Conduction-Electron-Spin–Impurity-Electron-Spin Correlation Function Using the t-Matrix Formalism for the Exchange Interaction*

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The conduction-electron-spin–impurity-electron-spin correlation function $\langle \mathbf{S}^{\rm el}(r)\cdot\mathbf{S}^{\rm imp}\rangle$ in a dilute magnetic alloy arising from the contact exchange interaction is computed using the t-matrix method. Nonperturbational as well as perturbational expressions are formulated. The nonperturbational expression for the correlation function can only be expressed in terms of certain integrals involving the t matrix. A general expression for the computation of the perturbation terms in powers of the exchange coupling parameter J has been found. Under specific approximations, a second-order expression along with the Ruderman-Kittel-Kasuya-Yosida term is found to be in agreement with the direct perturbational results.

I. INTRODUCTION

THERE have already appeared several controversial papers concerning how the conduction-electron spin polarization [henceforth referred to as $p(r)$] around a magnetic impurity is modified by the Kondo effect.[1] This polarization, strictly speaking, consists of two contributions: firstly, that due to conduction-electron-spin–conduction-electron-spin correlation in the presence of exchange interaction, $\langle \mathbf{S}^{\rm el}(r)\cdot\mathbf{S}^{\rm el}\rangle$, and secondly, that due to conduction-electron-spin–impurity-electron-spin correlation $\langle \mathbf{S}^{\rm el}(r)\cdot\mathbf{S}^{\rm imp}\rangle$. In some papers[2,3] $\langle \mathbf{S}^{\rm el}(r)\cdot\mathbf{S}^{\rm imp}\rangle$ was erroneously identified as the total conduction-electron spin polarization around the impurity spin. Recently, we have computed the quantity $\langle \mathbf{S}^{\rm el}(r)\cdot(\mathbf{S}^{\rm el}+\mathbf{S}^{\rm imp})\rangle$ using perturbation theory.[4] In order to fix the direction of the impurity spin we have applied a finite magnetic field. Assuming that the magnetic energy is small compared to the thermal energy, a linear response theory was adopted in calculating $p(r)$.

The purpose of the present paper is to formulate a nonperturbational expression for the conduction-electron-spin–impurity-electron-spin correlation function in terms of the t matrix for the s-d exchange interaction, and to investigate the approximations under which the nonperturbative expression for $\langle \mathbf{S}^{\rm el}(r)\cdot\mathbf{S}^{\rm imp}\rangle$ gives the perturbational result. In Sec. II we give a general outline of the t-matrix formulation of the exchange interaction. In Sec. III we obtain an exact, nonperturbational expression for the correlation function in terms of the non-spin-flip t matrix. We then perform a perturbational expansion of the resulting expression for temperature region $T>T_k$, where T_k is the "Kondo temperature" defined elsewhere in the text. We found that under certain approximations one can derive the perturbational result for $\langle \mathbf{S}^{\rm el}(r)\cdot\mathbf{S}^{\rm imp}\rangle$, which we have already obtained in the Appendix D of Ref. 4. We conclude with a few remarks on our final result for the correlation function $\langle \mathbf{S}^{\rm el}(r)\cdot\mathbf{S}^{\rm imp}\rangle$.

II. t-MATRIX FORMULATION OF THE EXCHANGE INTERACTION

The contact s-d exchange interaction between a conduction-electron system and a localized magnetic moment is described by the Hamiltonian

$$H=\sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}\sigma}-\frac{J}{2N}\sum_{\mathbf{k},\mathbf{k}'}\{(c_{\mathbf{k}\uparrow}^{\dagger}c_{\mathbf{k}'\uparrow}-c_{\mathbf{k}\downarrow}^{\dagger}c_{\mathbf{k}'\downarrow})S_z+c_{\mathbf{k}\uparrow}^{\dagger}c_{\mathbf{k}'\downarrow}S_-+c_{\mathbf{k}\downarrow}^{\dagger}c_{\mathbf{k}'\uparrow}S_+\}, \quad (2.1)$$

where $c_{\mathbf{k}\sigma}^{\dagger}(c_{\mathbf{k}\sigma})$ is the creation (annihilation) operator for an electron in state $|k\sigma\rangle$ and $S_{\pm}$ and S_z are the components of the spin operator $\mathbf{S}$ associated with the impurity atom. J is the exchange coupling constant. Following Nagaoka,[2] the Green's functions are defined as

$$G_{\mathbf{k}\mathbf{k}'}(\omega)=\langle c_{\mathbf{k}\uparrow}|c_{\mathbf{k}\uparrow}^{\dagger}\rangle, \quad (2.2)$$

