

Anisotropy in binary metallic spin-glass alloys. II. Rare earths

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We derive the anisotropic pair interaction for binary spin-glass systems where the magnetic scattering at the spin-orbit scattering site comes from the Coulomb exchange interaction. Its form is identical to that found in binary systems in which the spin scattering comes from the *s-d* mixing interaction.

I. INTRODUCTION

We have been studying the origins of anisotropy in metallic spin glasses. In the preceding paper¹ (hereafter denoted as I) we derived the pair interaction that gives rise to anisotropy in noble metals (Ag, Au, and Cu) with transition-metal impurities. For these alloys it is the *s-d* mixing interaction² which gives rise to the scattering of the conduction electrons by the local moments. For transition-metal impurities such as manganese in copper, the *s-d* mixing is sufficiently strong compared to intra-atomic energies that it is not correct to represent the effects of mixing by $\Gamma\mathbf{S}\cdot\mathbf{s}$, a spin scattering of the conduction electrons. Therefore in I, we derived the anisotropic pair interaction between impurities by using the method of phase shifts.³ Here, we will consider alloys in which the spin scattering of conduction electrons by the local moments can be represented by $\Gamma\mathbf{S}\cdot\mathbf{s}$. This interaction can be used when the Coulomb exchange interaction is the origin of the scattering or when the *s-d* mixing is sufficiently weak compared to intra-atomic terms that the Schrieffer-Wolff transformation is valid.

By using this form of the spin scattering we find that the form of the anisotropic pair interaction between impurities in rare-earth binary spin glasses is the same as that found in I. This is reassuring in that the derivation we present here maintains rotational invariance. In I this was not possible as we had to choose an axis of quantization for the spin-dependent phase-shift analysis. In Sec. II we derive our pair interaction and in Appendix A we show how the expression for the fifth-order correction to the energy of a gas of electrons is obtained. In Appendix B we show how terms of leading order in the interaction are selected.

II. CALCULATION OF THE INTERACTION

At an impurity site the conduction electrons are described by the Friedel or virtual bound state (VBS) wave function,²

$$\psi_{\mathbf{k}\sigma}(\eta) = \left[e^{i\mathbf{k}\cdot\mathbf{r}} + e^{i\eta_2(k)} \sin[\eta_2(k)] \frac{V_{dk}}{\Delta} \sum_m Y_{2m}^*(\hat{\mathbf{k}}) \phi_{2m}(\mathbf{r}) \right] \chi_\sigma, \quad (1a)$$

and at distant sites *A* and *B* far from the impurity the wave function is

$$\psi_{\mathbf{k}\sigma}(\eta) = [e^{i\mathbf{k}\cdot\mathbf{r}} - 4\pi e^{i\eta_2(k)} \sin[\eta_2(k)] h_2^{(+)}(kr) \times Y^2(\hat{\mathbf{k}}) \cdot Y^2(\hat{\mathbf{r}})] \chi_\sigma, \quad (1b)$$

where the scalar product is given by

$$Y^2(\theta, \phi) \cdot Y^2(\theta', \phi') = \sum_m (-1)^m Y_m^2(\theta, \phi) Y_{-m}^2(\theta', \phi'). \quad (2)$$

In Eq. (1), $\phi_{2m}(\mathbf{r})$ is a core *d* orbital, Δ is the half width of the VBS resonance, $h_2^{(+)}$ is an outgoing spherical Hankel function, and the phase shift is given by

$$\eta(k) \equiv \eta_2(k) = \arctan \left[\frac{\Delta}{E_{\text{res}} - E_k} \right], \quad (3)$$

where E_{res} is the center of the VBS resonance.

The electron gas is subject to a four component perturbation given by

$$V_{ABT\lambda} = -\frac{\Gamma}{N} [\mathbf{S}_A \cdot \mathbf{s} \delta(\mathbf{r} - \mathbf{R}_A) + \mathbf{S}_B \cdot \mathbf{s} \delta(\mathbf{r} - \mathbf{R}_B)] - \Gamma \mathbf{S}_T \cdot \mathbf{s} + \lambda(r) I \cdot \mathbf{s}. \quad (4)$$

An interaction with an odd number of impurity spins is zero because of time-reversal invariance; the lowest-order anisotropic interaction incorporating spin scattering at three sites requires at least two spin scatterings at one of the sites. Therefore, to obtain the effect of spin scattering from a ternary impurity, one must calculate the fifth-order perturbation energy $E_{ABT^2\lambda}^{(5)}[\psi(\eta)]$ by using Eq. (4) with the term in $\mathbf{S}_T \cdot \mathbf{s}$ taken to second order. Then the perturbation energy calculated to second order in the ternary moment is $E_{AB\lambda}^{(3)}[\psi(\eta)] + E_{ABT^2\lambda}^{(5)}[\psi(\eta)]$ where $E_{AB\lambda}^{(3)}[\psi(\eta)]$ is given by Eqs. (51a) and (51b) of I. Note that we do not literally use a constant Γ in the evaluation of the matrix elements of the spin scattering at site *T*, Eq. (7) below, because an expression such as $\langle \mathbf{k}_i | \Gamma | \mathbf{k}_j \rangle$ yields zero unless $\mathbf{k}_i = \mathbf{k}_j$. Rather, we mean to denote by Γ a coupling at site *T* given by an expansion of the form $\sum_l \Gamma_l(k, k') Y^l(\hat{\mathbf{k}}) \cdot Y^l(\hat{\mathbf{k}}')$, so Γ must be interpreted as $\Gamma_2(k_F, k_F)$.

