Anisotropy in binary metallic spin-glass alloys. I. Transition metals

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We derive the anisotropic pair interaction for binary spin-glass systems for the case where the ternary site which scatters electrons by means of the spin-orbit interaction is a magnetic site characterized by spin-split virtual bound states. We find that there are two distinctly different types of anisotropic Dzyaloshinsky-Moriya couplings. One depends only upon the magnitude of the third magnetic moment and has the vector coupling form familiar from ternary spin glasses: $(\hat{\mathbf{R}}_i\times\hat{\mathbf{R}}_j)\cdot(\mathbf{S}_i\times\mathbf{S}_j)$. The second type depends upon both the magnitude and direction of the third moment and has the coupling structure $(\hat{\mathbf{R}}_i\times\hat{\mathbf{R}}_j)\cdot\hat{\mathbf{S}}_k\,(\mathbf{S}_i\times\mathbf{S}_j)\cdot\hat{\mathbf{S}}_k$. We define spin-dependent critical distances $R_c^{\pm}$ in terms of which the coefficients of the two anisotropic interactions, acting relatively independently, take on preasymptotic or asymptotic forms according to whether the average interparticle spacings are less than or greater than the $R_c^{\pm}$. These critical distances are themselves variable, depending upon the separation of the virtual bound-state resonances from the Fermi surface. When the resonances are sufficiently close to E_F, there will be large regions where the interactions exhibit preasymptotic behavior $(1/R^3)$. If the resonances are sufficiently far from E_F, the interactions quickly reach their asymptotic forms. In the practical cases of *Cu*Mn and *Au*Fe, we find that the critical distances are of the order of a nearest-neighbor distance so that the interactions fall off as $1/R^4$. This feature has great consequence in calculations of the macroscopic anisotropy energy.

I. INTRODUCTION

Experimental data showing the influence of added impurities with spin-orbit coupling on the behavior of spin glasses led two of us to propose a model of anisotropy based on the Dzyaloshinsky-Moriya mechanism.[1,2] In this model, the s-d mixing interaction V_{sd} at a nonmagnetic impurity site enhances the $l=2$ component of the conduction-electron wave function about the site and gives rise to a virtual bound state (VBS).[3] This mixing enables the conduction electron to feel more strongly the intra-atomic spin-orbit force within the impurity. The electron in a VBS is described by Friedel wave functions.[3] An effective coupling between localized moments, mediated by the conduction electrons, is obtained by calculating to third order the change in energy of the electron gas due to spin scatterings at the magnetic sites and spin-orbit scattering at the nonmagnetic impurity site,[1] and is of the Dzyaloshinsky-Moriya (DM) form. Of considerable interest is the effect on the DM interaction of a magnetic moment on the ternary site. In particular, one would like to understand the origin of anisotropy in binary spin glasses for which all three sites are identical. In *Au*Fe, for example, one may conceptualize a "$\mathrm{AuFe}_x\mathrm{Fe}_y$" system in the sense that iron ions are acting as their own ternary impurities, modifying the wave function by s-d mixing and providing *both* spin-orbit and spin-spin scattering.

One must at the outset distinguish two possibilities. For transition-metal spin-glass alloys such as *Cu*Mn and *Au*Fe there are spin-split magnetic VBS's,[4] so that we have to consider the effects of spin-orbit scattering on spin-split states. The second case is that of alloys in which the magnetic ions interact with the conduction electrons through nonmagnetic VBS's; e.g., in noble-metal rare-earth alloys. Then we consider the spin-spin and spin-orbit scatterings on an equal footing.

In this paper we confine ourselves to the transition-metal alloys: the case of the magnetic VBS. The following paper[5] (hereafter denoted as II) will consider the rare-earth case. We use the Hartree-Fock approximation so that the effect of the third moment is built into the zeroth-order Hamiltonian H_0. The conduction electrons are described by spin-polarized Friedel wave functions defined with spin-dependent phase shifts. We find that in the binary spin-glass alloys there are two different Dzyaloshinsky-Moriya couplings, one depending only upon the magnitude of the third moment and the other depending upon both its magnitude and direction. Specifically, the interaction has the form

$$E\sim\alpha(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot(\mathbf{S}_A\times\mathbf{S}_B)+\beta(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot\hat{\mathbf{S}}_T\,(\mathbf{S}_A\times\mathbf{S}_B)\cdot\hat{\mathbf{S}}_T\ , \tag{1}$$

where $\mathbf{S}_T$ is the spin of the third moment. As we will show, in the limit as the magnetic moment on the third site vanishes, the coefficient β goes to zero while the term in α reproduces the "nonmagnetic" result given earlier when the VBS resonance is near E_F. At the opposite extreme, in the limit when the separation of the spin-split VBS's is very large, the term in α vanishes and the entire coupling is given by the second term in Eq. (1). The absence of terms of the form $(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)_{\pm}(\mathbf{S}_A\times\mathbf{S}_B)_{\mp}$ in this

limit merely reflects the fact that there can be no spin-flip contributions; i.e., terms arising from $l_{\pm}s_{\mp}$, between well-separated states.