$$\Gamma_{\mathbf{k}\mathbf{k}'}(\omega)=\langle c_{\mathbf{k}'\uparrow}S_z+c_{\mathbf{k}'\downarrow}S_-|c_{\mathbf{k}\uparrow}^{\dagger}\rangle, \quad (2.3)$$

where $\langle\ldots\rangle$ indicates the thermal average. These Green's functions satisfy the following equations of motion in the "total spin conservation" decoupling approximation:

$$(\omega-\epsilon_{\mathbf{k}'})G_{\mathbf{k}\mathbf{k}'}(\omega)+\frac{J}{2N}\sum_{l}\Gamma_{\mathbf{k}l}(\omega)=\frac{1}{2\pi}\delta_{\mathbf{k}\mathbf{k}'}, \quad (2.4)$$

$$(\omega-\epsilon_{\mathbf{k}'})\Gamma_{\mathbf{k}\mathbf{k}'}(\omega)+\frac{J}{2N}(n_{\mathbf{k}'}-\tfrac{1}{2})\sum_{l}\Gamma_{\mathbf{k}l}(\omega)+\frac{J}{2N}[S(S+1)-m_{\mathbf{k}'}]\sum_{l}G_{\mathbf{k}'l}(\omega)=0, \quad (2.5)$$

with

$$n_{\mathbf{k}'}=\sum_{l}\langle c_{l\uparrow}^{\dagger}c_{\mathbf{k}'\uparrow}\rangle, \quad (2.6)$$

$$m_{\mathbf{k}'}=3\sum_{l}\langle c_{l\uparrow}^{\dagger}c_{\mathbf{k}'\downarrow}S_-\rangle. \quad (2.7)$$

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The coupled equations (2.4) and (2.5) can be solved in a self-consistent manner and the solutions for $G_{kk'}$ and $\Gamma_{kk'}$ are given by

$$G_{kk'}(\omega)=\frac{1}{2\pi}\left(\frac{\delta_{kk'}}{\omega-\epsilon_{k'}}-\frac{J^2}{4N}\frac{1}{(\omega-\epsilon_k)(\omega-\epsilon_{k'})}\frac{\Gamma(\omega)}{1+JG(\omega)+\frac{1}{4}J^2F(\omega)\Gamma(\omega)}\right), \tag{2.8}$$

$$\Gamma_{kk'}(\omega)=(2\pi)^{-1}(J/2N)[(\omega-\epsilon_k)(\omega-\epsilon_{k'})]^{-1}\frac{[m_{k'}-S(S+1)][1+JG(\omega)]-(n_{k'}-\frac{1}{2})J\Gamma(\omega)}{1+JG(\omega)+\frac{1}{4}J^2F(\omega)\Gamma(\omega)}, \tag{2.9}$$

where

$$F(\omega)=\frac{1}{N}\sum_k\frac{1}{\omega-\epsilon_k}, \tag{2.10}$$

$$G(\omega)=\frac{1}{N}\sum_k\frac{n_k-\frac{1}{2}}{\omega-\epsilon_k}, \tag{2.11}$$

$$\Gamma(\omega)=\frac{1}{N}\sum_k\frac{m_k-S(S+1)}{\omega-\epsilon_k}. \tag{2.12}$$

In analogy with one-particle scattering theory, $t_R(\omega)$ given by the equation

$$t_R(\omega)=-\frac{J^2}{4N}\frac{\Gamma(\omega)}{1+JG(\omega)+\frac{1}{4}J^2F(\omega)\Gamma(\omega)} \tag{2.13}$$

can be identified as the one-particle "t matrix" for non-spin-flip scattering for the present problem. Now one can express $G_{kk'}(\omega)$ in terms of the t matrix. A consideration of the analytic property of $G_{kk'}(\omega)$ suggests that the discontinuity of $t_R(\omega)$ across the real axis is purely imaginary, i.e., $t_R(\omega)=t_A{}^*(\omega)$, where $t_R(\omega)\equiv t(\omega)$ for $\mathrm{Im}\omega>0$ and $t_A(\omega)\equiv t(\omega)$ for $\mathrm{Im}\omega<0$. The decoupled equations of motion [Eqs. (2.8) and (2.9)] can be reduced to the following nonlinear, singular integral equation for the t matrix[5]:

$$\psi_R(\omega)=1-2\pi i\rho t_R(\omega)$$

$$=\left[1-S(S+1)(\tfrac{1}{2}\gamma\pi)^2+\gamma\int_{-D}^{D}d\omega'\frac{f(\omega')-\frac{1}{2}}{\omega-\omega'+i\delta}\right]\Big/\left[1+S(S+1)(\tfrac{1}{2}\gamma\pi)^2+\gamma\int_{-D}^{D}d\omega'\frac{f(\omega')-\frac{1}{2}}{\omega-\omega'+i\delta}\psi_A(\omega')\right], \tag{2.14}$$