Our starting point is the fifth-order term of the Rayleigh-Schrödinger perturbation theory whose derivation is indicated in Appendix A:

$$\begin{aligned}
E^{(5)} &= \frac{1}{5} \left[\frac{1}{8\pi^3} \right]^5 \int_0^{k_F} dk_0 k_0^2 \int_0^\infty dk_1 k_1^2 \cdots \int_0^\infty dk_4 k_4^2 \\
&\times \left\{ \left[\mathbf{P} \left[\frac{1}{E_{k_0} - E_{k_1}} \right] \mathbf{P} \left[\frac{1}{E_{k_0} - E_{k_4}} \right] - \pi^2 \delta(E_{k_0} - E_{k_1}) \delta(E_{k_0} - E_{k_4}) \right] \right. \\
&\times \left[\mathbf{P} \left[\frac{1}{E_{k_0} - E_{k_2}} \right] \mathbf{P} \left[\frac{1}{E_{k_0} - E_{k_3}} \right] - \pi^2 \delta(E_{k_0} - E_{k_2}) \delta(E_{k_0} - E_{k_3}) \right] \\
&+ 2\mathbf{P} \left[\frac{1}{E_{k_0} - E_{k_1}} \right] \mathbf{P} \left[\frac{1}{E_{k_0} - E_{k_2}} \right] \left[\mathbf{P} \left[\frac{1}{E_{k_0} - E_{k_3}} \right] \mathbf{P} \left[\frac{1}{E_{k_0} - E_{k_4}} \right] - 2\pi^2 \delta(E_{k_0} - E_{k_3}) \delta(E_{k_0} - E_{k_4}) \right] \\
&\left. + 2\mathbf{P} \left[\frac{1}{E_{k_0} - E_{k_1}} \right] \mathbf{P} \left[\frac{1}{E_{k_0} - E_{k_3}} \right] \left[\mathbf{P} \left[\frac{1}{E_{k_0} - E_{k_2}} \right] \mathbf{P} \left[\frac{1}{E_{k_0} - E_{k_4}} \right] - 2\pi^2 \delta(E_{k_0} - E_{k_2}) \delta(E_{k_0} - E_{k_4}) \right] \right\} \\
&\times \text{Re}V(k_0, k_1, \dots, k_4), \tag{5a}
\end{aligned}$$

where

$$V(k_0, k_1, \dots, k_4) = \sum_{\sigma_0, \sigma_1, \dots, \sigma_4} \int d\Omega_{k_0} \cdots \int d\Omega_{k_4} V_{\mathbf{k}_0\sigma_0, \mathbf{k}_1\sigma_1} \cdots V_{\mathbf{k}_4\sigma_4, \mathbf{k}_0\sigma_0}. \tag{5b}$$

If one examines the discrete eigenfunction prototype of this formula,⁴ one observes what appears to be 14 distinctly different scattering processes. In Eq. (5) which is valid for continuous eigenfunctions, there is only *one* scattering process during which an electron in the initial state $|\mathbf{k}_0\sigma_0\rangle$ methodically hops from one intermediate state to another before returning to $|\mathbf{k}_0\sigma_0\rangle$. Since the two formulas are equivalent—see Appendix A—we believe that the appearance of scattering terms with structures other than that of Eq. (5b) appearing in the traditional method of derivation,⁵ for example, the term

$$V_{\mathbf{k}_0\sigma_0, \mathbf{k}_1\sigma_1} V_{\mathbf{k}_1\sigma_1, \mathbf{k}_0\sigma_0} V_{\mathbf{k}_0\sigma_0, \mathbf{k}_0\sigma_0}$$

in third order are not independent processes.