Our calculation has been performed using a spin-polarized Friedel wave function $\psi(\eta^{\sigma})$. For $\psi(\eta^{\sigma})$ to be an eigenfunction of H_0, the direction along which σ takes on the values $\pm$ must be that of $\mathbf{S}_T$ since we view the electron gas as being polarized by the moment itself. Thus, rotational invariance has been lost so that one may ask if the term in $(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot\hat{\mathbf{S}}_T(\mathbf{S}_A\times\mathbf{S}_B)\cdot\hat{\mathbf{S}}_T$ is an artifact of the Hartree-Fock approximation. In Appendix A, we show by general symmetry arguments that the effective Hamiltonian describing the perturbation about the spin-orbit scattering site is given by

$$H_{\text{eff}}(\lambda)=a\boldsymbol{l}\cdot\mathbf{s}+b(\boldsymbol{l}\cdot\hat{\mathbf{S}}_T)(\mathbf{s}\cdot\hat{\mathbf{S}}_T)+c\boldsymbol{l}\cdot\hat{\mathbf{S}}_T\ . \tag{2}$$

This perturbation operates in the space spanned by the uncoupled basis $|km_l\sigma\rangle$. When Eq. (2) is combined with spin scatterings at site A and B, we show that the resultant third-order perturbation energy of the electron gas is given by Eq. (1). Note that the term $\boldsymbol{l}\cdot\hat{\mathbf{S}}_T$ in Eq. (2) makes no contribution $\sim(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B\cdot\hat{\mathbf{S}}_T)$ to the energy in Eq. (1): From time-reversal invariance, there can be no contribution from an odd number of impurity spins.

In passing, we note that both types of DM terms in Eq. (1) yield the same form of macroscopic anisotropy for rigid rotations. For such rotations of the spin system with respect to the lattice, the vector $(\mathbf{S}_A\times\mathbf{S}_B)\cdot\hat{\mathbf{S}}_T$ is a constant, and the vector $(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot\hat{\mathbf{S}}_T$ yields the same result under rotation as does $(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot(\mathbf{S}_A\times\mathbf{S}_B)$. Thus, both terms in Eq. (1) contribute to the *unidirectional* anisotropy of binary spin glasses when the rotations of the spin system can be considered as rigid.

In Sec. II we calculate the form of the anisotropic pair interaction that comes from scattering by magnetic spin-orbit coupled impurities. In Sec. III, we discuss the coefficients of the interaction and, in particular, demonstrate the variable range dependence of the coupling. Section IV is devoted to a discussion of the binary spin glasses *Cu*Mn and *Au*Fe. We point out that numerical results depend upon four parameters for each material: the number of d electrons at the impurity site, the magnetic moment, and either the width or position of the resonance for each spin state. None of these parameters are known with sufficient precision for us to give more than somewhat general results for these alloys. We will show the effects of variations in these quantities and our conclusions will be presented in Sec. V.

II. CALCULATION OF THE INTERACTION

We now proceed with a sketch of the calculation of the Dzyaloshinsky-Moriya interaction in the Hartree-Fock approximation for the binary transition-metal spin glass. The scattering of the conduction electrons by the ternary site is described by the VBS wave functions,[3]

$$\psi_{\mathbf{k}\sigma}(\eta^{\sigma})=\left[e^{i\mathbf{k}\cdot\mathbf{r}}+e^{i\eta^{\sigma}(k)}\sin[\eta^{\sigma}(k)]\frac{V^{\sigma}_{dk}}{\Delta^{\sigma}}\sum_m Y^*_{2m}(\hat{\mathbf{k}})\phi_{2m}(\mathbf{r})\right]\chi_{\sigma} \tag{3a}$$

and

$$\psi_{\mathbf{k}\sigma}(\eta^{\sigma})=\left[e^{i\mathbf{k}\cdot\mathbf{r}}-4\pi e^{i\eta^{\sigma}(k)}\sin[\eta^{\sigma}(k)]h_2^{(+)}(kr)\sum_m Y^*_{2m}(\hat{\mathbf{k}})Y_{2m}(\hat{\mathbf{r}})\right]\chi_{\sigma} \tag{3b}$$

for the regions near to and far from the ternary site, respectively. In these equations, $\phi_{2m}(\mathbf{r})$ is a core d orbital, Δ^{σ} is the half width of the associated VBS, $h_2^{(+)}$ is an outgoing spherical Hankel function, χ_{σ} is the electron's spin state, and $\eta^{\sigma}(k)$ is the phase shift imparted to the electron by the mixing at the impurity site:

$$\eta^{\sigma}(k)\equiv\eta_2^{\sigma}(k)=\tan^{-1}\left[\frac{\Delta^{\sigma}}{E^{\sigma}_{\text{res}}-E_k}\right], \tag{4}$$

where E^{σ}_{res} is the center of the resonance.

Our starting point is the expression for the third-order energy correction for an electron gas due to perturbations as derived in Ref. 1,

$$E^{(3)}=\left[\frac{1}{8\pi^3}\right]^3\int_0^{k_F}dk_0\,k_0^2\int_0^{\infty}dk_1\,k_1^2\int_0^{\infty}dk_2\,k_2^2\left[\mathrm{P}\left[\frac{1}{E_{k_0}-E_{k_1}}\right]\mathrm{P}\left[\frac{1}{E_{k_0}-E_{k_2}}\right]-\frac{\pi^2}{3}\delta(E_{k_0}-E_{k_1})\delta(E_{k_0}-E_{k_2})\right]V(k_0,k_1,k_2)\ , \tag{5}$$

where

$$V(k_0,k_1,k_2)=\sum_{\sigma_0,\sigma_1,\sigma_2}\int d\Omega_{k_0}\int d\Omega_{k_1}\int d\Omega_{k_2}\,V_{\mathbf{k}_0\sigma_0,\mathbf{k}_1\sigma_1}V_{\mathbf{k}_1\sigma_1,\mathbf{k}_2\sigma_2}V_{\mathbf{k}_2\sigma_2,\mathbf{k}_0\sigma_0}\ ,$$

and the potential is given by

$$V_{AB\lambda}=\frac{-\Gamma}{N}[\mathbf{S}_A\cdot\mathbf{s}\,\delta(\mathbf{r}-\mathbf{R}_A)+\mathbf{S}_B\cdot\mathbf{s}\,\delta(\mathbf{r}-\mathbf{R}_B)]+\lambda(r)\boldsymbol{l}\cdot\mathbf{s}\ . \tag{6}$$

