce several new functions, which allow an explicit separation of the interaction terms from the functions that occur when the impurities are isolated, and we then truncate the higher-order Green's functions, using the same general approximation method as was outlined in I. In Sec. 4, we solve the chainbroken set of equations and reduce these solutions to terms of leading order in $J_0\rho/N$, where ρ is the conduction-electron density of states at the Fermi surface, and N is the number of atoms in the crystal. In this section we also set up the integral relations that determine all quantities involved in our equations in terms of the single-particle t matrix. In Sec. 5, we determine the average energy of the system, using both the Nagaoka and BH solutions for the t matrix, and present our conclusions.

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2. HAMILTONIAN AND GREEN'S FUNCTIONS

We will drop all reference to an external field here, so that the Hamiltonian is given by

$$H'=H-NE_F$$

$$=\sum_{\mathbf{k},\sigma} n_{\mathbf{k}\sigma}\xi_{\mathbf{k}} - \frac{J_0}{N}\sum_{\mathbf{k}_1,\mathbf{k}_2,j} e^{i(\mathbf{k}_2-\mathbf{k}_1)\cdot\mathbf{R}_j} 2\mathbf{S}_j\cdot\mathbf{s}_{\mathbf{k}_1,\mathbf{k}_2}, \quad (2.1)$$

where it is to be understood that we are dealing with only two impurities, $j=1,2$. The operator notation appearing here has already been defined in I. We will once again direct our attention to the average value of the Hamiltonian, and for this purpose we will use a particular retarded Green's function $\langle\langle A(\lambda_1 t)\,|\,B(\lambda_2)\rangle\rangle$ as defined by Eq. (2.6) in I. In order to conform more closely to other work relating to the single-impurity problem, we define the Fourier transforms of the Green's function of (2.6) in I by the following relations:

$$\langle\langle A(\lambda_1,\xi)\,|\,B(\lambda_2)\rangle\rangle = \lim_{\epsilon\to 0^+}\int_{-\infty}^{\infty} e^{i\xi t-\epsilon t}\langle\langle A(\lambda_1,t)\,|\,B(\lambda_2)\rangle\rangle dt, \quad (2.2)$$

$$\langle\langle A(\lambda_1,t)\,|\,B(\lambda_2)\rangle\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\xi t}\langle\langle A(\lambda_1,\xi)\,|\,B(\lambda_2)\rangle\rangle d\xi, \quad (2.3)$$

where the energy is $\xi=E-E_F$ and t is the time. Thermal averages are to be calculated using the standard formula[6]

$$\langle B(\lambda_2)A(\lambda_1)\rangle = -\frac{1}{\pi}\int_{-\infty}^{\infty} f(\xi)\,\mathrm{Im}\langle\langle A(\lambda_1,\xi)\,|\,B(\lambda_2)\rangle\rangle d\xi, \quad (2.4)$$

where $f(\xi)$ is the Fermi function. The Fourier-transformed equation of motion for a Green's function takes the form

$$\xi\langle\langle A(\lambda_1,\xi)\,|\,B(\lambda_2)\rangle\rangle = \langle[A(\lambda_1),B(\lambda_2)]_+\rangle + \langle\langle[A(\lambda_1,\xi),H']_-\,|\,B(\lambda_2)\rangle\rangle. \quad (2.5)$$

The calculation of the average value of Eq. (2.1) necessitates the introduction of the Green's functions

$$G_\sigma(\mathbf{k}'\mathbf{k}\,|\,\xi)=\langle\langle a_{\mathbf{k}'\sigma}(\xi)\,|\,a_{\mathbf{k}\sigma}^\dagger\rangle\rangle, \quad (2.6)$$

$$\Gamma_\sigma(j\mathbf{k}'\mathbf{k}\,|\,\xi)=\langle\langle a_{\mathbf{k}'\sigma}M_{j\sigma}(\xi)\,|\,a_{\mathbf{k}\sigma}^\dagger\rangle\rangle + \langle\langle a_{\mathbf{k}'-\sigma}S_{j-\sigma}(\xi)\,|\,a_{\mathbf{k}\sigma}^\dagger\rangle\rangle, \quad (2.7)$$

where $\sigma=(+,-)$ represents the two possible spin projections, and

$$M_{j\sigma}=\sigma S_{jz}. \quad (2.8)$$

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

The average energy of the system is given by the expression

$$\langle H'\rangle = -\frac{1}{\pi}\sum_{\mathbf{k},\sigma}\int_{-\infty}^{\infty}\xi f(\xi)\,\mathrm{Im}G^+(\mathbf{k}\mathbf{k}\,|\,\xi)d\xi, \quad (2.9)$$

where, in general, a superscript $+$ or $-$ on a Green's function Z means

$$Z^\pm=\tfrac{1}{2}(Z_+\pm Z_-). \quad (2.10)$$

We will complete this section by determining the equations of motion for the functions defined by Eqs. (2.6) and (2.7), using Eq. (2.5). We have

$$(\xi-\xi_{\mathbf{k}'})G^\sigma(\mathbf{k}'\mathbf{k}\,|\,\xi) = \tfrac{1}{2}(1+\sigma)\delta_{\mathbf{k}'\mathbf{k}} - \frac{J_0}{N}\sum_{1,j} e^{i(1-\mathbf{k}')\cdot\mathbf{R}_j}\Gamma^\sigma(j\mathbf{l}\mathbf{k}\,|\,\xi); \quad (2.11)$$

$$\begin{aligned}(\xi-\xi_1)\Gamma^\sigma(j\mathbf{l}\mathbf{k}\,|\,\xi) &= \tfrac{1}{2}(1-\sigma)\langle S_{jz}\rangle - \frac{J_0}{N}\mathbf{S}_j{}^2\sum_{\mathbf{k}_1} e^{i(\mathbf{k}_1-1)\cdot\mathbf{R}_j}G^\sigma(\mathbf{k}_1\mathbf{k}\,|\,\xi)\\ &+\frac{J_0}{N}\sum_{\mathbf{k}_1} e^{i(\mathbf{k}_1-1)\cdot\mathbf{R}_j}\Gamma^\sigma(j\mathbf{k}_1\mathbf{k}\,|\,\xi)\\ &-\frac{J_0}{N}\sum_{\mathbf{k}_1} e^{i(\mathbf{k}_1-1)\cdot\mathbf{R}_{j'}}\Omega^\sigma(j'j\mathbf{k}_1\mathbf{k}\,|\,\xi)\\ &+\frac{J_0}{N}\sum_{\mathbf{k}_1,\mathbf{k}_2} e^{i(\mathbf{k}_2-\mathbf{k}_1)\cdot\mathbf{R}_j}Q^\sigma(j\mathbf{k}_1\mathbf{l}\mathbf{k}_2\mathbf{k}\,|\,\xi), \quad (2.12)\end{aligned}$$

where once again we adopt the convention that $j'\neq j$ in this equation and in all that follow. The two new Green's functions that appear in Eq. (2.12) are defined by the relations