A priori, there are $5!/2! = 60$ matrix elements contributing to $V(k_0, k_1, \dots, k_4)$ which are quintilinear in the individual terms of $V_{ABT^2\lambda}$. Only 30 of these contribute in leading order in $1/R$, one of which is $M_{AT\lambda TB}$ defined by

$$\begin{aligned}
M_{AT\lambda TB} &= \sum_{\sigma_0, \sigma_1, \dots, \sigma_4} \langle \mathbf{k}_0\sigma_0 | (\Gamma/N) \mathbf{S}_A \cdot \mathbf{s} \delta(\mathbf{r} - \mathbf{R}_A) | \mathbf{k}_1\sigma_1 \rangle \langle \mathbf{k}_1\sigma_1 | \Gamma \mathbf{S}_T \cdot \mathbf{s} | \mathbf{k}_2\sigma_2 \rangle \\
&\times \langle \mathbf{k}_2\sigma_2 | \lambda(r) \mathbf{l} \cdot \mathbf{s} | \mathbf{k}_3\sigma_3 \rangle \langle \mathbf{k}_3\sigma_3 | \Gamma \mathbf{S}_T \cdot \mathbf{s} | \mathbf{k}_4\sigma_4 \rangle \langle \mathbf{k}_4\sigma_4 | (\Gamma/N) \mathbf{S}_B \cdot \mathbf{s} \delta(\mathbf{r} - \mathbf{R}_B) | \mathbf{k}_0\sigma_0 \rangle. \tag{6}
\end{aligned}$$

This includes the spin summations in Eq. (5). We evaluate the matrix elements of $\Gamma \mathbf{S}_T \cdot \mathbf{s}$ by using the VBS wave function Eq. (1a) and find

$$\langle \mathbf{k}_i | \Gamma | \mathbf{k}_j \rangle \simeq \frac{4\Gamma}{\Delta \mathcal{N}(E_F)} \exp\{-i[\eta(k_i) - \eta(k_j)]\} \sin[\eta(k_i)] \sin[\eta(k_j)] Y^2(\hat{\mathbf{k}}_i) \cdot Y^2(\hat{\mathbf{k}}_j), \tag{7}$$

where $\mathcal{N}(E_F)$ is the density of states for one spin direction evaluated at the Fermi level.

The remaining factors of Eq. (6) as well as the procedures for evaluating its contribution to the energy, Eq. (5), have been given elsewhere.¹ We obtain for the sum total of all 30 leading order contributions

$$\begin{aligned}
E_{ABT^2\lambda}^{(5)}[\psi(\eta)] &= -\frac{1}{2} \frac{135\pi}{32} \frac{\lambda \Gamma^4 \mathcal{S}_T^2}{\Delta^3 E_F k_F^7} \frac{P_1(\hat{\mathbf{R}}_A \cdot \hat{\mathbf{R}}_B)}{R_A R_B R_{AB}} \\
&\times \left[k_F^2 \int_0^{k_F} dk k \sin^4[\eta(k)] \cos^2[\eta(k)] \sin[k(R_A + R_B + R_{AB}) + 2\eta(k)] \right. \\
&\quad + 2k_F \int_0^{k_F} dk k^2 \sin^5[\eta(k)] \cos[\eta(k)] \cos[k(R_A + R_B + R_{AB}) + 2\eta(k)] \\
&\quad \left. - \int_0^{k_F} dk k^3 \sin^6[\eta(k)] \sin[k(R_A + R_B + R_{AB}) + 2\eta(k)] \right] \\
&\times (\hat{\mathbf{R}}_A \times \hat{\mathbf{R}}_B) \cdot [\mathbf{S}_A \times \mathbf{S}_B + 2\hat{\mathbf{S}}_T (\mathbf{S}_A \times \mathbf{S}_B) \cdot \hat{\mathbf{S}}_T], \tag{8}
\end{aligned}$$

where $P_1(x)=x$. Equation (8) explicitly shows the existence of the second type of Dzyaloshinsky-Moriya interaction, $(\hat{\mathbf{R}}_A \times \hat{\mathbf{R}}_B) \cdot \hat{\mathbf{S}}_T (\mathbf{S}_A \times \mathbf{S}_B) \cdot \hat{\mathbf{S}}_T$, demonstrated earlier in a Hartree-Fock calculation¹ but now obtained in a rotationally invariant context.

The integrals of Eq. (8) may be obtained analytically by using the methods in I (Ref. 1) but the result is not particularly illuminating. Instead we give both preasymptotic and asymptotic forms of the fifth-order term and present a plausibility argument to demonstrate that the asymptotic form is a good approximation in the regime of interest in spin-glass physics, the range from 1 to 15 lattice constants.