At sites A and B we have written the local moment-conduction electron spin interactions as if they were due to a term such as $\Gamma\mathbf{S}\cdot\mathbf{s}$ even though they should, in principle, be described by magnetic VBS's as we do at the ternary site. There is a seeming inconsistency in this but we are concerned primarily with the lowest-order correction of spin-orbit coupling to the energy. Thus, one takes it into account at only one site at which we must consider the effect of spin-orbit scattering from spin-split VBS's. At the other sites A and B we consider only spin scattering and for ease of calculation, model it as $\Gamma\mathbf{S}\cdot\mathbf{s}$. A proper description of the magnetic scattering at sites A and B requires consideration of the energy dependence of Γ. This has already been done for the two-site problem[6] but we cannot introduce this feature into three-site calculations at this time as it makes the phase-shift analysis very difficult.

Since the spin scattering at site T has been built into H_0, the energy denominators in Eq. (5) are, in principle, spin-dependent. However, as we are interested in dilute alloys with small concentrations of magnetic impurities, the spin dependence of the energy of the conduction electrons can be ignored.

When Eq. (6) is substituted into Eq. (5), one obtains 27 terms of which six are trilinear in the three particles. One particular term is

$$M^{(1)}_{A\lambda B}=\frac{\Gamma^2\lambda_d}{N^2}\sum_{\sigma_0,\sigma_1,\sigma_2}M^{(1)}_{\sigma_0\sigma_1\sigma_2}\ , \tag{7a}$$

where

$$M^{(1)}_{\sigma_0\sigma_1\sigma_2}=\langle\mathbf{k}_0\sigma_0\,|\,\mathbf{S}_A\cdot\mathbf{s}\,\delta(\mathbf{r}-\mathbf{R}_A)\,|\,\mathbf{k}_1\sigma_1\rangle\langle\mathbf{k}_1\sigma_1\,|\,\boldsymbol{l}\cdot\mathbf{s}\,|\,\mathbf{k}_2\sigma_2\rangle\langle\mathbf{k}_2\sigma_2\,|\,\mathbf{S}_B\cdot\mathbf{s}\,\delta(\mathbf{r}-\mathbf{R}_B)\,|\,\mathbf{k}_0\sigma_0\rangle$$

and the spin-orbit constant λ_d is defined by

$$\lambda_d=\int_0^\infty dr\,r^2\,|f_{3d}(r)|^2\ , \tag{7b}$$

where $f_{3d}(r)$ is the radial part of the $3d$ core wave function. The subscripts $A\lambda B$ refer to the order of individual scatterings. The remaining five matrix elements $M^{(l)}$, $2<l<6$, are obtained by permuting the operators in Eq. (7).

The individual factors of Eq. (7) have been given earlier without the σ indices.[1] Their product is quite long and will not be given. As we are interested only in the leading terms of the coupling, we can extract these from the general expression. After performing on these terms the angular integrations and summation over the initial spin variable σ_0, we obtain

$$\sum_{\sigma_0}\int d\Omega_{k_0}\int d\Omega_{k_1}\int d\Omega_{k_2}M^{(1)}_{\sigma_0\sigma_1\sigma_2}=\frac{-i}{4}\,\frac{\Gamma^2\lambda_d}{N^2}\,(4\pi)^3\,\frac{V^{\sigma_1}_{dk_F}V^{\sigma_2}_{k_Fd}}{\Delta^{\sigma_1}\Delta^{\sigma_2}}\,\frac{\sin(k_0R_{AB})}{k_0R_{AB}}\,\Gamma^{\sigma_1\sigma_2}_{k_1R_A,k_2R_B}A^{(1)}_{\sigma_1\sigma_2}\ , \tag{8}$$

where

$$\begin{aligned}\Gamma^{\sigma\sigma'}_{kR,k'R'}=&j_2(kR)j_2(k'R')\exp\{-i[\eta^\sigma(k)-\eta^{\sigma'}(k')]\}+j_2(kR)h_2^{(-)}(k'R')\exp[-i\eta^\sigma(k)]\sin[\eta^{\sigma'}(k')]\\&+h_2^{(+)}(kR)j_2(k'R')\sin[\eta^\sigma(k)]\exp[i\eta^{\sigma'}(k')]+h_2^{(+)}(kR)h_2^{(-)}(k'R')\sin[\eta^\sigma(k)]\sin[\eta^{\sigma'}(k')]\end{aligned} \tag{9}$$

and

$$\tilde{A}^{(1)}=-i\sqrt{10}\begin{bmatrix}[Y^2(\hat{\mathbf{R}}_A)\times Y^2(\hat{\mathbf{R}}_B)]^1_0(S_{A_+}S_{B_-}-\frac{1}{2}S_{A_0}S_{B_0}) & -[Y^2(\hat{\mathbf{R}}_A)\times Y^2(\hat{\mathbf{R}}_B)]^1_{-1}(S_{A_+}S_{B_0}-S_{A_0}S_{B_+})\\ -[Y^2(\hat{\mathbf{R}}_A)\times Y^2(\hat{\mathbf{R}}_B)]^1_1(S_{A_0}S_{B_-}-S_{A_-}S_{B_0}) & [Y^2(\hat{\mathbf{R}}_A)\times Y^2(\hat{\mathbf{R}}_B)]^1_0(-S_{A_-}S_{B_+}+\frac{1}{2}S_{A_0}S_{B_0})\end{bmatrix}\ . \tag{10}$$