where $\gamma\equiv J\rho/N\ll 1$, ρ is the density of states at the Fermi surface, $2D$ is the width of the conduction band, and $\psi_R(\omega)$ ($\psi_A(\omega)$) is the analytic continuation of the function $\psi(\omega)$ in the upper (lower) ω half-plane. ψ_R (ψ_A) can be obtained in the lower (upper) ω half-plane by analytically continuing ψ_R (ψ_A) through the real-axis cut of $\psi(\omega)$. From the properties of $t_{R,A}(\omega)$ it is clear that $\psi_R{}^*(\omega)=\psi_A(\omega^*)$ for all points on the ω plane. Equation (2.14) is an exact equation for the t matrix if we assume the validity of Nagaoka's decoupling scheme.

Hammann[5] found the following approximate solution for $\psi_R(\omega)$:

$$\psi_R(\omega)=\frac{X}{[X^2+S(S+1)\pi^2]^{1/2}}, \tag{2.15}$$

where

$$X=\ln[(\omega+iT)/iT_k], \tag{2.16}$$

$$T_k=D\exp\{[1-S(S+1)\pi^2(\tfrac{1}{2}\gamma)^2]\gamma^{-1}\}. \tag{2.17}$$

From Eq. (2.15) it is clear that $t_R(\omega)$ is analytic in the upper ω half-plane. On the unphysical sheet of the lower ω half-plane $t_R(\omega)$ has three branch points at $\omega=iT_k\exp\pm i\pi[S(S+1)]^{1/2}-iT$; $-iT$. It should be noted that for $S\geq\frac{1}{2}$, these branch points do not cross the real axis for temperatures $T\gtrless T_k$. Recently Bloomfield and Hamann[6] have obtained an improved solution for $\psi_R(\omega)$, given by

$$\psi_R(\omega)=\psi_R{}^{\mathrm{Hamann}}(\omega)\exp\left[\frac{1}{2\pi i}\int_{-D}^{D}d\omega'\frac{\ln|H(\omega')|}{\omega-\omega'+i\delta}\right], \tag{2.18}$$

where

$$\ln|H(\omega)|\approx A(T)\theta(T_k-|\omega|). \tag{2.19}$$

θ is a unit step function and

$$\begin{aligned}A(T)&=1 \quad \text{for} \quad T=0\\ &=0 \quad \text{for} \quad T>T_k.\end{aligned} \tag{2.20}$$

As can be seen from Eq. (2.20), the solution (2.18) differs from the approximate solution of Hamann only in the temperature range $T_k\geq T\geq 0$. For temperatures $T>T_k$, Hamann's approximate solution provides us with fairly accurate solution. More recently, Zittartz *et al.*[7] have obtained an exact solution for $t_R(\omega)$. It should be noted that the Bloomfield-Hamann solution gives a negative susceptibility contribution at $T=0$. This seems to raise a question of the accuracy of the decoupling approximation.

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III. CALCULATION OF THE CONDUCTION-ELECTRON-SPIN–IMPURITY-ELECTRON-SPIN CORRELATION FUNCTION

The conduction-electron-spin–impurity-electron-spin correlation function can be expressed as

$$\langle \mathbf{S}^{\mathrm{el}}(r)\cdot\mathbf{S}^{\mathrm{imp}}\rangle=\sum_{\mathbf{kk'}}\langle c_{\mathbf{k}\uparrow}^{\dagger}c_{\mathbf{k'}\downarrow}S_{-}\rangle e^{i(\mathbf{k}-\mathbf{k'})\cdot\mathbf{r}}. \quad (3.1)$$

Making use of the relation

$$\langle BA\rangle=\int_{-\infty}^{+\infty}(-2\,\mathrm{Im}\langle A\,|\,B\rangle)f(\omega)d\omega, \quad (3.2)$$

where $f(\omega)=(e^{\omega/T}-1)^{-1}$, we can write

$$\langle \mathbf{S}^{\mathrm{el}}(r)\cdot\mathbf{S}^{\mathrm{imp}}\rangle=\tfrac{2}{3}\sum_{\mathbf{kk'}}\int_{-\infty}^{+\infty}d\omega\, f(\omega)\times[-2\,\mathrm{Im}\Gamma_{\mathbf{kk'}}(\omega)]e^{i(\mathbf{k}-\mathbf{k'})\cdot\mathbf{r}}. \quad (3.3)$$