The preasymptotic form may be obtained by means of the identity

$$k dk = \frac{m\Delta}{\hbar^2} \frac{d\eta}{\sin^2\eta}, \quad (9)$$

which derives from Eq. (3) and the relationship $E(k) = \hbar^2 k^2 / 2m$, and the assumption that the dominant contributions come from a narrow band of wave vectors at E_{res} which is close to E_F . Then the three integrals add to

$$\frac{m\Delta}{\hbar^2} k_F^2 \int_0^{\eta_2(k_F)} d\eta \sin^2\eta \sin[k(R_A + R_B + R_{AB}) + 4\eta] = \frac{1}{6} \left[\frac{k_F^4}{E_F} \Delta \right] \sin^3[\eta_2(k_F)] \sin[k_F(R_A + R_B + R_{AB}) + 3\eta_2(k_F)] \quad (10)$$

and the fifth-order term in Eq. (8) takes the form

$$E_{ABT^2\lambda}^{(5)}[\psi(\eta)] = - \frac{1}{12} \frac{135\pi}{32} \frac{\lambda\Gamma^4 S_T^2}{\Delta^2 E_F^2 k_F^3} \frac{P_1(\hat{\mathbf{R}}_A \cdot \hat{\mathbf{R}}_B)}{R_A R_B R_{AB}} \sin^3[\eta_2(k_F)] \\ \times \sin[k_F(R_A + R_B + R_{AB}) + 3\eta_2(k_F)] (\hat{\mathbf{R}}_A \times \hat{\mathbf{R}}_B) \cdot [\mathbf{S}_A \times \mathbf{S}_B + 2\hat{\mathbf{S}}_T (\mathbf{S}_A \times \mathbf{S}_B) \cdot \hat{\mathbf{S}}_T]. \quad (11)$$

This form is valid when the average interparticle distance R_{av} in the interacting triads satisfy the condition $3 |k_F - k_{\text{res}}| R_{\text{av}} \ll 1$; i.e., when $E_{\text{res}} \simeq E_F$ in real materials. It is also the correct mathematical solution in the nonphysical regime for which R_{av} is less than a nearest-neighbor distance.

For sufficiently large R , defined by $3 |k_F - k_{\text{res}}| R_{\text{av}} \gg 1$, we obtain the asymptotic form

$$E_{ABT^2\lambda}^{(5)}[\psi(\eta)] = + \frac{1}{2} \frac{135\pi}{32} \frac{\lambda\Gamma^4 S_T^2}{\Delta^3 E_F k_F^4} \frac{P_1(\hat{\mathbf{R}}_A \cdot \hat{\mathbf{R}}_B)}{R_A R_B R_{AB} (R_A + R_B + R_{AB})} \\ \times \sin^4[\eta_2(k_F)] \cos[k_F(R_A + R_B + R_{AB}) + 4\eta_2(k_F)] (\hat{\mathbf{R}}_A \times \hat{\mathbf{R}}_B) \cdot [\mathbf{S}_A \times \mathbf{S}_B + 2\hat{\mathbf{S}}_T (\mathbf{S}_A \times \mathbf{S}_B) \cdot \hat{\mathbf{S}}_T]. \quad (12)$$

Thus, the range dependence varies from R^{-3} to R^{-4} as R increases.

Now we demonstrate that Eq. (12) is valid over the whole range of interest, $1 < R/a < 15$ where a is the lattice constant. We have previously shown for the case of the binary transition-metal spin glass that if the average interparticle spacing is larger than a critical distance defined by

$$R_c \equiv (3 |k_F - k_{\text{res}}|)^{-1}, \quad (13)$$

where $k_{\text{res}} = (2mE_{\text{res}})^{1/2} / \hbar$, then the Dzyaloshinsky-Moriya interaction may be approximated by its asymptotic form. This observation resulted from the analysis of the coefficients which were given by integrals of the form

$$K \sim \int_0^{k_F} dk k \sin^2[\eta(k)] \sin[k(R_A + R_B + R_{AB}) + 2\eta(k)]. \quad (14)$$

Equation (13) follows from the behavior of the denominator of the oscillatory factor

$$\sin^2[\eta(k)] = \frac{k_\Delta^4}{(k^2 - k_{\text{res}}^2)^2 + k_\Delta^4}, \quad (15)$$

where $k_\Delta = (2m\Delta)^{1/2} / \hbar$. The integrals appearing in our present calculation, Eq. (8), differ from Eq. (14) only by the appearance of additional factors of $\sin^2\eta$ and $\sin\eta \cos\eta$, where

$$\sin[\eta(k)] \cos[\eta(k)] = \frac{k_\Delta^2 (k_{\text{res}}^2 - k^2)}{(k^2 - k_{\text{res}}^2)^2 + k_\Delta^4}. \quad (16)$$

Since the denominators of these additional factors are the same, the definition of R_c remains valid.