We are using spherical tensor notation

$$S_0=S_z,\quad S_\pm=\mp\frac{1}{\sqrt{2}}(S_x\pm iS_y)\ , \tag{11}$$

and the vector product of the Y^2 tensor is defined as

$$[Y^2(\theta,\phi)\times Y^2(\theta',\phi')]^1=\sum_{m''}\hat{\boldsymbol{\varepsilon}}_{m''}\sum_{m,m'}(2m,2m'\,|\,1m'')Y_{2m}(\theta,\phi)Y_{2m'}(\theta',\phi')\ , \tag{12}$$

where $\hat{\epsilon}_{m''}$ is a generalized unit vector with the property $\hat{\epsilon}^*_n \cdot \hat{\epsilon}_{n'} = \delta_{nn'}$, and the symbol $(lm,l'm' \mid l''m'')$ is a Clebsch-Gordan coefficient.[7]

The matrix $\tilde{A}^{(1)}$ has the property that

$$\sum_{\sigma_1,\sigma_2} A^{(1)}_{\sigma_1\sigma_2} = \sqrt{10}[Y^2(\hat{\mathbf{R}}_A) \times Y^2(\hat{\mathbf{R}}_B)]^1 \cdot (\mathbf{S}_A \times \mathbf{S}_B) \tag{13}$$

which follows from[8]

$$\begin{aligned}\mathbf{S}_A \times \mathbf{S}_B &= -i\sqrt{2} \sum_{m''} \hat{\epsilon}_{m''} \sum_{m,m'} (1m,1m' \mid 1m'')(\mathbf{S}_A)_m (\mathbf{S}_B)_{m'} \\ &= -i[(S_{A_+} S_{B_0} - S_{A_0} S_{B_+})\hat{\epsilon}_1 \\ &\quad + (S_{A_+} S_{B_-} - S_{A_-} S_{B_+})\hat{\epsilon}_0 \\ &\quad + (S_{A_0} S_{B_-} - S_{A_-} S_{B_0})\hat{\epsilon}_{-1}] ,\end{aligned} \tag{14}$$

and

$$\begin{aligned}&[Y^2(\hat{\mathbf{R}}_A) \times Y^2(\hat{\mathbf{R}}_B)]^1 \cdot (\mathbf{S}_A \times \mathbf{S}_B) \\ &\quad = \sum_m (-)^m [Y^2(\hat{\mathbf{R}}_A) \times Y^2(\hat{\mathbf{R}}_B)]^1_m (\mathbf{S}_A \times \mathbf{S}_B)_{-m} .\end{aligned} \tag{15}$$

Since

$$i\sqrt{10}[Y^2(\hat{\mathbf{R}}_A) \times Y^2(\hat{\mathbf{R}}_B)]^1 = \frac{15}{4\pi} P_1(\hat{\mathbf{R}}_A \cdot \hat{\mathbf{R}}_B)\hat{\mathbf{R}}_A \times \hat{\mathbf{R}}_B \tag{16}$$

it follows that

$$\sum_{\sigma_1,\sigma_2} A^{(1)}_{\sigma_1\sigma_2} \sim (\hat{\mathbf{R}}_A \times \hat{\mathbf{R}}_B) \cdot (\mathbf{S}_A \times \mathbf{S}_B) . \tag{17}$$

Thus, when the space and spin variables are decoupled, i.e., if the ternary impurity is nonmagnetic so that the function Γ in Eq. (8) is independent of σ_1,σ_2 there is only one anisotropic coupling of the form of Eq. (17).

For dilute spin glasses the average distance between magnetic ions is large; furthermore, the dominant contributions to the interaction come from wave vectors around the Fermi level. Thus, kR is large and the function $\Gamma^{\sigma\sigma'}_{kR,k'R'}$ may be replaced by its asymptotic form

$$\Gamma^{\sigma\sigma'}_{kR,k'R'} \simeq \frac{\sin[kR + \eta^{\sigma}(k)]}{kR} \frac{\sin[k'R' + \eta^{\sigma'}(k')]}{k'R'} . \tag{18}$$

By substituting this expression into Eq. (8) and after multiplying by the factor $(k_0k_1k_2)^2$ of Eq. (5), we obtain for the contribution of the matrix element $M^{(1)}_{A\lambda B}$ to the quantity $(k_0k_1k_2)^2 V(k_0,k_1,k_2)$ of Eq. (5):

$$\begin{aligned}(k_0k_1k_2)^2 V^{(1)}(k_0,k_1,k_2) &= \sum_{\sigma_1,\sigma_2} \alpha_{\sigma_1\sigma_2}(k) \sin(k_0R_{AB}) \sin[\eta^{\sigma_1}(k_1)] \sin[k_1R_A + \eta^{\sigma_1}(k_1)] \\ &\quad \times \sin[\eta^{\sigma_2}(k_2)] \sin[k_2R_B + \eta^{\sigma_2}(k_2)] A^{(1)}_{\sigma_1\sigma_2} ,\end{aligned} \tag{19}$$

where

$$\alpha_{\sigma_1\sigma_2}(k) = \frac{-i}{4} \frac{\Gamma^2\lambda_d}{N^2} (4\pi)^3 \frac{V^{\sigma_1}_{dk_F} V^{\sigma_2}_{k_Fd}}{\Delta^{\sigma_1}\Delta^{\sigma_2}} \frac{k_0k_1k_2}{R_AR_BR_{AB}} .$$