In writing the above equation we have exploited the rotational invariance of the impurity spin. $\Gamma_{\mathbf{kk'}}(\omega)$, occurring in the above expression, can be expressed in terms of the t matrix as

$$\Gamma_{\mathbf{kk'}}(\omega)=\frac{1}{2\pi}\frac{1}{(\omega-\epsilon_{\mathbf{k}})(\omega-\epsilon_{\mathbf{k'}})}\Big[\frac{J}{2N}(m_{\mathbf{k'}}-S(S+1))-\tfrac{1}{2}J(m_{\mathbf{k'}}-S(S+1))F(\omega)t_R(\omega)+2(n_{\mathbf{k'}}-\tfrac{1}{2})t_R(\omega)\Big]. \quad (3.4)$$

In the following calculations we approximate $F(\omega)$ by the purely imaginary constant $-i\pi\rho/N$. Furthermore, we put

$$\tilde{\Gamma}_k(\omega)=-\frac{\rho}{\pi}\frac{t_R(\omega)}{\omega-\epsilon_{\mathbf{k}}+i\delta}. \quad (3.5)$$

These simplifications yield

$$\Gamma_{\mathbf{kk'}}(\omega)=\frac{1}{2\pi}\frac{1}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k'}}}\Big[\frac{J}{2N}(m_{\mathbf{k'}}-S(S+1))\Big(\frac{1}{\omega-\epsilon_{\mathbf{k}}+i\delta}-\frac{1}{\omega-\epsilon_{\mathbf{k'}}+i\delta}\Big)-\frac{2\pi J}{N}(n_{\mathbf{k'}}-\tfrac{1}{2})(\tilde{\Gamma}_{\mathbf{k}}(\omega)-\tilde{\Gamma}_{\mathbf{k'}}(\omega))+\frac{J}{2N}(m_{\mathbf{k'}}-S(S+1))\Big(\frac{i\pi^2J\rho}{N}\Big)(\tilde{\Gamma}_{\mathbf{k}}(\omega)-\tilde{\Gamma}_{\mathbf{k'}}(\omega))\Big]. \quad (3.6)$$

We have replaced ω by $\omega+i\delta$ in the above energy denominator so as to ensure the retarded character of the Green's functions. The imaginary part of $\Gamma_{\mathbf{kk'}}(\omega)$ is given by

$$\mathrm{Im}\Gamma_{\mathbf{kk'}}(\omega)=[2\pi(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k'}})]^{-1}\Big[\frac{J}{2N}(m_{\mathbf{k'}}-S(S+1))(\delta(\omega-\epsilon_{\mathbf{k'}})-\delta(\omega-\epsilon_{\mathbf{k}}))+\frac{J\pi^2\gamma}{2N}(m_{\mathbf{k'}}-S(S+1))\,\mathrm{Re}(\tilde{\Gamma}_{\mathbf{k}}(\omega)-\tilde{\Gamma}_{\mathbf{k'}}(\omega))-\frac{2\pi\gamma}{\rho}(n_{\mathbf{k'}}-\tfrac{1}{2})\,\mathrm{Im}(\tilde{\Gamma}_{\mathbf{k}}(\omega)-\tilde{\Gamma}_{\mathbf{k'}}(\omega))\Big]. \quad (3.7)$$

In a similar way $n_{\mathbf{k}}$ and $m_{\mathbf{k}}$ occurring in the above expression can be expressed in terms of the t matrix as

$$n_{\mathbf{k'}}=f(\epsilon_{\mathbf{k'}})+\rho\pi f(\epsilon_{\mathbf{k'}})\,\mathrm{Im}t_R(\epsilon_{\mathbf{k'}})+\rho P\int_{-\infty}^{+\infty}d\omega\frac{\mathrm{Re}t_R(\omega)}{\omega-\epsilon_{\mathbf{k'}}}f(\omega), \quad (3.8)$$

$$m_{\mathbf{k'}}=-4\frac{N\rho}{J}f(\epsilon_{\mathbf{k'}})\,\mathrm{Re}t_R(\epsilon_{\mathbf{k'}})+\frac{4N}{\pi J}P\int_{-\infty}^{+\infty}d\omega\frac{\mathrm{Im}t_R(\omega)}{\omega-\epsilon_{\mathbf{k'}}}f(\omega). \quad (3.9)$$

P in front of the integration sign indicates the principle part of the integration. Equation (3.3) in conjunction with Eqs. (3.7)–(3.9) gives us an exact, nonperturbational expression for $\langle \mathbf{S}^{\mathrm{el}}(r)\cdot\mathbf{S}^{\mathrm{imp}}\rangle$. Now one can use the correct solution for the t matrix and perform the relevant integrations in order to get the conduction-electron-spin–impurity-electron-spin correlation function. Unfortunately, the integrations involved are too complicated to carry out analytically.