Consequently, it is easy to show that $R_c \approx a$ for both silver and gold rare-earth alloys so that the regime of interest to us, $R/a > 1$, is also the asymptotic regime. In noble-metal-rare-earth alloys, the $5d$ states of the rare-earth ion are split by the crystal field and mix with the conduction band. The lowest state is the triplet T_{2g} (Ref. 6) so that the effective angular momentum of the $5d$ electron is $l=1$. Then the phase shift imparted to the conduction-electron wave function by the s - d mixing, evaluated at the Fermi surface, is given by the Friedel sum rule³ $\eta(k_F) = [\pi/2(2l+1)]Z_d$ which equals $\pi/6$ since $Z_d=1$. The halfwidths Δ of the nonmagnetic VBS's for both $Ag\mathcal{R}$ and $Au\mathcal{R}$ may be taken as those values which have been used to explain transport properties in these materials.⁶

For $Ag\mathcal{R}$:

$$\Delta=0.45 \text{ eV}, E_{\text{res}}=6.27 \text{ eV}, E_F=5.49 \text{ eV}.$$

For $Au\mathcal{R}$:

$$\Delta=0.60 \text{ eV}, E_{\text{res}}=6.56 \text{ eV}, E_F=5.53 \text{ eV}.$$

Then the critical distances are for $Ag\mathcal{R}$:

$$R_c=4.4 \text{ \AA},$$

and for $Au\mathcal{R}$:

$$R_c=3.09 \text{ \AA},$$

while the lattice constants are $a_{Ag}=4.09 \text{ \AA}$, $a_{Au}=4.08 \text{ \AA}$. It follows that the fifth-order term may be approximated by its asymptotic form so that the Dzyaloshinsky-Moriya interaction is given by the sum of the asymptotic form of $E_{AB\lambda}^{(3)}[\psi(\eta)]$, Eq. (51b) of I, and Eq. (12) of this paper.

In conclusion, we have calculated the Dzyaloshinsky-Moriya interaction in fifth-order perturbation theory, appropriate for noble-metal-rare-earth spin glasses. In particular, we have demonstrated in a rotationally invariant manner the existence of a second type of DM term. Previously, this term was found from a Hartree-Fock calculation and it was not entirely clear whether symmetry breaking associated with the Hartree-Fock approximation induced this new term.

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APPENDIX A: RAYLEIGH-SCHRÖDINGER ALGORITHM

Here, we present an algorithm with which the Rayleigh-Schrödinger perturbation series can be generated

$$E^{(3)} = \left[\frac{1}{8\pi^3} \right]^3 \int_0^{k_F} dk_0 k_0^2 \int_0^\infty dk_1 k_1^2 \int_0^\infty dk_2 k_2^2 \left[\mathcal{P} \left[\frac{1}{E_{k_0} - E_{k_1}} \right] \mathcal{P} \left[\frac{1}{E_{k_0} - E_{k_2}} \right] - \frac{\pi^2}{3} \delta(E_{k_0} - E_{k_1}) \delta(E_{k_0} - E_{k_2}) \right] \times V(k_0, k_1, k_2), \quad (\text{A2})$$

where, in general,

$$V(k_0, k_1, \dots, k_n) = \sum_{\sigma_0, \sigma_1, \dots, \sigma_n} \int d\Omega_{k_0} \cdots \int d\Omega_{k_n} V_{k_0\sigma_0, k_1\sigma_1} \cdots V_{k_n\sigma_n, k_0\sigma_0}$$

and an integration over the initial state $|k_0\sigma_0\rangle$ has been included. The double pole contribution is represented by the product of the two δ functions.

The fourth-order Rayleigh-Schrödinger term has been given by Niessen⁸ while the fifth- and sixth-order terms have been given by Levy.⁴ To convert these expressions to useful form would require the evaluation of triple and quadrupole pole singularities involving the simultaneous convergence of 8 three-dimensional integrals, 16 four-

in *decoupled*, integral form to arbitrary order of a perturbation. The principle difficulty in adapting the Rayleigh-Schrödinger series to the situation where the intermediate states as well as the initial states form a continuum is the evaluation of multipole singularities. For example, the third-order term,⁵

$$E_{k_0}^{(3)} = \sum_{k_1} \frac{V_{k_0 k_1}}{E_{k_0} - E_{k_1}} \left[\sum_{k_2} \frac{V_{k_1 k_2} V_{k_2 k_0}}{E_{k_0} - E_{k_2}} - \frac{V_{k_1 k_0} V_{k_0 k_0}}{E_{k_0} - E_{k_1}} \right], \quad (\text{A1})$$

contains a two-dimensional double pole of the form

$$\mathcal{P} \int_0^\infty dk_1 \int_0^\infty dk_2 \frac{f(k_1, k_2)}{(k_1 - k_0)(k_2 - k_0)},$$

where $f(k_1, k_2)$ is analytic. By writing the integral as a product of single pole contributions

$$\mathcal{P} \int_0^\infty dk_1 \frac{1}{k_1 - k_0} \mathcal{P} \int_0^\infty dk_2 \frac{f(k_1, k_2)}{k_2 - k_0}$$

one fails to delete the region in the (k_1, k_2) plane for which $k_1 = k_2 = k_0$. In other words, in a one-dimensional integral of the form

$$\mathcal{P} \int_0^\infty dk \frac{f(k)}{(k - k_0)^2},$$

one evaluates the two contributions $\int_0^{k_0 - \epsilon}$ and $\int_{k_0 + \epsilon}^\infty$ where ϵ is an infinitesimal, taking the limit $\epsilon \rightarrow 0$. The pole region on a line has two edges. For the two-dimensional case, the pole region is a square bounded by lines drawn through the four points $(k_0 \pm \epsilon, k_0 \pm \epsilon)$. One must evaluate four two-dimensional integrals and calculate their contribution in the limit where all four corners of the square converge to the point (k_0, k_0) . Levy and Fert found the correct solution⁷

dimensional integrals, etc. This is a formidable mathematical problem if undertaken with the original method. However, one may approach the problem differently by noting that the Rayleigh-Schrödinger series is a special case of many-body theory.