By a permutation of the operators, we obtain the contribution of the matrix element

$$M^{(2)}_{B\lambda A} = \frac{\Gamma^2\lambda_d}{N^2} \sum_{\sigma_0,\sigma_1,\sigma_2} M^{(2)}_{\sigma_0\sigma_1\sigma_2} , \tag{20}$$

with

$$M^{(2)}_{\sigma_0\sigma_1\sigma_2} = \langle \mathbf{k}_0\sigma_0 \mid \mathbf{S}_B \cdot \mathbf{s}\, \delta(\mathbf{r} - \mathbf{R}_B) \mid \mathbf{k}_1\sigma_1 \rangle \langle \mathbf{k}_1\sigma_1 \mid l \cdot \mathbf{s} \mid \mathbf{k}_2\sigma_2 \rangle \langle \mathbf{k}_2\sigma_2 \mid \mathbf{S}_A \cdot \mathbf{s}\, \delta(\mathbf{r} - \mathbf{R}_A) \mid \mathbf{k}_0\sigma_0 \rangle$$

to the coupling in Eq. (5):

$$\begin{aligned}(k_0k_1k_2)^2 V^{(2)}(k_0,k_1,k_2) &= \sum_{\sigma_1,\sigma_2} \alpha_{\sigma_1\sigma_2}(k) \sin(k_0R_{AB}) \sin[\eta^{\sigma_1}(k)] \sin[k_1R_B + \eta^{\sigma_1}(k_1)] \\ &\quad \times \sin[\eta^{\sigma_2}(k_2)] \sin[k_2R_A + \eta^{\sigma_2}(k_2)] A^{(2)}_{\sigma_1\sigma_2} ,\end{aligned} \tag{21}$$

where

$$\tilde{A}^{(2)} = \begin{bmatrix} A^{(1)}_{--} & A^{(1)}_{+-} \\ A^{(1)}_{-+} & A^{(1)}_{++} \end{bmatrix} , \tag{22}$$

so that

$$\sum_{\sigma_1,\sigma_2} A^{(2)}_{\sigma_1\sigma_2} = \sum_{\sigma_1,\sigma_2} A^{(1)}_{\sigma_1\sigma_2} .$$

The remaining four contributions come from the matrix elements $M^{(3)}_{BA\lambda}$, $M^{(4)}_{AB\lambda}$, $M^{(5)}_{\lambda BA}$, and $M^{(6)}_{\lambda AB}$. When the principal-value integrals are performed, we obtain for the total of all six contributions

$$E^{(3)}_{AB\lambda}[\psi(\eta^\sigma)]=\frac{-i}{128\pi^4}\frac{\Gamma^2\lambda_d}{N^2}\left[\frac{2m}{\hbar^2}\right]^2\frac{1}{R_AR_BR_{AB}}\sum_{l=1}^{6}\sum_{\sigma,\sigma'}\frac{V^\sigma_{dk_F}V^{\sigma'}_{k_Fd}}{\Delta^\sigma\Delta^{\sigma'}}I^{(l)}_{\sigma\sigma'}A^{(l)}_{\sigma\sigma'}\ , \tag{23}$$

where we have set all pairs of dummy spin variables equal to (σ,σ'). The integrals $I^{(l)}_{\sigma\sigma'}$ are given by

$$I^{(1)}_{\sigma\sigma'}=\int_0^{k_F}dk\,k\sin(kR_{AB})\sin[\eta^\sigma(k)]\sin[\eta^{\sigma'}(k)]$$
$$\times\{\cos[kR_A+\eta^\sigma(k)]\cos[kR_B+\eta^{\sigma'}(k)]-\tfrac{1}{3}\sin[kR_A+\eta^\sigma(k)]\sin[kR_B+\eta^{\sigma'}(k)]\}\ , \tag{24a}$$

$$I^{(2)}_{\sigma\sigma'}=I^{(1)}_{\sigma'\sigma}\ , \tag{24b}$$

$$I^{(3)}_{\sigma\sigma'}=\int_0^{k_F}dk\,k\cos(kR_{AB})\sin[\eta^\sigma(k)]\sin[\eta^{\sigma'}(k)]$$
$$\times\{\cos[kR_A+\eta^\sigma(k)]\sin[kR_B+\eta^{\sigma'}(k)]-\tfrac{1}{3}\sin[kR_A+\eta^\sigma(k)]\sin[kR_B+\eta^{\sigma'}(k)]\}\ , \tag{24c}$$

$$I^{(4)}_{\sigma\sigma'}=\int_0^{k_F}dk\,k\cos(kR_{AB})\sin[\eta^\sigma(k)]\sin[\eta^{\sigma'}(k')]$$
$$\times\{\cos[kR_B+\eta^\sigma(k)]\sin[kR_A+\eta^{\sigma'}(k)]-\tfrac{1}{3}\sin[kR_A+\eta^\sigma(k)]\sin[kR_B+\eta^{\sigma'}(k)]\}\ , \tag{24d}$$

$$I^{(5)}_{\sigma\sigma'}=I^{(4)}_{\sigma'\sigma}\ , \tag{24e}$$

and

$$I^{(6)}_{\sigma\sigma'}=I^{(3)}_{\sigma'\sigma}\ , \tag{24f}$$

and for the matrices $\tilde{A}^{(l)}$, we have

$$\tilde{A}^{(1)}=\tilde{A}^{(3)}=\tilde{A}^{(5)}\ \text{ and }\ \tilde{A}^{(2)}=\tilde{A}^{(4)}=\tilde{A}^{(6)}\ . \tag{25}$$