In order to compute (3.7), let us define the following functions of complex argument:

$$G(z)=\frac{\rho}{N}\int_{-D}^{D}d\omega'\frac{f(\omega')-\frac{1}{2}}{z-\omega'}, \quad (3.10)$$

$$\phi^1(z)=\gamma\int_{-D}^{D}d\omega'\frac{f(\omega')-\frac{1}{2}}{z-\omega'}\psi_R(\omega'), \quad (3.11)$$

$$\phi^2(z)=\gamma\int_{-D}^{D}d\omega'\frac{f(\omega')-\frac{1}{2}}{z-\omega'}\psi_A(\omega'). \quad (3.12)$$

We note that

$$G_R(\omega)\equiv G(\omega), \quad \text{if } \mathrm{Im}z>0 \qquad G_A(\omega)\equiv G(\omega), \quad \text{if } \mathrm{Im}z<0$$
$$\phi_R{}^{1,2}(\omega)\equiv\phi^{1,2}(\omega), \quad \text{if } \mathrm{Im}z>0 \qquad \phi_A{}^{1,2}(\omega)\equiv\phi^{1,2}(\omega), \quad \text{if } \mathrm{Im}z<0.$$

In terms of the above functions, n_k and m_k are given by

$$n_k=\tfrac{1}{2}[f(\epsilon_k)-\tfrac{1}{2}]+(2\pi\gamma)^{-1}\,\mathrm{Im}\phi_A{}^1(\epsilon_k), \tag{3.13}$$

$$m_k=(2/\pi^2\gamma^2)\,\mathrm{Re}[JG_A(\epsilon_k)-\phi_A{}^1(\epsilon_k)]. \tag{3.14}$$

Making use of the properties of $\psi_R(\omega)$ and $\psi_A(\omega)$, one can easily show that

$$\phi_{R,A}{}^1(z)=[\phi_{A,R}{}^2(z)]^*. \tag{3.15}$$

Using Eqs. (3.3), (3.7), (3.13), (3.14) and carrying out the ω integration, we obtain

$$\langle \mathbf{S}^{el}(r)\cdot\mathbf{S}^{imp}\rangle=-\tfrac{4}{3}\sum_{kk'}e^{i(k-k')\cdot r}[2\pi(\epsilon_k-\epsilon_{k'})]^{-1}\Big\{\frac{1}{\pi\rho\gamma}(n_{k'}-\tfrac{1}{2})\,\mathrm{Re}[JG_A(\epsilon_k)-\phi_A{}^1(\epsilon_k)-JG_A(\epsilon_{k'})+\phi_A{}^1(\epsilon_{k'})]$$
$$+\frac{J\pi}{2N}(m_{k'}-S(S+1))[(f(\epsilon_{k'})-\tfrac{1}{2})-(f(\epsilon_k)-\tfrac{1}{2})]+\frac{J}{4N\gamma}(m_{k'}-S(S+1))$$
$$\times\mathrm{Im}[JG_A(\epsilon_k)-\phi_A{}^1(\epsilon_k)-JG_A(\epsilon_{k'})+\phi_A{}^1(\epsilon_{k'})]\Big\}. \tag{3.16}$$

The real and the imaginary parts of $G_A(\omega)$ are given by

$$J\,\mathrm{Re}G_A(\omega)=-\gamma\ln[(\omega^2+T^2)/D^2]^{1/2}, \tag{3.17}$$

$$J\,\mathrm{Im}G_A(\omega)=\pi\gamma[f(\omega)-\tfrac{1}{2}]. \tag{3.18}$$

The above relations are consistent with Hamann's approximation[5]:

$$\frac{f(\omega',T)-\frac{1}{2}}{\omega-\omega'+i\delta}\cong\frac{f(\omega',0)-\frac{1}{2}}{\omega-\omega'+iT}. \tag{3.19}$$

In the Appendix we discuss, in some detail, how one can avoid this approximation in doing the relevant integrals. Making use of the identity (3.15) in the integral equation (2.14) we derive

$$\phi_A{}^1(\omega)=-[1+S(S+1)(\tfrac{1}{2}\gamma\pi)^2+\gamma(X^2+S(S+1)\pi^2)^{1/2}]^*. \tag{3.20}$$