One starts with the well-known expression for the change in the grand potential arising from some arbitrary perturbations, selects only those diagrams for which there are neither exchange processes between electrons nor

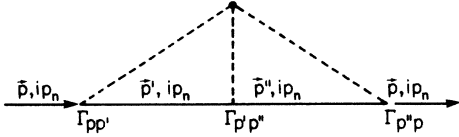


FIG. 1. Diagram for the evaluation of the change in the grand potential due to triple scattering from a single impurity site, Eq. (A3).

internal excitations such as phonons nor internal interactions such as electron-electron scatterings, and then takes the limit as the temperature goes to zero. This generates the correction to the ground-state energy in general, and for this special case, the integral form of the Rayleigh-Schrödinger series. Thus, we have⁹

$$\Omega - \Omega_0 = \frac{1}{\beta} \sum_{\mathbf{p}, \sigma, ip_n} \int_0^1 \frac{d\alpha}{\alpha} G(\alpha, \mathbf{p}, ip_n) \Sigma(\alpha, \mathbf{p}, ip_n), \quad (\text{A3})$$

where α is the coupling constant, ip_n is the set of thermal poles, G is the electron Green function, and Σ is the set of relevant self-energy diagrams.

Since our principle task is to evaluate the multipole singularities, it is sufficient to evaluate only those contributions to $\Delta\Omega$ which are linear in the impurity concentration; i.e., we consider the case of multiple scatterings from a single impurity site. That the resultant expressions may be used to calculate the corrections to the energy of the

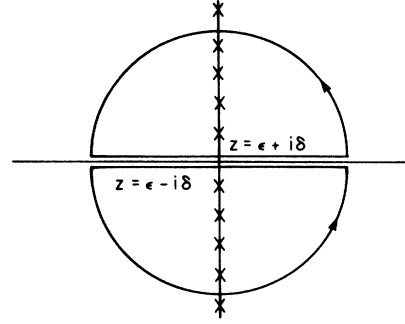


FIG. 2. Contour of integration and the poles of the integrand of J , Eq. (A7).

conduction-electron gas arising from single scatterings from multiple sites has been shown by Ruderman and Kittel.¹⁰ Consequently, to obtain the n th perturbation term, we use in Eq. (A3) the zero-order Green function G^0 and the single n th-order self-energy diagram $\Sigma^{(n)}$ so that

$$\lim_{V \rightarrow \infty} \lim_{T \rightarrow 0} (\Omega - \Omega_0)^{(n)} = (E - E_0)^{(n)} N_i \equiv E^{(n)} N_i, \quad (\text{A4})$$

where N_i is the number of impurities.

To illustrate our method, we rederive Eq. (A2). The impurity potential is treated as an external field and there are no energy transfers in the intermediate states. The only relevant third-order diagram is shown in Fig. 1. Then

$$(\Delta\Omega)^{(3)} = n_i \frac{V}{\beta} \sum_{\sigma, ip_n} \int_0^1 \frac{d\alpha}{\alpha} \alpha^3 \int \frac{d^3 p}{(2\pi)^3} G^0(\mathbf{p}, ip_n) \int \frac{d^3 p'}{(2\pi)^3} \int \frac{d^3 p''}{(2\pi)^3} G^0(p', ip_n) G^0(p'', ip_n) \Gamma_{pp'} \Gamma_{p'p''} \Gamma_{p''p}, \quad (\text{A5})$$

where n_i is the impurity concentration, $\beta = 1/k_B T$, and the $\Gamma_{p_i p_j}$ are the scattering matrix elements. The dependence on the coupling constant α is trivial in this example: $G^0(\alpha, \mathbf{p}, ip_n) = G^0(\mathbf{p}, ip_n)$, and $\Sigma^{(3)}(\alpha, \mathbf{p}, ip_n) = \alpha^3 \Sigma^{(3)}(\mathbf{p}, ip_n)$; i.e., the single third-order contribution to $\Delta\Omega$ is cubic in the scattering potential.