In Eq. (24), we have set the initial wave vector k_0 equal to k. Now Eq. (23) may be written as

$$E^{(3)}_{AB\lambda}[\psi(\eta^\sigma)]\sim\sum_{n=1}^{2}\sum_{\sigma,\sigma'}\frac{V^\sigma_{dk_F}V^{\sigma'}_{k_Fd}}{\Delta^\sigma\Delta^{\sigma'}}J^{(n)}_{\sigma\sigma'}A^{(n)}_{\sigma\sigma'}\ , \tag{26}$$

where

$$J^{(1)}_{\sigma\sigma'}=\sum_{(l\ \text{odd})}I^{(l)}_{\sigma\sigma'}$$

and

$$J^{(2)}_{\sigma\sigma'}=\sum_{(l\ \text{even})}I^{(l)}_{\sigma\sigma'}=J^{(1)}_{\sigma'\sigma}\ .$$

By adding the integrands of the $I^{(l)}$, we find

$$J^{(1)}_{\sigma\sigma'}=\int_0^{k_F}dk\,k\sin[\eta^\sigma(k)]\sin[\eta^{\sigma'}(k)]\sin[k(R_A+R_B+R_{AB})+\eta^\sigma(k)+\eta^{\sigma'}(k)]\ . \tag{27}$$

This is symmetric in (σ,σ') so that

$$J^{(2)}_{\sigma\sigma'}=J^{(1)}_{\sigma\sigma'}\equiv J_{\sigma\sigma'}\ . \tag{28}$$

Then Eq. (26) becomes

$$E^{(3)}_{AB\lambda}[\psi(\eta^\sigma)]\sim\sum_{\sigma,\sigma'}\frac{V^\sigma_{dk_F}V^{\sigma'}_{k_Fd}}{\Delta^\sigma\Delta^{\sigma'}}J_{\sigma\sigma'}A_{\sigma\sigma'}\ , \tag{29}$$

where

$$\tilde{A}=\tilde{A}^{(1)}+\tilde{A}^{(2)}=\begin{bmatrix}A^{(1)}_{++}+A^{(1)}_{--} & 2A^{(1)}_{+-}\\ 2A^{(1)}_{-+} & A^{(1)}_{++}+A^{(1)}_{--}\end{bmatrix}\ . \tag{30}$$

and from Eqs. (10), (14), and (16), we find

$$\tilde{A}=-i\frac{15}{4\pi}P_1(\hat{\mathbf{R}}_A\cdot\hat{\mathbf{R}}_B)\times\begin{bmatrix}(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)_0(\mathbf{S}_A\times\mathbf{S}_B)_0 & -2(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)_-(\mathbf{S}_A\times\mathbf{S}_B)_+\\ -2(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)_+(\mathbf{S}_A\times\mathbf{S}_B)_- & (\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)_0(\mathbf{S}_A\times\mathbf{S}_B)_0\end{bmatrix}. \tag{31}$$

From Eqs. (23) and (31), and by defining

$$K_{\sigma\sigma'}=\frac{\hbar^2}{2m}\frac{V^{\sigma}_{dk_F}V^{\sigma'}_{k_Fd}}{\Delta^{\sigma}\Delta^{\sigma'}}J_{\sigma\sigma'}$$
$$=\frac{V^{\sigma}_{dk_F}V^{\sigma'}_{k_Fd}}{\Delta^{\sigma}\Delta^{\sigma'}}\int_0^{E_F}dE_k\sin[\eta_2^{\sigma}(k)]\sin[\eta_2^{\sigma'}(k)]\sin[k(R_A+R_B+R_{AB})+\eta_2^{\sigma}(k)+\eta_2^{\sigma'}(k)]\,, \tag{32}$$

we obtain

$$E^{(3)}_{AB\lambda}[\psi(\eta^{\sigma})]=-\frac{135}{512\pi}\frac{\lambda_d\Gamma^2}{E_F^3}\frac{P_1(\hat{\mathbf{R}}_A\cdot\hat{\mathbf{R}}_B)}{R_AR_BR_{AB}}(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot\overleftrightarrow{\mathbf{K}}\cdot(\mathbf{S}_A\times\mathbf{S}_B)\,, \tag{33}$$

where the dyadic $\overleftrightarrow{\mathbf{K}}$ is given by

$$\overleftrightarrow{\mathbf{K}}=K_{+-}\overleftrightarrow{\mathbf{I}}+[\tfrac{1}{2}(K_{++}+K_{--})-K_{+-}]\hat{\mathbf{S}}_T\hat{\mathbf{S}}_T\,. \tag{34}$$

We have used the relationship $E_F=h^2k_F^2/2m$, $k_F^3=3\pi^2\mathcal{N}_e$, where $\mathcal{N}_e$ is the density of states for one spin direction, and the fact that for noble metals there is one electron per atom so that $\mathcal{N}_e=N$. Since the quantization axis was that of $\hat{\mathbf{S}}_T$ itself, we have set $\hat{\boldsymbol{\epsilon}}_0=\hat{\mathbf{S}}_T$; also K_{+-} is equal to K_{-+}.