Equation (3.20) is valid for all temperatures. For $T>T_k$, $\phi_A{}^1(\omega)$ can be expanded in powers of X. In the lowest order, the real and the imaginary parts of $\phi_A{}^1(\omega)$ are given by

$$\mathrm{Re}\phi_A{}^1(\omega)=-\{1+S(S+1)(\tfrac{1}{2}\gamma\pi)^2+\gamma\ln[(\omega^2+T^2)/D^2]^{1/2}\}, \tag{3.21}$$

$$\mathrm{Im}\phi_A{}^1(\omega)=\pi\gamma[f(\omega)-\tfrac{1}{2}]. \tag{3.22}$$

It is now trivial to verify that

$$\mathrm{Re}[JG_A(\epsilon_k)-\phi_A{}^1(\epsilon_k)-JG_A(\epsilon_{k'})+\phi_A{}^1(\epsilon_{k'})]=0, \tag{3.23}$$

$$\mathrm{Im}[JG_A(\epsilon_k)-\phi_A{}^1(\epsilon_k)-JG_A(\epsilon_{k'})+\phi_A{}^1(\epsilon_{k'})]=0, \tag{3.24}$$

$$\mathrm{Re}[JG_A(\epsilon_k)-\phi_A{}^1(\epsilon_k)]=1+\gamma\ln(D/T_k)+S(S+1)(\tfrac{1}{2}\gamma\pi)^2. \tag{3.25}$$

Direct substitution of Eqs. (3.23)–(3.25) in Eq. (3.16) results in

$$\langle \mathbf{S}^{el}(r)\cdot\mathbf{S}^{imp}\rangle=0. \tag{3.26}$$

The expression (3.26) indicates an entire lack of correlation between the conduction-electron spins and the impurity-electron spins. To get an insight into the above result let us examine how the scattering matrix $\psi_R(\omega)$ behaves in this lowest-order limit. We can easily verify that $t_R(\omega)=0$ in this limit. From Eq. (2.14) we find that for the temperature $T\gg T_k$, which is true in the lowest-order limit, the scattering matrix $\psi_R(\omega)$ approaches unity. This result indicates that at temperatures well above T_K electrons do not see the magnetic impurity potential and that the conduction-electron-spin–impurity-electron-spin interaction is completely smeared out by the thermal fluctuation in the system. It is instructive to note that the improved Hamann-Bloomfield solution[6] for $\psi_R(\omega)$, which is given by

$$\psi_R(\omega)\cong\exp(2\pi i)^{-1}A\,(T)\int_{-T_k}^{T_k}\frac{d\omega'}{\omega-\omega'+i\delta}$$

and valid for all temperatures, also shows that $\psi_R(\omega)$ tends to unity for $T\gg T_k$.

In what follows, we shall calculate the next higher-order contribution to $\langle \mathbf{S}^{el}(r)\cdot\mathbf{S}^{imp}\rangle$. The relevant quantities are given by

$$\mathrm{Re}[JG_A(\epsilon_k)-\phi_A{}^1(\epsilon_k)-JG_A(\epsilon_{k'})+\phi_A{}^1(\epsilon_{k'})]=-\tfrac{1}{2}\gamma\pi^2S(S+1)[\Theta(\epsilon_k)-\Theta(\epsilon_{k'})], \tag{3.27}$$

$$\mathrm{Im}[JG_A(\epsilon_k)-\phi_A{}^1(\epsilon_k)-JG_A(\epsilon_{k'})+\phi_A{}^1(\epsilon_{k'})]=-\tfrac{1}{2}\gamma\pi^2S(S+1)[\Phi(\epsilon_k)-\Phi(\epsilon_{k'})], \tag{3.28}$$

$$(n_{k'}-\tfrac{1}{2})=\tfrac{1}{2}[f(\epsilon_{k'})-\tfrac{1}{2}]+\frac{1}{4\pi}S(S+1)\pi^2\Phi(\epsilon_{k'}), \quad (3.29)$$

$$m_{k'}=S(S+1)-\frac{1}{2\pi^2\gamma}S(S+1)\pi^2\Theta(\epsilon_{k'}), \quad (3.20)$$

where

$$\Theta(\omega)=\frac{\mathrm{Re}X(\omega)}{[\mathrm{Re}X(\omega)]^2+[\mathrm{Im}X(\omega)]^2}, \quad (3.21)$$

$$\Phi(\omega)=\frac{\mathrm{Im}X(\omega)}{[\mathrm{Re}X(\omega)]^2+[\mathrm{Im}X(\omega)]^2}. \quad (3.32)$$

Using Eqs. (3.27)–(3.30) in Eq. (3.16), we get

$$\langle \mathbf{S}^{el}(r)\cdot\mathbf{S}^{imp}\rangle=\frac{S(S+1)}{6\rho}\sum_{kk'}\frac{e^{i(k-k')\cdot r}}{\epsilon_k-\epsilon_{k'}}\times\{[f(\epsilon_{k'})-\tfrac{1}{2}]\Theta(\epsilon_k)-[f(\epsilon_k)-\tfrac{1}{2}]\Theta(\epsilon_{k'})+S(S+1)[\Theta(\epsilon_k)\Phi(\epsilon_{k'})-\Theta(\epsilon_{k'})\Phi(\epsilon_k)]\}. \quad (3.33)$$