$$\begin{aligned}\Omega_\sigma(j'j\mathbf{k}_1\mathbf{k}\,|\,\xi) &= \langle\langle a_{\mathbf{k}_1\sigma}M_{j'\sigma}M_{j\sigma}\,|\,a_{\mathbf{k}\sigma}^\dagger\rangle\rangle\\ &+\langle\langle a_{\mathbf{k}_1-\sigma}S_{j'-\sigma}M_{j\sigma}\,|\,a_{\mathbf{k}\sigma}^\dagger\rangle\rangle\\ &+\langle\langle a_{\mathbf{k}_1\sigma}S_{j'\sigma}S_{j-\sigma}\,|\,a_{\mathbf{k}\sigma}^\dagger\rangle\rangle\\ &-\langle\langle a_{\mathbf{k}_1-\sigma}M_{j\sigma}S_{j-\sigma}\,|\,a_{\mathbf{k}\sigma}^\dagger\rangle\rangle, \quad (2.13)\end{aligned}$$

$$\begin{aligned}Q_\sigma(j'\mathbf{k}_1\mathbf{l}\mathbf{k}_2\mathbf{k}\,|\,\xi) &= \langle\langle a_{\mathbf{k}_1-\sigma}{}^\dagger a_{1\sigma}a_{\mathbf{k}_2\sigma}S_{j\sigma}\,|\,a_{\mathbf{k}\sigma}^\dagger\rangle\rangle\\ &-\langle\langle a_{\mathbf{k}_1\sigma}{}^\dagger a_{1\sigma}a_{\mathbf{k}_2-\sigma}S_{j-\sigma}\,|\,a_{\mathbf{k}\sigma}^\dagger\rangle\rangle\\ &+\langle\langle a_{\mathbf{k}_1\sigma}{}^\dagger a_{1-\sigma}a_{\mathbf{k}_2\sigma}S_{j-\sigma}\,|\,a_{\mathbf{k}\sigma}^\dagger\rangle\rangle\\ &-\langle\langle a_{\mathbf{k}_1-\sigma}{}^\dagger a_{1-\sigma}a_{\mathbf{k}_2-\sigma}S_{j-\sigma}\,|\,a_{\mathbf{k}\sigma}^\dagger\rangle\rangle\\ &-2\langle\langle a_{\mathbf{k}_1-\sigma}{}^\dagger a_{1-\sigma}a_{\mathbf{k}_2\sigma}M_{j\sigma}\,|\,a_{\mathbf{k}\sigma}^\dagger\rangle\rangle. \quad (2.14)\end{aligned}$$

3. CHAINBREAKING RELATIONS

In I, we described in some detail a method of chain-breaking that was basically designed to determine the average energy exactly to at least the third power in the s-d coupling J_0, the expectation being that deviations from these approximate relationships are un-

important if $|J_0|/E_F \ll 1$, a requirement that is usually satisfied in dilute magnetic alloys. Our method of chain-breaking the functions defined by Eqs. (2.13) and (2.14) is based on this same approach, and therefore we will not trace through any of the lengthy calculations inherent to determining the proper approximations that were carried out in I.

We shall look for solutions that have contributions proportional to $\langle S_j \cdot S_{j'} \rangle$. Therefore, we start by making a separation of terms as follows:

$$G^+(\mathbf{k}'\mathbf{k}|\xi) = G^N(\mathbf{k}'\mathbf{k}|\xi) + \langle \mathbf{S}_j \cdot \mathbf{S}_{j'} \rangle G(\mathbf{k}'\mathbf{k}|\xi), \tag{3.1}$$

$$\Gamma^+(j\mathbf{k}'\mathbf{k}|\xi) = \langle \mathbf{S}_j \cdot \mathbf{S}_j \rangle \Gamma^N(j\mathbf{k}'\mathbf{k}|\xi) + \langle \mathbf{S}_j \cdot \mathbf{S}_{j'} \rangle \Lambda(j'\mathbf{k}'\mathbf{k}|\xi). \tag{3.2}$$

Such a separation is consistent with the results of Sec. 3 of I. Here, $G^N(\mathbf{k}'\mathbf{k}|\xi)$ and $\mathbf{S}_j^2\Gamma^N(j\mathbf{k}'\mathbf{k}|\xi)$ are the functions relevant to the problem dealing with *isolated* impurities. The expansions of the functions are similar in form, and therefore we will use

$$\Omega^+(j'j\mathbf{l}\mathbf{k}|\xi) = \langle \mathbf{S}_j \cdot \mathbf{S}_{j'} \rangle P(j'j\mathbf{l}\mathbf{k}|\xi), \tag{3.3}$$

$$Q^+(j\mathbf{k}_1\mathbf{l}\mathbf{k}_2\mathbf{k}|\xi) = \langle \mathbf{S}_j \cdot \mathbf{S}_j \rangle Q^N(j\mathbf{k}_1\mathbf{l}\mathbf{k}_2\mathbf{k}|\xi) + \langle \mathbf{S}_j \cdot \mathbf{S}_{j'} \rangle X(j'\mathbf{k}_1\mathbf{l}\mathbf{k}_2\mathbf{k}|\xi), \tag{3.4}$$

where in Eq. (3.3), only interaction terms occur because Ω^+ is a function involving two impurity operators explicitly, and therefore it vanishes unless there are indirect interactions between impurities.

Equations (3.1)–(3.4) are to be substituted into the Z^+ forms of Eqs. (2.11) and (2.12). Separating off terms proportional to $\langle S_j \cdot S_{j'} \rangle$ from the rest, we first get two equations independent of $\langle S_j \cdot S_{j'} \rangle$:

$$(\xi - \xi_{\mathbf{k}'}) G^N(\mathbf{k}'\mathbf{k}|\xi) = \delta_{\mathbf{k}'\mathbf{k}} - \frac{J_0}{N} \sum_{\mathbf{l},j} e^{i(\mathbf{l}-\mathbf{k}')\cdot\mathbf{R}_j} \mathbf{S}_j^2 \Gamma^N(j\mathbf{l}\mathbf{k}|\xi), \tag{3.5}$$

$$(\xi - \xi_{\mathbf{l}}) \Gamma^N(j\mathbf{l}\mathbf{k}|\xi) = -\frac{J_0}{N} \sum_{\mathbf{k}_1} e^{i(\mathbf{k}_1-\mathbf{l})\cdot\mathbf{R}_j} G^N(\mathbf{k}_1\mathbf{k}|\xi) + \frac{J_0}{N} \sum_{\mathbf{k}_1} e^{i(\mathbf{k}_1-\mathbf{l})\cdot\mathbf{R}_j} \Gamma^N(j\mathbf{k}_1\mathbf{k}|\xi) + \frac{J_0}{N} \sum_{\mathbf{k}_1,\mathbf{k}_2} e^{i(\mathbf{k}_2-\mathbf{k}_1)\cdot\mathbf{R}_j} Q^N(j\mathbf{k}_1\mathbf{k}_2\mathbf{k}|\xi). \tag{3.6}$$