Therefore,

$$(\Delta\Omega)^{(3)} = \frac{N_i}{3} \sum_{\sigma} \int \frac{d^3 p}{(2\pi)^3} \frac{d^3 p'}{(2\pi)^3} \frac{d^3 p''}{(2\pi)^3} \left[\frac{1}{\beta} \sum_{ip_n} \frac{1}{ip_n - \epsilon_p} \frac{1}{ip_n - \epsilon_{p'}} \frac{1}{ip_n - \epsilon_{p''}} \right] \Gamma_{pp'} \Gamma_{p'p''} \Gamma_{p''p}. \quad (\text{A6})$$

We have used $G^0(\mathbf{p}, ip_n) = 1/(ip_n - \epsilon_p)$, where $p_n = (2n + 1)\pi/\beta$, $\epsilon_p = E_p - \mu$, and sums over the internal spin variables are implicit.

The quantity in large parentheses in Eq. (A6) may be evaluated by defining the integral

$$J = \frac{1}{2\pi i} \oint_C dz n_F(z) \frac{1}{z - \epsilon_p} \frac{1}{z - \epsilon_{p'}} \frac{1}{z - \epsilon_{p''}}, \quad (\text{A7})$$

where

$$n_F(z) = \frac{1}{e^{\beta z} + 1},$$

and the contour of integration is shown in Fig. 2. There is a branch cut along the real axis and the only poles within C are those of $n_F(z)$, the thermal poles on the imaginary axis, for which the sum of the residues of the integrand of J is the negative of the quantity in parentheses in Eq. (A6). By direct evaluation of J along the contour, we obtain¹¹

$$J = -\frac{1}{\pi} \int_{-\infty}^{+\infty} d\epsilon n_F(\epsilon) \text{Im} \prod_j \frac{1}{\epsilon - \epsilon_{p_j} - i\delta}, \quad (\text{A8})$$

where we have set $(p, p', p'') \equiv (p_0, p_1, p_2)$. Substitution of Eq. (A8) into Eq. (A6) together with the cyclical permutability of the Γ product leads directly to Eq. (A2) since $\epsilon_{p_i} - \epsilon_{p_j} \equiv E_{p_i} - E_{p_j}$, and $n_F(\epsilon_{p_i}) \equiv n_F(E_{p_i} - E_F)$, the usual Fermi function.

$$\begin{aligned}
E^{(4)} = & \left[\frac{1}{8\pi^3} \right]^4 \int_0^{k_F} dk_0 k_0^2 \int_0^\infty dk_1 k_1^2 \cdots \int_0^\infty dk_3 k_3^2 P \left[\frac{1}{E_{k_0} - E_{k_1}} \right] \left\{ P \left[\frac{1}{E_{k_0} - E_{k_2}} \right] P \left[\frac{1}{E_{k_0} - E_{k_3}} \right] \right. \\
& \left. - \pi^2 \delta(E_{k_0} - E_{k_2}) \delta(E_{k_0} - E_{k_3}) \right\} \\
& \times \text{Re} V(k_0, k_1, k_2, k_3). \tag{A9}
\end{aligned}$$

Note that there is no triple pole (δ^3) contribution.

Equation (A9) may be used to calculate the effect on the coupling between two spins of two orders of spin-orbit scattering at a third site. For $R > R_c$ it is

$$\begin{aligned}
E_{AB\lambda^2}^{(4)}[\psi(\eta)] = & \frac{135\pi}{32} \frac{\lambda^2 \Gamma^2}{\Delta^2 E_F k_F^4} \frac{\sin^3[\eta_2(k_F)] \cos[k_F(R_A + R_B + R_{AB}) + 3\eta_2(k_F)]}{R_A R_B R_{AB} (R_A + R_B + R_{AB})} \\
& \times [P_1(\hat{\mathbf{R}}_A \cdot \hat{\mathbf{R}}_B)(\hat{\mathbf{R}}_A \times \hat{\mathbf{R}}_B) \cdot (\mathbf{S}_A \times \mathbf{S}_B) + 2P_2(\hat{\mathbf{R}}_A \cdot \hat{\mathbf{R}}_B) \mathbf{S}_A \cdot \mathbf{S}_B], \tag{A10}
\end{aligned}$$

which shows both anisotropic and isotropic components. The functions P_1 and P_2 are the usual Legendre polynomials of order 1 and 2.

The fifth-order term is given by Eq. (5). That one picks up the real part of $V(k_0, k_1, \dots, k_4)$ in Eq. (A9) and Eq. (5) is an algebraic consequence of the derivation and is not an imposed condition.

We reiterate that Eqs. (A2), (A9), and (5) are only valid for a continuous set of eigenfunctions.