With the idea of simplifying the above equation we make the assumption that $\mathrm{Re}X\gg\mathrm{Im}X$. This assumption is quite justified in the energy range $T_k\ll|\omega|<D$. This gives $\Theta(\omega)\approx(\mathrm{Re}X)^{-1}$ and allows us to neglect terms of the order of $\mathrm{Im}X(\mathrm{Re}X)^{-2}$ compared to those of order $(\mathrm{Re}X)^{-1}$. Subjected to the above approximations, Eq. (3.33) becomes

$$\langle \mathbf{S}^{el}(r)\cdot\mathbf{S}^{imp}\rangle=\frac{S(S+1)}{6\rho}\sum_{k,k'}\frac{e^{i(k-k')\cdot r}}{\epsilon_k-\epsilon_{k'}}\left\{[f(\epsilon_{k'})-\tfrac{1}{2}]\left[\ln\left(\frac{\epsilon_k^2+T^2}{T_k^2}\right)^{1/2}\right]^{-1}-[f(\epsilon_k)-\tfrac{1}{2}]\left[\ln\left(\frac{\epsilon_k^2+T^2}{T_k^2}\right)^{1/2}\right]^{-1}\right\}. \quad (3.34)$$

Assuming an antiferromagnetic interaction between spin systems, for $T>T_k$ we can rewrite the Eq. (3.34) in powers of J as

$$\langle \mathbf{S}^{el}(r)\cdot\mathbf{S}^{imp}\rangle\cong\frac{S(S+1)}{6\rho}\frac{|J|\rho}{N}\sum_{kk'}\frac{e^{i(k-k')\cdot r}}{\epsilon_k-\epsilon_{k'}}[f(\epsilon_{k'})-f(\epsilon_k)]+\frac{S(S+1)}{12\rho}\left(\frac{|J|\rho}{N}\right)^2\sum_{kk'}\frac{e^{i(k-k')\cdot r}}{\epsilon_k-\epsilon_{k'}}\times\left\{[f(\epsilon_{k'})-\tfrac{1}{2}]\ln\left(\frac{\epsilon_k^2+T^2}{D^2}\right)^{1/2}-[f(\epsilon_k)-\tfrac{1}{2}]\ln\left(\frac{\epsilon_{k'}^2+T^2}{D^2}\right)^{1/2}\right\}. \quad (3.35)$$

The spatial character of the above expression for the conduction-electron-spin–impurity-spin correlation function is the same as that obtained by the direct second-order perturbation theory. The first term of the Eq. (3.35) shows precisely the oscillations of the Ruderman-Kittel-Kasuya-Yosida (RKKY) type. The second term has been evaluated explicitly in the Appendix D of Ref. 4.

IV. CONCLUDING REMARKS

The calculations in the preceding sections give us a perturbational and a nonperturbational expression for the conduction-electron-spin–impurity-electron-spin correlation function. The nonperturbational expression, which is an exact one, could only be expressed in terms of certain integrals involving the t matrix. These integrals are, to the author's knowledge, too involved to carry out analytically. However, these integrals can be carried out numerically since a numerical plot of $t_R(\omega)$ versus ω is presently known. So far as the perturbational approach is concerned, we have developed a fairly straightforward method of evaluating $\langle \mathbf{S}^{el}(r)\cdot\mathbf{S}^{imp}\rangle$ to all orders in J. To get an explicit expression for this correlation function beyond second order, one encounters complicated integrals which can be done numerically.

In the lowest-order expansion in X, which is important at very high temperatures ($T\gg T_k$), we have found that there exists no correlation between the conduction-electron spin and the impurity-electron spin. Physically this result is plausible because at very high temperature the effect of exchange interaction is destroyed by the thermal fluctuations in the system. The next-higher-order term in X contributes to the conduction-electron-spin–impurity-electron-spin correlation function, giving an RKKY term to first order in J. In the second order in J, apart from some oscillatory terms involving Si and Ci functions, we get a *nonoscillatory* term which, in turn, is responsible for the *Kondo-type* logarithmic singularity in the susceptibility.[4]