We could, if we wish, *define* G^N and Γ^N by these equations. The remaining parts of Eqs. (2.11) and (2.12) are

$$(\xi - \xi_{\mathbf{k}'}) G(\mathbf{k}'\mathbf{k}|\xi) = -\frac{J_0}{N} \sum_{\mathbf{l},j} e^{i(\mathbf{l}-\mathbf{k}')\cdot\mathbf{R}_j} \Lambda(j'\mathbf{l}\mathbf{k}|\xi), \tag{3.7}$$

$$(\xi - \xi_{\mathbf{l}}) \Lambda(j'\mathbf{l}\mathbf{k}|\xi) = -\frac{J_0}{N} \mathbf{S}_j^2 \sum_{\mathbf{k}_1} e^{i(\mathbf{k}_1-\mathbf{l})\cdot\mathbf{R}_j} G(\mathbf{k}_1\mathbf{k}|\xi) + \frac{J_0}{N} \sum_{\mathbf{k}_1} e^{i(\mathbf{k}-\mathbf{l})\cdot\mathbf{R}_j} \Lambda(j'\mathbf{k}_1\mathbf{k}|\xi) - \frac{J_0}{N} \sum_{\mathbf{k}_1} e^{i(\mathbf{k}_1-\mathbf{l})\cdot\mathbf{R}_{j'}} P(j'j\mathbf{k}_1\mathbf{k}|\xi) + \frac{J_0}{N} \sum_{\mathbf{k}_1,\mathbf{k}_2} e^{i(\mathbf{k}_2-\mathbf{k}_1)\cdot\mathbf{R}_j} X(j'\mathbf{k}_1\mathbf{l}\mathbf{k}_2\mathbf{k}|\xi). \tag{3.8}$$

Equations (3.5) and (3.6) bear a close resemblance to those used in the single-impurity problem,[4] and hence we have denoted the functions contained there with the superscript N. The method being used here has the advantage that the results of the single-impurity problem are contained in the solutions obtained from Eqs. (3.5) and (3.6).

In the single-impurity problem formulated by Nagaoka,[4] certain symmetry relations are utilized (e.g., $\langle S_{j+} s_{\mathbf{l}_1\mathbf{l}_2-} \rangle = \langle S_{j-} s_{\mathbf{l}_1\mathbf{l}_2+} \rangle$) to simplify the equations, but these relations are valid only if $\langle S_{jz} \rangle = \langle S_{j'z} \rangle = 0$, as one may see from Eq. (3.5f) in I; in this case there is no difference between the spin-up and spin-down functions, e.g., $G_+(\mathbf{k}'\mathbf{k}|\xi) = G_-(\mathbf{k}'\mathbf{k}|\xi)$. If we envision the possibility that $\langle S_{jz} \rangle$ and $\langle S_{j'z} \rangle$ do not vanish, however, then the Z^- functions of the form defined by Eq. (2.10) do not vanish. Since the only change being made here from the Nagaoka formulation is to allow the possibility that $\langle S_{jz} \rangle$ and $\langle S_{j'z} \rangle$ are not zero, it is clear that the Z^- functions can be proportional only to these latter two averages. Thus the following separations are quite useful:

$$G^-(\mathbf{k}'\mathbf{k}|\xi) = \langle S_{jz} \rangle G^{(j)}(\mathbf{k}'\mathbf{k}|\xi) + \langle S_{j'z} \rangle G^{(j')}(\mathbf{k}'\mathbf{k}|\xi), \tag{3.9}$$

$$\Gamma^-(j\mathbf{l}\mathbf{k}|\xi) = \langle S_{jz} \rangle \Gamma^{(j)}(j\mathbf{l}\mathbf{k}|\xi) + \langle S_{j'z} \rangle \Phi^{(j')}(j'\mathbf{l}\mathbf{k}|\xi), \tag{3.10}$$

$$Q^-(j\mathbf{k}_1\mathbf{l}\mathbf{k}_2\mathbf{k}|\xi) = \langle S_{jz} \rangle Q^{(j)}(j\mathbf{k}_1\mathbf{l}\mathbf{k}_2\mathbf{k}|\xi) + \langle S_{jz} \rangle Y^{(j')}(j'\mathbf{k}_1\mathbf{l}\mathbf{k}_2\mathbf{k}|\xi), \tag{3.11}$$

$$\Omega^-(j'j\mathbf{k}_1\mathbf{k}|\xi) = \langle S_{jz} \rangle \Omega^{(j)}(j'j\mathbf{k}_1\mathbf{k}|\xi) + \langle S_{j'z} \rangle \Omega^{(j')}(jj'\mathbf{k}_1\mathbf{k}|\xi). \tag{3.12}$$

The averages $\langle S_{jz} \rangle$ and $\langle S_{j'z} \rangle$ refer to different impurities, and it is suggested that separate equations of

motion can be generated from the original equations for the Z^- functions in much the same manner that the separation for the Z^+ functions was carried out above. Hence, we will isolate all the terms in a Z^- equation that are proportional to $\langle S_{jz}\rangle$ (or $\langle S_{j'z}\rangle$) and thus determine a separate equation of motion from these terms; the advantage of this method is that once again we will in this way have the equations of motion involved for the problem of a single impurity contained in our resultant equations. The equations obtained in this way are

$$(\xi-\xi_{\mathbf{k}'})G^{(j)}(\mathbf{k}'\mathbf{k}|\xi) = -\frac{J_0}{N}\sum_{\mathbf{l}} e^{i(\mathbf{l}-\mathbf{k}')\cdot\mathbf{R}_j}\Gamma^{(j)}(j\mathbf{l}\mathbf{k}|\xi) - \frac{J_0}{N}\sum_{\mathbf{l}} e^{i(\mathbf{l}-\mathbf{k}')\cdot\mathbf{R}_{j'}}\Phi^{(j)}(j\mathbf{l}\mathbf{k}|\xi), \quad (3.13)$$

$$(\xi-\xi_{\mathbf{l}})\Gamma^{(j)}(j\mathbf{l}\mathbf{k}|\xi) = \delta_{\mathbf{l}\mathbf{k}} - \frac{J_0}{N}\mathbf{S}_j^2\sum_{\mathbf{k}_1} e^{i(\mathbf{k}_1-\mathbf{l})\cdot\mathbf{R}_j}G^{(j)}(\mathbf{k}_1\mathbf{k}|\xi) + \frac{J_0}{N}\sum_{\mathbf{k}_1} e^{i(\mathbf{k}_1-\mathbf{l})\cdot\mathbf{R}_j}\Gamma^{(j)}(j\mathbf{l}\mathbf{k}|\xi) - \frac{J_0}{N}\sum_{\mathbf{k}_1} e^{i(\mathbf{k}_1-\mathbf{l})\cdot\mathbf{R}_{j'}}\Omega^{(j)}(j'j\mathbf{k}_1\mathbf{k}|\xi) + \frac{J_0}{N}\sum_{\mathbf{k}_1,\mathbf{k}_2} e^{i(\mathbf{k}_2-\mathbf{k}_1)\cdot\mathbf{R}_j}Q^{(j)}(j\mathbf{k}_1\mathbf{l}\mathbf{k}_2\mathbf{k}|\xi), \quad (3.14)$$