Equations (33) and (34) together with Eq. (32) represent the Dzyaloshinsky-Moriya coupling between two magnetic moments in the presence of the third *magnetic* impurity. The effect of the spin scattering at the ternary site is fully contained in the phase shifts $\eta_2^{\sigma}(k)$. We will discuss these equations in Sec. III. For the moment, we point out two obvious limits. When the ternary impurity is nonmagnetic, we have $\eta^+=\eta^-=\eta$. All the coefficients $K_{\sigma\sigma'}$ collapse into a single function. The second term of Eq. (34) vanishes and the interaction goes as $(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot(\mathbf{S}_A\times\mathbf{S}_B)$ as is well known.[1] At the opposite extreme, if the spin scattering is sufficiently strong so that the spin-split VBS's are well separated, $\eta^+(k)$ goes to π as E_k increases from zero to E_F before $\eta^-(k)$ differs significantly from zero. The product $\sin[\eta^+(k)]\sin[\eta^-(k)]$ of the integrand of K_{+-} vanishes throughout the range of integration. Then K_{+-} vanishes so that the interaction is dominated by the term in $(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot\hat{\mathbf{S}}_T(\mathbf{S}_A\times\mathbf{S}_B)\cdot\hat{\mathbf{S}}_T$.

III. RANGE DEPENDENCE OF THE COUPLING

To complete the calculation, it is necessary to evaluate the integrals $K_{\sigma\sigma'}$, Eq. (32). With the use of

$$\begin{aligned}&\Delta^{\sigma}=\frac{\hbar^2}{2m}(k_{\Delta}^{\sigma})^2,\quad E^{\sigma}_{\rm res}=\frac{\hbar^2}{2m}(k_r^{\sigma})^2\,,\\ &\alpha^{\sigma}=[(k_r^{\sigma})^4+(k_{\Delta}^{\sigma})^4]^{1/4}/k_F\,,\\ &\tan\phi^{\sigma}=-\tan[\eta_2^{\sigma}(0)]=-\left[\frac{k_{\Delta}^{\sigma}}{k_r^{\sigma}}\right],\\ &\beta^{\sigma}=\alpha^{\sigma}e^{i\phi^{\sigma}/2}\,,\end{aligned} \tag{35}$$

and

$$G_{\sigma}(R)=\int_0^{k_F}dk\frac{e^{ikR}}{k^2-(k_r^{\sigma})^2+i(k_{\Delta}^{\sigma})^2}\,, \tag{36}$$

we show in Appendix B that[9]

$$K_{\sigma\sigma}=\frac{|V^{\sigma}_{dk_F}|^2}{\Delta^{\sigma}}\{\sin[\eta_2^{\sigma}(k_F)]\sin[3k_FR_{\rm av}+\eta_2^{\sigma}(k_F)]-\sin^2[\eta_2^{\sigma}(0)]+3R_{\rm av}(k_{\Delta}^{\sigma})^2{\rm Re}G_{\sigma}(3R_{\rm av})\} \tag{37}$$

and

$$K_{\sigma-\sigma}=V^{\sigma}_{dk_F}V^{-\sigma}_{k_Fd}\{\tfrac{1}{2}[(E^{-}_{\rm res}-E^{+}_{\rm res})^2+(\Delta^{-}-\Delta^{+})^2]\}^{-1}{\rm Re}\left\{[(E^{-}_{\rm res}-E^{+}_{\rm res})+i(\Delta^{-}-\Delta^{+})]\left[\Delta\left[\frac{dG_{\sigma}(R)}{dR}\right]\right]_{R=3R_{\rm av}}\right\}, \tag{38}$$

where

$$3R_{\rm av} \equiv R_A + R_B + R_{AB}$$

and

$$\Delta\left[\frac{dG_\sigma}{dR}\right] \equiv \frac{dG_+}{dR} - \frac{dG_-}{dR} .$$

The integral $G_\sigma(3R_{\rm av})$ is given by[10]

$$G_\sigma(3R_{\rm av}) = (2k_F\beta^\sigma)^{-1}\{\exp(-i\,3k_F R_{\rm av}\beta^\sigma)[E_1(-i\,3k_F R_{\rm av}(1+\beta^\sigma)) - E_1(-i\,3k_F R_{\rm av}\beta^\sigma)] - \exp(i\,3k_F R_{\rm av}\beta^\sigma)[E_1(-i\,3k_F R_{\rm av}(1-\beta^\sigma)) - E_1(i\,3k_F R_{\rm av}\beta^\sigma)]\} , \quad (39)$$

where $E_1(z)$ is the exponential integral defined by

$$E_1(z) = \int_z^\infty dt \frac{e^{-t}}{t}, \quad |\arg z| < \pi . \quad (40)$$

The derivative of $G_\sigma(3R_{\rm av})$ is given by

$$\left.\frac{dG_\sigma(R)}{dR}\right|_{R=3R_{\rm av}} = \frac{-i}{2}\{\exp(-i\,3k_F R_{\rm av}\beta^\sigma)[E_1(-i\,3k_F R_{\rm av}(1+\beta^\sigma)) - E_1(-i\,3k_F R_{\rm av}\beta^\sigma)] + \exp(i\,3k_F R_{\rm av}\beta^\sigma)[E_1(-i\,3k_F R_{\rm av}(1-\beta^\sigma)) - E_1(i\,3k_F R_{\rm av}\beta^\sigma)]\} . \quad (41)$$

First, we derive analytic expressions for the range dependence in the two regimes of large and small average interparticle spacings, "large" and "small" being defined relative to *spin-dependent critical distances* R_c^σ which, as we show, are themselves dependent upon the positions of the VBS resonances with respect to the position of the Fermi level. We then discuss the Dzyloshinsky-Moriya interaction itself. Our key point is that the interaction displays a variable range dependence. If both resonances are far from the Fermi level, the interaction can be represented by its asymptotic form even for nearest-neighbor triads. At the other extreme, if the resonances are close to k_F, the interaction will display its preasymptotic form even at large average interparticle spacings.