APPENDIX B: LEADING ORDER CONTRIBUTIONS

We show how the order of scattering in the fifth-order matrix elements determines whether their contribution to the preasymptotic form of the interaction will go as $1/R^3$ or $1/R^4$. Consider the partial matrix element

$$M \dots_{AB} \dots = \cdots \langle k_1 | \delta(\mathbf{r} - \mathbf{R}_A) | k_2 \rangle \langle k_2 | \delta(\mathbf{r} - \mathbf{R}_B) | k_3 \rangle \cdots \tag{B1}$$

and assume for simplicity that the states $|k_i\rangle$ are plane waves. Then

$$M \sim e^{-i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{R}_A} e^{-i(\mathbf{k}_2 - \mathbf{k}_3) \cdot \mathbf{R}_B} = e^{-\mathbf{k}_1 \cdot \mathbf{R}_A} e^{i\mathbf{k}_2 \cdot (\mathbf{R}_A - \mathbf{R}_B)} e^{i\mathbf{k}_3 \cdot \mathbf{R}_B}. \tag{B2}$$

The integration over the angles of $\hat{\mathbf{k}}_2$ gives a factor $\sin(k_2 R_{AB})/k_2 R_{AB}$, while the integrations over Ω_{k_1} and Ω_{k_3} give $\sin(k_1 R_A) \sin(k_3 R_B)/k_1 k_3 R_A R_B$ so that $M \sim (R_A R_B R_{AB})^{-1}$. On the other hand, for the matrix element

$$M \dots_{A\lambda B} \dots = \cdots \langle k_1 | \delta(\mathbf{r} - \mathbf{R}_A) | k_2 \rangle \langle k_2 | \lambda(r) I | k_3 \rangle \langle k_3 | \delta(\mathbf{r} - \mathbf{R}_B) | k_4 \rangle \cdots, \tag{B3}$$

we obtain the expression

$$M \sim e^{-i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{R}_A} [Y^2(\hat{\mathbf{k}}_2) \times Y^2(\hat{\mathbf{k}}_3)]^1 e^{-i(\mathbf{k}_3 - \mathbf{k}_4) \cdot \mathbf{R}_B} \tag{B4}$$

which, after integrating over Ω_{k_2} and Ω_{k_3} , gives

$$M \sim e^{-i\mathbf{k}_1 \cdot \mathbf{R}_A} \frac{\sin(k_2 R_A)}{k_2 R_A} [Y^2(\hat{\mathbf{R}}_A) \times Y^2(\hat{\mathbf{R}}_B)]^1 \frac{\sin(k_3 R_B)}{k_3 R_B} e^{i\mathbf{k}_4 \cdot \mathbf{R}_B} \tag{B5}$$

and we find after integrating over Ω_{k_1} and Ω_{k_4} that $M \sim (R_A^2 R_B^2)^{-1}$. We conclude that if the scatterings \mathbf{S}_A 's and \mathbf{S}_B 's have a common state between them; e.g.,

$$\cdots | \mathbf{S}_A \cdot \mathbf{s} | \mathbf{k}_i \sigma_i \rangle \langle \mathbf{k}_i \sigma_i | \mathbf{S}_B \cdot \mathbf{s} | \cdots \quad \text{or} \quad \langle \mathbf{k}_i \sigma_i | \mathbf{S}_A \cdot \mathbf{s} | \cdots | \mathbf{S}_B \cdot \mathbf{s} | \mathbf{k}_i \sigma_i \rangle, \tag{B6}$$

then to leading order in $1/R$, the matrix element is proportional to $1/R^3$; otherwise, it goes as $1/R^4$. This is independent of the behavior of the coefficient which introduces an additional factor of $1/R$ for large interparticle distances. Thus, to leading order in $1/R$, we may concern ourselves only with those matrix elements for which the \mathbf{S}_A 's and \mathbf{S}_B 's factors are cyclically consecutive; e.g., $M_{TTAB\lambda}$, $M_{A\lambda TT B}$, etc., of which there are 30 in all.

- ¹S. M. Goldberg, P. M. Levy, and A. Fert, preceding paper, Phys. Rev. B **33**, 276 (1986), referred to as I.
- ²P. W. Anderson, Phys. Rev. **124**, 41 (1961).
- ³E. Daniel and J. Friedel, in *Proceedings of the 9th International Conference on Low Temperature Physics*, edited by J. Daunt, P. Edwards, F. Milford, and M. Yaqub (Plenum, New York, 1965), p. 933.
- ⁴P. M. Levy, Phys. Rev. **147**, 320 (1966).
- ⁵L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1968).
- ⁶G. Lacueva, P. M. Levy, and A. Fert, Phys. Rev. B **26**, 1099 (1982).
- ⁷P. M. Levy and A. Fert, Phys. Rev. B **23**, 4667 (1981).
- ⁸K. F. Niessen, Phys. Rev. **34**, 253 (1929).
- ⁹A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971), p. 268.
- ¹⁰M. A. Ruderman and C. Kittel, Phys. Rev. **96**, 99 (1954).
- ¹¹S. D. Silverstein and C. B. Duke, Phys. Rev. **161**, 546 (1967); G. D. Mahan, *Many-Particle Physics* (Plenum, New York, 1981), p. 157. Mahan's discussion of impurity scattering provided the inspiration for Appendix A.