$$(\xi-\xi_{\mathbf{l}})\Phi^{(j')}(j'\mathbf{l}\mathbf{k}|\xi) = -\frac{J_0}{N}\mathbf{S}_j^2\sum_{\mathbf{k}_1} e^{i(\mathbf{k}_1-\mathbf{l})\cdot\mathbf{R}_j}G^{(j')}(\mathbf{k}_1\mathbf{k}|\xi) + \frac{J_0}{N}\sum_{\mathbf{k}_1} e^{i(\mathbf{k}_1-\mathbf{l})\cdot\mathbf{R}_j}\Phi^{(j')}(j'\mathbf{k}_1\mathbf{k}|\xi) - \frac{J_0}{N}\sum_{\mathbf{k}_1} e^{i(\mathbf{k}_1-\mathbf{l})\cdot\mathbf{R}_{j'}}\Omega^{(j')}(jj'\mathbf{k}_1\mathbf{k}|\xi) + \frac{J_0}{N}\sum_{\mathbf{k}_1,\mathbf{k}_2} e^{i(\mathbf{k}_2-\mathbf{k}_1)\cdot\mathbf{R}_j}Y^{(j')}(j'\mathbf{k}_1\mathbf{l}\mathbf{k}_2\mathbf{k}|\xi). \quad (3.15)$$

Equations (3.5)–(3.8) and (3.13)–(3.15) are those that we now wish to solve, and this can be accomplished only after some chainbreaking approximations have been made. As was mentioned previously, we will employ the same sort of method used in I, which depends upon expanding functions such as $\Omega_\sigma(j'j\mathbf{l}\mathbf{k}|\xi)$ and $Q_\sigma(j\mathbf{k}_1\mathbf{l}\mathbf{k}_2\mathbf{k}|\xi)$ to first power via their respective equations of motion; after this is accomplished, it is possible to infer relationships between the latter expansions and terms to first power in $G_\sigma(\mathbf{k}'\mathbf{k}|\xi)$ and $\Gamma_\sigma(j\mathbf{k}'\mathbf{k}|\xi)$, and averages that can be computed from these functions using Eq. (2.4).

The list of decouplings found in this manner follows:

$$P(j'j\mathbf{l}\mathbf{k}|\xi) = G^N(\mathbf{l}\mathbf{k}|\xi)+\Gamma^{(j)}(j\mathbf{l}\mathbf{k}|\xi) - \Gamma^{(j')}(j'\mathbf{l}\mathbf{k}|\xi), \quad (3.16)$$

$$Q^N(j\mathbf{k}_1\mathbf{l}\mathbf{k}_2\mathbf{k}|\xi) = \langle 2S_j\cdot\mathbf{s}_{\mathbf{k}_1\mathbf{l}}\rangle^N G^N(\mathbf{k}_2\mathbf{k}|\xi) - 2\langle n_{\mathbf{k}_1\mathbf{l}}\rangle^N\Gamma^N(j\mathbf{k}_2\mathbf{k}|\xi), \quad (3.17)$$

$$X(j'\mathbf{k}_1\mathbf{l}\mathbf{k}_2\mathbf{k}|\xi) = \langle 2S_{j'}\cdot\mathbf{s}_{\mathbf{k}_1\mathbf{l}}\rangle^N G^N(\mathbf{k}_2\mathbf{k}|\xi) - 2\langle n_{\mathbf{k}_1\mathbf{l}}\rangle^N\Lambda(j'\mathbf{k}_2\mathbf{k}|\xi), \quad (3.18)$$

$$Q^{(j)}(j\mathbf{k}_1\mathbf{l}\mathbf{k}_2\mathbf{k}|\xi) = p(j\mathbf{k}_1\mathbf{k}_2)G^N(\mathbf{l}\mathbf{k}|\xi) - 2\langle n_{\mathbf{k}_1\mathbf{l}}\rangle^N\Gamma^{(j)}(j\mathbf{k}_2\mathbf{k}|\xi), \quad (3.19)$$

$$Y^{(j')}(j'\mathbf{k}_1\mathbf{k}_2\mathbf{k}|\xi) = 0, \quad (3.20)$$

where the superscript N on an average means that it is to be calculated from a function with the same superscript, e.g.,

$$\langle n_{\mathbf{k}_1\mathbf{l}}\rangle^N = -\frac{1}{\pi}\int_{-\infty}^{\infty} f(\xi)\,\mathrm{Im}G^N(\mathbf{l}\mathbf{k}_1|\xi)\,d\xi, \quad (3.21)$$

$$\langle 2\mathbf{S}_j\cdot\mathbf{s}_{\mathbf{k}_1\mathbf{l}}\rangle^N = -\frac{2}{\pi}\int_{-\infty}^{\infty} f(\xi)\,\mathrm{Im}\Gamma^N(j\mathbf{l}\mathbf{k}_1|\xi)\,d\xi. \quad (3.22)$$

These averages are, moreover, the same as those used by Nagaoka,[4] except that the common factor $\mathbf{S}_j^2=S(S+1)$ has been removed from Eq. (3.20).

In Eq. (3.22), the quantity $p(j\mathbf{k}_1\mathbf{k}_2)$ is defined by the relation

$$\langle S_{jz}\rangle p(j\mathbf{k}_1\mathbf{k}_2) = \langle S_{j+}s_{\mathbf{k}_1\mathbf{k}_2-}\rangle - \langle S_{j-}s_{\mathbf{k}_1\mathbf{k}_2}\rangle. \quad (3.23)$$

When the equations of motion are constructed, the term $p(j\mathbf{k}_1\mathbf{k}_2)$ leads directly to the function $p(j\sigma)$ defined by (3.16) in I, and, as was noted there, it is a strictly second-order term, which can therefore contribute at best a third-order term to $G^\sigma(\mathbf{k}'\mathbf{k}|\xi)$. We will neglect this term at the outset on this basis, since it contributes no anomalous terms to $G^\sigma(\mathbf{k}'\mathbf{k}|\xi)$.

Equations (3.16)–(3.20) comprise the chainbreaking relations that will be used.

4. SOLUTIONS TO EQUATIONS

From here on the algebra becomes extremely tedious, although it is quite straightforward. We shall therefore only outline the procedure and actually write only the final approximated solutions that we use.

The basic equations are as follows: (a) Eq. (3.5), no chainbreaking required; (b) Eq. (3.6), with Q^N from Eq. (3.17); (c) Eq. (3.7); (d) Eq. (3.8), with P from Eq. (3.16) and X from Eq. (3.18); (e) Eq. (3.13); (f) Eq. (3.14), with $Q^{(j)}$ from Eq. (3.19) and Ω from Eqs. (2.3) and (3.16); (g) Eq. (3.15), with Y from Eq. (3.20) and Ω from Eqs. (3.3) and (3.16).