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APPENDIX

The purpose of this Appendix is to illustrate the procedure for evaluating the integral

$$I\equiv P\int_{-\infty}^{+\infty}\frac{t_R(\omega')}{\omega-\omega'+i\delta}f(\omega')d\omega', \quad (A1)$$

occurring in the course of our calculation without restricting ourselves to the approximation (3.17). The

integrand in Eq. (A1) has the following analytical properties: (a) $t_R(\omega')$, although regular in the upper ω' half-plane at all temperatures, has three branch points on unphysical sheet of the lower ω' half-plane at $\omega'=iT_k \exp\pm i\pi[S(S+1)]^{1/2}-iT$; $-iT$; (b) the Fermi function $f(\omega')$ has a series of first-order poles at $\omega'=i\omega_n$; $\omega_n=(2n+1)\pi T$ with $n=0, \pm1, \pm2, \cdots$; (c) pole due to energy denominator at $\omega'=\omega+i\delta$; (d) $t_R(\omega')$ behaves as $\ln^{-2}|\omega'/T_k|$ in the asymptotic limit.[5] Now since the integrand vanishes fast enough at $\pm\infty$, we can close the integration contour in the upper ω half-plane. The use of dispersion relation gives

$$I=T\sum_{n>0}^{\infty}\frac{t_R(i\omega_n)}{i\omega_n-\omega}-i\pi t_R(\omega)f(\omega). \tag{A2}$$

It is very difficult to estimate the contributions from the poles of $f(\omega')$ because of the complex analytic structure of the summand. For low enough temperature one can show in the following way that for asymptotic values of $t_R(\omega')$ the contribution from these poles is negligible. Using the asymptotic form of $t_R(\omega')$ in (A2), we get (for estimation purpose we put $\omega=0$)

$$T\sum_{n>0}^{\infty}\frac{t_R(i\omega_n)}{i\omega_n-\omega}\bigg|_{\omega=0}\cong T\sum_{n>0}^{\infty}\frac{1}{i\omega_n}\ln^{-2}\left|\frac{i\omega_n}{T_k}\right|. \tag{A3}$$

Making a change of variable and converting summation into intergration we can write (A3) as

$$T\sum_{n>0}^{\infty}\frac{t_R(i\omega_n)}{i\omega_n-\omega}\bigg|_{\omega=0}\cong\frac{1}{2\pi}\int_{\pi T}^{\infty}\frac{d\omega_n}{i\omega_n}\ln^{-2}\frac{i\omega_n}{T_k}. \tag{A4}$$

Let us make another change of variable by substituting z for $\ln|i\omega_n/T_k|$ in (A4). We get

$$T\sum_{n>0}^{\infty}\frac{t_R(i\omega_n)}{i\omega_n-\omega}\bigg|_{\omega=0}\cong\frac{i}{2\pi}\int_{\ln(i\pi T/T_k)}^{\infty}dz\,z^{-2}=\frac{1}{2\pi i}\ln^{-1}\left|\frac{i\pi T}{T_k}\right|. \tag{A5}$$

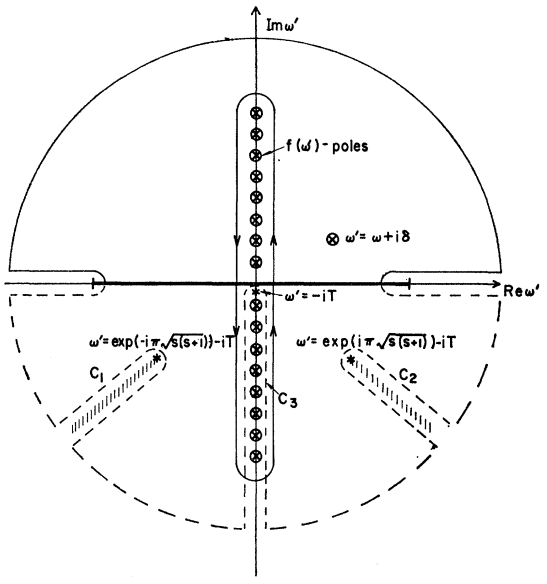

FIG. 1. Integration contour for the integral in (A6). The full line of the contour is on the physical sheet, and the dashed line on the unphysical sheet.

From (A5) it is clear that for very low temperature the contribution from the poles of $f(\omega')$ function in the large ω' region is negligible.

In order to compute the contribution from the poles of $f(\omega')$ function in arbitrary ω' region, we make use of Poisson summation formula:

$$T\sum_{n=-\infty}^{+\infty}\frac{t_R(i\omega_n)}{i\omega_n-\omega}=-\frac{1}{2\pi i}\int_C\frac{t_R(\omega')}{\omega'-\omega}f(\omega')d\omega', \tag{A6}$$

where the contour C encircles the imaginary ω' axis. Now we can stretch the contour to infinity as shown in Fig. 1, picking up the contributions from the singularities of $t_R(\omega')/(\omega-\omega')$. Assuming that $t_R(\omega')$ vanishes on the infinite circle, the $f(\omega')$ pole contribution will be given by the values of the integrals along the branch cuts and the residue of the pole at $\omega'=\omega+i\delta$.