These form a set of seven equations for the seven unknowns G^N, Γ^N, G, Λ, $G^{(j)}$, $\Gamma^{(j)}$, and $\Phi^{(j)}$. The equa-

tions can be solved at this stage without approximation, but we shall not write the solutions here; they have been tabulated elsewhere.[7]

The solutions can be simplified enormously by making use of the smallness of $J_0\rho/N$, as we did in I. Powers of J_0 are not reliable guides when dealing with the anomalous Kondo terms because of the peculiar nature of a function like $g_j(0|\xi)$, which, for $T>T_K$ at any rate, has a logarithmic behavior that can overcome the smallness of the *s-d* coupling J_0 if this function is evaluated near $\xi=0$. However, we can simplify $G^N(\mathbf{k}'\mathbf{k}|\xi)$ and $G(\mathbf{k}'\mathbf{k}|\xi)$ by keeping only the terms of leading *order* in $J_0\rho/N$, i.e., we can use the fact that the functions $J_0h(0|\xi)$ and $J_0h(\mathbf{R}|\xi)$ are first-order quantities in $J_0\rho/N$, irrespective of the temperature range under consideration, where

$$h(\mathbf{r}|\xi)=N^{-1}\sum_{\mathbf{k}}\frac{1}{\xi-\xi_{\mathbf{k}}}e^{i\mathbf{k}\cdot\mathbf{r}}\cdots\mathbf{r}=\mathbf{0},\mathbf{R}. \tag{4.1}$$

What is involved here is an appeal to *comparative* orders of smallness with respect to the various functions involved. Let us therefore assume, for the sake of argument, that the combination $J_0g_j(\mathbf{r}|\xi)$ is a zeroth-order term; then, whenever this occurs in our equations, multiplied by J_0h, as in $J_0^2h(\mathbf{r}|\xi)g_j(\mathbf{r}|\xi)$, we consider the latter combination to be an order of magnitude smaller than $J_0g_j(\mathbf{r}|\xi)$. Applying this argument to all the expressions in the exact solutions, we emerge finally with the approximate solutions

$$G^N(\mathbf{k}'\mathbf{k}|\xi)=\frac{1}{\xi-\xi_{\mathbf{k}'}}\delta_{\mathbf{k}'\mathbf{k}}-\frac{J_0}{N}\frac{1}{(\xi-\xi_{\mathbf{k}'})(\xi-\xi_{\mathbf{k}})}\sum_j e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j}\times\frac{J_0\mathbf{S}_j^2B_j(0|\xi)}{1+2J_0g_j(0|\xi)+J_0^2\mathbf{S}_j^2h(0|\xi)B_j(0|\xi)}, \tag{4.2}$$

$$G(\mathbf{k}'\mathbf{k}|\xi)=\sum_j[G_{\mathrm{RKKY}}{}^j(\mathbf{k}'\mathbf{k}|\xi)+G_N{}^j(\mathbf{k}'\mathbf{k}|\xi)+G_{\mathrm{rest}}{}^j(\mathbf{k}'\mathbf{k}|\xi)], \tag{4.3}$$

where

$$G_{\mathrm{RKKY}}{}^j=+\frac{J_0}{2N}\frac{1}{(\xi-\xi_{\mathbf{k}'})(\xi-\xi_{\mathbf{k}})}e^{-i\mathbf{k}'\cdot\mathbf{R}_j+i\mathbf{k}\cdot\mathbf{R}_j}\times\frac{J_0h(R|\xi)[1+\psi_{j'}(\xi)]}{1+2J_0g_j(0|\xi)}, \tag{4.4}$$

$$G_N{}^j=-\frac{J_0}{2N}\frac{1}{(\xi-\xi_{\mathbf{k}'})(\xi-\xi_{\mathbf{k}})}e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}_j}\times\frac{J_0H(j'j|\xi)[1+\psi_j(\xi)]}{1+2J_0g_j(0|\xi)}, \tag{4.5}$$

$$G_{\mathrm{rest}}{}^j=-\frac{J_0}{N}\frac{1}{(\xi-\xi_{\mathbf{k}'})(\xi-\xi_{\mathbf{k}})}\frac{2J_0^2h(R|\xi)}{[1+2J_0g_j(0|\xi)]^2}\times[g_j(0|\xi)e^{i\mathbf{k}\cdot\mathbf{R}_{j'}-i\mathbf{k}'\cdot\mathbf{R}_j}-g_j(R|\xi)e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}_j}]. \tag{4.6}$$

G_{RKKY} is the term that reduces to the standard RKKY interaction when all Kondo effects are neglected. G_N is the term that leads to an interaction resembling the Nagaoka bound-state polarization, when the Nagaoka t matrix is used. We shall be interested in this paper with what these two interactions become in terms of an arbitrary t matrix. However, there comes out of this calculation a third term G_{rest}, which at first glance seems to be small (being proportional directly to products gh), but which we shall not pursue any further here.

We shall also use the result in the same approximation for Γ:

$$\Gamma^N(j'\mathbf{l}\mathbf{k}|\xi')=[1/(\xi'-\xi_{\mathbf{l}})][1/(\xi'-\xi_{\mathbf{k}})]e^{i(\mathbf{k}-\mathbf{l})\cdot\mathbf{R}_{j'}}\times\{[J_0/2N][\langle 2\mathbf{S}_{j'}\cdot\mathbf{s}_{\mathbf{l}}{}^{j'}\rangle^N-1][1+\psi_{j'}(\xi')]-[1-\psi_{j'}(\xi')/Nh(0|\xi')S_{j'}{}^2][\langle n_{\mathbf{l}}{}^{j'}\rangle^N-\tfrac{1}{2}]\}. \tag{4.7}$$

In these and in future equations, functions are defined as follows:

$$H(j'j|\xi)=N^{-1}\sum_{\mathbf{l}}\frac{2\langle\mathbf{S}_{j'}\cdot\mathbf{s}_{\mathbf{l}}{}^j\rangle^N}{\xi-\xi_{\mathbf{l}}}, \tag{4.8}$$

$$g_j(\mathbf{r}|\xi)=N^{-1}\sum_{\mathbf{l}}\frac{\langle n_{\mathbf{l}}{}^j\rangle-\frac{1}{2}}{\xi-\xi_{\mathbf{l}}}e^{i\mathbf{l}\cdot\mathbf{r}}\cdots\mathbf{r}=\mathbf{0},\mathbf{R}, \tag{4.9a}$$

$$B_j(0|\xi)=N^{-1}\sum_{\mathbf{l}}\frac{\langle 2\mathbf{S}_j\cdot\mathbf{s}_{\mathbf{l}}{}^j\rangle^N-1}{\xi-\xi_{\mathbf{l}}} \tag{4.9b}$$

where

$$\langle 2\mathbf{S}_{j'}\cdot\mathbf{s}_{\mathbf{l}}{}^j\rangle^N=\sum_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{R}_j}\langle 2\mathbf{S}_{j'}\cdot\mathbf{s}_{\mathbf{k}\mathbf{l}}\rangle^N \tag{4.10}$$

is obtained from Γ^N, Eq. (4.7), and

$$\langle n_{\mathbf{l}}{}^j\rangle^N=\sum_{\mathbf{k}}e^{i(\mathbf{l}-\mathbf{k})\cdot\mathbf{R}_j}\langle n_{\mathbf{k}\mathbf{l}}\rangle^N \tag{4.11a}$$

is obtained from G^N, Eq. (4.2); finally,

$$\langle 2\mathbf{S}_j\cdot\mathbf{s}_{\mathbf{l}}{}^j\rangle^N=\sum_{\mathbf{k}}e^{i(\mathbf{l}-\mathbf{k})\cdot\mathbf{R}_j}\langle 2\mathbf{S}_j\cdot\mathbf{s}_{\mathbf{k}\mathbf{l}}\rangle^N \tag{4.11b}$$

is obtained from Γ^N, Eq. (4.7).

One of the advantages of the present calculation is that the result for G_N can be written in terms of the one-impurity t matrix $t_j(\xi)$. In Eqs. (4.4)–(4.9) we have used the ψ function introduced by Hamann.[8] The relation between ψ and t is

$$\psi_j{}^r(\xi)=1-2i\pi\rho t_j(\xi), \tag{4.12}$$

[7] R. H. Bresemann, Ph.D. thesis, Northwestern University, 1968 (unpublished).

[8] D. R. Hamann, Phys. Rev. **158**, 570 (1967).

where $t_j(\xi)$ is defined through G^N by

$$G^N(\mathbf{k}'\mathbf{k}|\xi)=\frac{\delta_{\mathbf{k}'\mathbf{k}}}{\xi-\xi_{\mathbf{k}'}}+\frac{1}{(\xi-\xi_{\mathbf{k}'})(\xi-\xi_{\mathbf{k}})}\sum_j e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j}t_j(\xi). \quad (4.13)$$

Now in Eq. (4.8) $\langle\mathbf{S}_{j'}\cdot\mathbf{s}_{\mathbf{l}^j}\rangle^N$ refers to both impurities. We can use Γ^N, Eq. (4.7), and the definition in Eq. (2.4) to reduce $H(j'j|\xi)$ to functions depending on a single impurity. After some algebra we find

$$H(j'j|\xi)=-\frac{2J_0{}^2}{N}\sum_{\mathbf{k}\mathbf{k}'}e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}}\times(\langle 2\mathbf{S}_{j'}\cdot\mathbf{s}_{\mathbf{k}'j'}\rangle^N-1)(\langle n_{\mathbf{k}}{}^{j'}\rangle^N-\tfrac{1}{2})\times(\xi_{\mathbf{k}'}-\xi_{\mathbf{k}})^{-1}[(\xi-\xi_{\mathbf{k}'})^{-1}+(\xi-\xi_{\mathbf{k}})^{-1}], \quad (4.14)$$

where now only one-impurity functions appear, which are determined from

$$\langle 2\mathbf{S}_j\cdot\mathbf{s}_{\mathbf{k}}{}^j\rangle^N=\frac{2N}{\pi J_0\mathbf{S}_j{}^2}\int_{-\infty}^{\infty}f(\xi'')\,\mathrm{Im}''\frac{t_j(\xi'')}{\xi''-\xi_{\mathbf{k}}}d\xi'', \quad (4.15)$$

$$\langle n_{\mathbf{k}}{}^j\rangle^N=-\tfrac{1}{2}\pi^{-1}\int_{-\infty}^{\infty}f(\xi'')\times\mathrm{Im}''(\xi''-\xi_{\mathbf{k}})^{-1}[1+\psi_j(\xi'')]\,d\xi'', \quad (4.16)$$

where Im″ means

$$\mathrm{Im}''(\xi,\xi'')=(2i)^{-1}\lim_{\epsilon\to 0^+}[F(\xi,\xi''+i\epsilon)-F(\xi,\xi''-i\epsilon)]. \quad (4.17)$$

The one-impurity functions, such as g_j, $\langle n_{\mathbf{k}}{}^j\rangle$, etc., no longer need the index j' on them, so we shall drop them in what follows.

Thus, once a solution for t (or ψ) is obtained, we can use Eqs. (4.15) and (4.16) to obtain $H(j'j|\xi)$ [from Eq. (4.14)] and $g(r|\xi)$ [from Eq. (4.9)]. These are then substituted into Eqs. (4.4)–(4.6) to obtain G_N. From G_N we obtain the interaction energy directly.

5. CALCULATION OF AVERAGE ENERGY

To get the average energy, we use the formula Eq. (2.9). There are, corresponding to Eq. (4.3), three terms proportional to

$$\langle H'\rangle=\sum_j\langle\mathbf{S}_j\cdot\mathbf{S}_{j'}\rangle[J_{\mathrm{RKKY}}+E'+J_{\mathrm{rest}}]. \quad (5.1)$$

In this paper, we shall not discuss J_{rest}. The other two terms are generalizations of well-known effects, and are now discussed in turn.

A. RKKY Interaction

The first term comes from Eq. (4.4), and in the absence of any Kondo effects, yields the ordinary RKKY interaction. Using the definitions of Sec. 4, we have

$$G_{\mathrm{RKKY}}(\xi)\equiv\sum_k G_{\mathrm{RKKY}}(\mathbf{k}\mathbf{k}|\xi)=i\frac{J_0{}^2}{4}\frac{1+\psi(\xi)}{1+2J_0g(0)}\frac{d}{d\xi}h^2(R|\xi)\equiv-\alpha(\xi)\frac{d}{d\xi}h^2(R|\xi), \quad (5.2)$$

which defines α. If we integrate the energy expression by parts, we obtain

$$J_{\mathrm{RKKY}}=-\mathrm{Im}\int_{-\infty}^{\infty}d\xi\,\xi f(\xi)\alpha(\xi)\frac{d}{d\xi}h^2(R|\xi)=-\mathrm{Im}\int d\xi\left(f\alpha+\xi\frac{d}{d\xi}f\alpha\right)h^2(R|\xi). \quad (5.3)$$

If we integrate by parts again, using $\int^{\xi}h^2$ to indicate the indefinite integral of $h^2(R|\xi)$, we get

$$J_{\mathrm{RKKY}}=+\mathrm{Im}\int d\xi\left(\frac{d}{d\xi}f\alpha\right)\int^{\xi}h^2+\mathrm{Im}\int d\xi\left(\frac{d}{d\xi}f\alpha\right)h^2(R|\xi). \quad (5.4)$$

Suhl has made an argument, which, when applied to this integral, says that if the Kondo effect concerns only the region of order k_BT_K near the Fermi surface, then this expression should yield the ordinary RKKY interaction. We can see how this would occur. First, the product $f\alpha$ would be slowly varying everywhere except very close to the Fermi level. Thus, the first term in Eq. (5.4) would be integrated by taking out $\int^{\xi}h^2$ evaluated close to the Fermi level, getting

$$J_{\mathrm{RKKY}}=\mathrm{Im}\int^{(\xi_F)}h^2[f\alpha]_{-\epsilon}{}^{+\epsilon}+\{\ \}, \quad (5.5)$$

where ϵ is some small energy of order k_BT_K (but not arbitrarily small), and where the curly brackets represent the second term in Eq. (5.4). The first term in Eq. (5.5) is the ordinary RKKY expression, if we set

$$[f\alpha]_{-\epsilon}{}^{\epsilon}=[f\alpha]_{-\epsilon}^{\epsilon}\cong-2. \quad (5.6)$$

The second term in Eq. (5.4) would be negligible, since in the region where the factor $d(f\alpha)/d\xi$ is not small, the factor ξ is.

The main interest of the present paper is not in the RKKY term, but we can test the premise of the above

argument by seeing whether the Bloomfield-Hamann t matrix (see Sec. 5 B) actually gives $-[f\alpha]_{-\epsilon}=2$. We find, in fact, for this expression at zero temperature the value 0.20, which indicates that at least one of the t matrices presently being discussed for the problem does not give back the ordinary RKKY interaction. If this t matrix is reliable, then the indications are that a temperature dependence in the ordinary RKKY interaction occurs. Of course, once the first term of Eq. (5.4) has alterations in it, the second term must also be considered. But this is beyond the scope of this paper.

In this connection, it should be noted that on our previous calculation I, *above* T_K the Suhl argument is valid, since the perturbation t matrix does satisfy the Suhl premise. We used in I the incorrect evaluation of Eq. (5.6) at $-\epsilon\approx 0$.

Before leaving the RKKY term, we mention one final thing. In Nagaoka's original paper, there was no RKKY interaction found below T_K. The reason for this was that he used for his self-consistency condition [see Eq. (4.1) of Ref. 4] $m_k-\frac{3}{4}=\alpha(n_k-\frac{1}{2})/\xi_k$. A close look at Falk and Fowler's[9] paper shows that the correct relation is $m_k=\alpha(n_k-\frac{1}{2})/\xi_k$. However, in Nagaoka's polarization expression, the combination $m_k-\frac{3}{4}$ actually appears. If m_k is converted away by the self-consistency condition to give the bound-state polarization, the remaining $-\frac{3}{4}$ can be shown to provide the ordinary RKKY interaction. Thus, the RKKY interaction does occur even in Nagaoka's approach to the solution of the problem.

B. Nagaoka Bound-State Interaction

The term G_N in Eq. (4.5) yields the $\sin^2 k_F R/R^2$ interaction of Nagaoka, if Nagaoka's t matrix is used. We therefore labeled it with a subscript N. The purpose here is to put it into a suitable form for calculation, using an arbitrary t matrix, and then to use both the Nagaoka and BH t matrices for specific calculations. First, we form the sum

$$G_N(\xi)=\sum_k G_{\mathrm{RKKY}}(\mathbf{kk}|\xi)$$
$$=\frac{1}{2\mathbf{S}_j^2}\frac{[1-\psi_j(\xi)]}{(-i\pi\rho/N)}\frac{d}{d\xi}h(0|\xi)\phi(R|\xi), \quad (5.7)$$

where

$$\phi(R|\xi)=H(j'j|\xi)/[H(jj|\xi)-h(0|\xi)]. \quad (5.8)$$

From this we get

$$E'=\mathrm{Im}\int_{-\infty}^{\infty}d\xi\,\xi f(\xi)G_N(\xi). \quad (5.9)$$

All the R dependence is in the ϕ function. If the energy associated with G_N were calculated according to the Suhl premise indicated in the previous pages, there would be no appreciable contribution to the interaction energy from it. We shall not proceed, however, on this premise, but actually work out the consequences by direct evaluation for particular t matrices. We do this for (1) the Nagaoka and (2) the BH solutions.

1. Nagaoka Solution

The problem is first to get $\phi[R(\xi)]$, and then to substitute into Eq. (5.9) for J_N. The s matrix on the Nagaoka model is given by

$$\psi(\xi)=(\xi-i\Delta)/(\xi+i\Delta), \quad (5.10)$$

as shown by BH, where

$$\lim_{T\to 0}\Delta(T)\cong k_B T_K. \quad (5.11)$$

Nagaoka's self-consistency condition is

$$m_k\equiv\langle 2\mathbf{S}_j\cdot\mathbf{s}_k{}^j\rangle^N$$
$$=[2\Delta/|J_0|\pi n_c S(S+1)](n_k-\tfrac{1}{2}/\xi_k), \quad (5.12)$$

from which $H(j'j|\xi)$ can be written

$$H(j'j|\xi)=2J_0\gamma(R)\sum_k\frac{m_k}{\xi-\xi_k}e^{i\mathbf{k}\cdot\mathbf{R}}, \quad (5.13)$$

where

$$\gamma(R)=N^{-1}\sum_k\frac{n_k-\frac{1}{2}}{\xi_k}e^{i\mathbf{k}\cdot\mathbf{R}}. \quad (5.14)$$

Nagaoka has evaluated $\gamma(R)$ as

$$\gamma(R)=(1/2J_0)(\sin k_F R/k_F R) \quad (5.15)$$

for $R\ll v_F/\Delta$, on the assumption that the variation of the exponential factor in Eq. (5.14) is small compared to the variation in m_k in the region where nonzero contributions from the latter quantity can occur. We will use Nagaoka's evaluation here, inserting $\gamma(R)$ into Eq. (5.13). Noting that the remaining exponential factor in the summand can be handled according to the same approximation, we have finally

$$\phi(R|\xi)=(\sin k_F R/k_F R)^2. \quad (5.16)$$

Thus the energy becomes

$$E'\cong(\sin k_F R/k_F R)^2 I(\Delta)/S_j^2, \quad (5.17)$$

where, according to the Nagaoka theory, the integral $I(\Delta)$ is

$$I(\Delta)=-(2/\pi)\Delta. \quad (5.18)$$

Thus we get an interaction that corresponds to Nagaoka's bound-state polarization. It is interesting to note that this simple result occurs because the ratio $\phi(R|\xi)$ is real and independent of ξ. In general this is not the case, as we will see below.

2. BH Solution

Once again we must first discuss the function $\phi(R|\xi)$. To evaluate it, we need $H(j'j|\xi)$, and this requires

[9] D. S. Falk and M. Fowler, Phys. Rev. **158**, 567 (1967).

the ψ function. In the BH solution, the retarded ψ is for $S=\frac{1}{2}$,

$$\psi(\xi) = -\frac{X^+(\xi)}{\{[X^+(\xi)]^2+\frac{3}{4}\pi^2\}^{1/2}} \times\exp\frac{1}{2\pi i}\int_{-D}^{D}\frac{\ln|H(\xi')|}{\xi-\xi'+i\epsilon}, \quad (5.19)$$

where the quantities involved here are defined in their paper.

We shall not evaluate ϕ or E' completely in the BH model, because the calculations, even when placed on a computer, are too complicated. But we shall, in the way of simplifications, do the following: (a) We restrict the calculation to $T=0$. (b) We look only at that part of the ϕ function that would go as $\sin^2k_FR/R^2$ so as to compare with the Nagaoka solution. (c) We approximate the $\ln|H(\xi')|$ appearing in Eq. (5.19), which at $T=0$ is rigorously

$$\ln|H(\xi)| = \ln\left(\frac{(\ln|\xi/T_K|)^2+\pi^2}{\{[(\ln|\xi|T_K|)^2+\frac{1}{2}\pi^2]^2+\pi^2\ln^2|\xi/T_K|\}^{1/2}}\right) \quad (5.20)$$

by

$$\ln|H(\xi)| \cong (\ln 2)\xi T_K\{[(\xi-T_K)^2+T_K^2]^{-1} -[(\xi+T_K)^2+T_K^2]^{-1}\}. \quad (5.21)$$

This last approximation follows from the remarks of BH that only the behavior of $\ln H(\xi)$ near $\pm k_BT_K$ is important. We have used other forms for this function and have found that the qualitative results are not very sensitive to the form used.

Item (b) above, restricting the calculation to the part of ϕ proportional to $\sin^2k_FR/R^2$, can be understood from Eq. (4.14) as follows. In this equation, the k and k' sums are formed separately, and the exponential $\exp(ik\cdot R)$ for each of these is evaluated on a parabolic band approximation, giving rise to a factor $R^{-1}\times\sin k_FR(1-\xi_k/D)^{1/2}$, where $2D$ is the bandwidth. If there is a peaking of the rest of the integrand[10] about $\xi_k=0$, then this factor can be taken out of the peaking region at the value $R^{-1}\sin k_FR$. Since both a k and a k' integral appear, there results a product of such factors, and it is the coefficient of this product that we are interested in. Thus, we eventually have the double integral over the peaked region. There is, in fact, a peaking, which we find well restricted to within $|\xi|/D\leq 0.001$, and we do find a finite value upon integration over this small region. In this way we obtained ϕ.

[10] The peaking occurs because the m_k function gets large logarithmically as $\xi_k\to 0$, both on the Nagaoka and BH models. (In fact, however, m_k can never diverge.)

There is still the question how to evaluate the $dh(0|\xi)/d\xi$ factor of Eq. (5.9). In general,

$$h(0|\xi)=N^{-1}\textstyle\sum_k P(\xi-\xi_k)^{-1}-i\pi N^{-1}\rho(\xi). \quad (5.22)$$

In order to be consistent with BH's solution, we use a Lorentzian density of states

$$\rho(\xi)=(1/N)\rho_0D^2/(\xi^2+D^2), \quad |\xi|<D$$
$$=0, \quad |\xi|>D \quad (5.23)$$

which leads to

$$h(0|\xi)=(\pi\rho_0D/N)1/(\xi+iD), \quad |\xi|<D$$
$$=0, \quad |\xi|>D. \quad (5.24)$$

The cutoff and, in fact, the details of the density of states in general give rise to great uncertainty in the actual value of the integral for the E'. BH have noted this problem in their calculation of the specific heat, but it has a more severe effect on the energy. In particular, the major contributions to the resultant E' come from the region far from $\xi=k_BT$ and also primarily from those parts of the integrand involving $\mathrm{Im}\psi_j$ and $\mathrm{Im}[(d/d\xi)h(0|\xi)]$, in much the same manner as the results obtained by BH in calculating the condensation energy. We find then for $|J_0|\rho/N=0.1$ that the part of E' proportional to $\sin^2k_FR$ at $T=0$ is

$$E'=-(0.046T_K/S(S+1))(\sin k_FR/k_FR)^2, \quad (5.25)$$

if we use the BH density of states. The factor 0.046 is to be compared with the $2/\pi$ obtained from the Nagaoka result.

Thus the BH t matrix gives a far smaller long-range effect than the Nagaoka polarization indicated. It is not clear, however, to what extent the actual numerical results are significant. As mentioned above, even the calculation for the condensation energy is greatly dependent on the density of states used. We have verified this with a number of numerical calculations, using different densities of states. If the Lorentzian density of states and the BH t matrix is used, we find the condensation energy to be approximately $+20k_BT_K$. This value emerges as a small difference between large-positive and large-negative contributions that extend all the way down to the bottom of the band.

The only significant difference between the integral for the condensation energy and the integral for E' lies in the factor $\phi(\xi|R)$. Further, the formula for ϕ is not very sensitive to the density-of-states function. In discussing E', therefore, it is perhaps best to concentrate on this factor. From the numerical calculations, we find that ϕ is small for all values of ξ, ranging from $\frac{1}{10}$ times the Nagaoka value for it near the Fermi level down to order 1/200 times Nagaoka near the bottom of the band. Thus, from this factor alone, it seems as if the Nagaoka polarization effect was overestimated by one to two orders of magnitude. These results depend entirely on the use of the BH t matrix. But we feel that even this result is an overestimate. The conclusion is

that the ordinary RKKY interaction is stronger than the bound-state interaction at all distances.

To summarize, we have derived an expression for the interaction between two magnetic impurities on the basis of the Nagaoka approach to the problem, and we have reduced the result to an expression that can be evaluated when the one-impurity t matrix is known. (This interaction is not reducible to a simple factor times the spin polarization about one impurity.) To estimate the effect, we have used two forms for the t matrix: Nagaoka's, and Bloomfield and Hamman's. In the former, we can obtain a result analogous to Nagaoka's long-range polarization if we make manipulations just as he did. But in the latter case, we get an effect an order or two smaller. The results can be adapted to any t-matrix solution,[11] but these seemed the most appropriate to use at this time.

[11] Recently after the completion of the present paper, E. Müller-Hartmann [Z. Physik **223**, 277 (1969)] published a calculation that indicates a nonoscillatory $(k_F R)^{-3}$ behavior in the spin correlation function at low temperatures. We have searched in this paper for a $(k_F R)^{-2}$ type of effect in the impurity-impurity correlation, but have not yet made an investigation of the details of the nonoscillatory $(k_F R)^{-3}$ terms that Müller-Hartmann suggests may be present.

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Study of the α-β Quartz Phase Transformation by Inelastic Neutron Scattering*

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An inelastic neutron scattering investigation of high-temperature β quartz by triple-axis spectrometry reveals the existence of a phonon branch with anomalously low and temperature-dependent frequencies. Near the Brillouin zone center, the mode is overdamped and unstable, and gives rise to a critical scattering intensity which diverges as $(T-T_c)^{-1}$. Here T_c is 10°C lower than the transition temperature $T_0=573$°C. Measurements of the relative intensity of the critical scattering about various reciprocal-lattice points establishes that the general pattern of displacements associated with the α-β transformation is determined by this soft mode. At room temperature, the zone center phonon at 25.8 meV (208 cm^{-1}) is shown to strongly resemble the α-β displacements. This confirms the proposal by Scott that the renormalized soft mode interacts with and passes through another low-lying excitation. It is suggested that the anomalous elastic behavior of β quartz results from virtual excitation of pairs of phonons in the soft branch with wave vectors directed oppositely along the hexagonal axis.

I. INTRODUCTION

At about 573°C, quartz undergoes a transformation from a high-temperature hexagonal β form (space group D_6^4 or its enantiomorph D_6^5) into a trigonal α form (D_3^4 or D_3^6) which differs from the former by loss of 180° rotational symmetry about the c axis. The atomic displacements involved are shown in Fig. 1. It has long been suspected that phonons were actively involved in the mechanism of the α-β transformation.[1-3] By analogy with the mechanism for several ferroelectric phase changes, one is tempted to suppose that the transformation results from an instability of a normal vibrational mode of the crystal.[4] The several problems encountered in applying these ideas to quartz have been reviewed by Scott,[5] and basically arise from the following points:

(1) Although recent light scattering experiments by Shapiro, O'Shea, and Cummins[6] have established the existence of an excitation whose frequency does decrease remarkably as the transformation temperature T_0 is approached from below, its presence has raised fundamental questions concerning the normal-mode assignments in quartz and leaves the nature of the unstable excitation unclear.

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