The behavior of the functions $G_\sigma(3R_{\rm av})$ and $[dG_\sigma(R)/dR]_{R=3R_{\rm av}}$ is determined for large $R_{\rm av}$ primarily by the term in $E_1(-i\,3k_F R_{\rm av}(1-\beta^\sigma))$ for which the argument is smallest for a given value of $R_{\rm av}$ of the four functions E_1 in Eqs. (39) and (40). Consider, therefore, the term

$$\exp(i\,3k_F R_{\rm av}\beta^\sigma)E_1(-i\,3k_F R_{\rm av}(1-\beta^\sigma)) \equiv e^{3ik_F R_{\rm av}} e^{z^\sigma} E_1(z^\sigma) , \quad (42)$$

where

$$z^\sigma = -i\,3k_F R_{\rm av}(1-\beta^\sigma) .$$

Then with $z^\sigma = x^\sigma + iy^\sigma$, we obtain

$$x^\sigma = 3k_F R_{\rm av}\alpha^\sigma \sin(\phi^\sigma/2)$$

and (43a)

$$y^\sigma = -3k_F R_{\rm av}[1-\alpha^\sigma\cos(\phi^\sigma/2)] .$$

Since the phase angle ϕ^σ is always small, and since $k_F\alpha^\sigma \approx k_r^\sigma$, we may write

$$x^\sigma \approx 3k_r^\sigma R_{\rm av}\phi^\sigma/2$$

and (43b)

$$y^\sigma \approx -3(k_F - k_r^\sigma)R_{\rm av} .$$

One may define two critical distances,

$$R_c^\sigma \equiv (3\,|\,k_F - k_r^\sigma\,|\,)^{-1} , \quad (44)$$

such that if the average interparticle spacing $R_{\rm av}$ is much greater than the larger of $R_c^\pm$, it follows that both of $|\,z^\pm\,|$ are sufficiently large that Eq. (42) as well as the remaining terms E_1 in Eqs. (39) and (41) may be replaced by their asymptotic forms. Then from the expansion

$$E_1(z) = \frac{e^{-z}}{z}\left[1 - \frac{1}{z} + \cdots\right] , \quad (45)$$

we obtain[9]

$$\mathrm{Re}G_0(3R_{\rm av}) \simeq [3(k_\Delta^\sigma)^2 R_{\rm av}]^{-1}\left[-\sin[\eta_2^\sigma(k_F)]\sin[3k_F R_{\rm av} + \eta_2^\sigma(k_F)] + \sin^2[\eta_2^\sigma(0)] - \frac{2k_F}{3(k_\Delta^\sigma)^2 R_{\rm av}}\sin^2[\eta_2^\sigma(k_F)]\cos[3k_F R_{\rm av} + 2\eta_2^\sigma(k_F)] + O(1/R_{\rm av}^2)\right] \quad (46)$$

and

$$\left.\frac{dG_\sigma(R)}{dR}\right|_{R=3R_{\rm av}} \simeq \frac{-k_F}{3(k_\Delta^\sigma)^2 R_{\rm av}} \sin[\eta_2^\sigma(k_F)] e^{i[3k_F R_{\rm av}+\eta_2^\sigma(k_F)]} + O(1/R_{\rm av}^2) \ . \tag{47}$$

We immediately note from Eqs. (37) and (46) that in this regime the first two terms of $K_{\sigma\sigma}$ are canceled by the first two terms of $\mathrm{Re}G_\sigma(3R_{\rm av})$. Then $K_{\sigma\sigma}$ and $K_{\sigma\,-\sigma}$ fall off as $R_{\rm av}^{-1}$ and the range dependence of the DM interaction, Eqs. (33) and (34), will have the general form $[R_A R_B R_{AB}(R_A+R_B+R_{AB})]^{-1}$. Specifically, for large $R_{\rm av}$ we have

$$K_{\sigma\sigma} = \frac{-32\pi^2 E_F}{k_F^2 (k_\Delta^\sigma)^2} \sin^2[\eta_2^\sigma(k_F)] \frac{\cos[3k_F R_{\rm av}+2\eta_2^\sigma(k_F)]}{3R_{\rm av}} \tag{48a}$$

and

$$\begin{aligned} K_{\sigma\,-\sigma} = {} & \frac{32\pi^2 E_F}{3k_F^2 R_{\rm av}} \frac{(\Delta^+\Delta^-)^{1/2}}{(E_{\rm res}^+ - E_{\rm res}^-)^2 + (\Delta^+ - \Delta^-)^2} \\ & \times \left[\frac{1}{(k_\Delta^+)^2} \sin[\eta_2^+(k_F)] \{ (E_{\rm res}^+ - E_{\rm res}^-) \cos[3k_F R_{\rm av} + \eta_2^+(k_F)] - (\Delta^+ - \Delta^-) \sin[3k_F R_{\rm av} + \eta_2^+(k_F)] \} \right. \\ & \left. - \frac{1}{(k_\Delta^-)^2} \sin[\eta_2^-(k_F)] \{ (E_{\rm res}^+ - E_{\rm res}^-) \cos[3k_F R_{\rm av} + \eta_2^-(k_F)] - (\Delta^+ - \Delta^-) \sin[3k_F R_{\rm av} + \eta_2^-(k_F)] \} \right] . \end{aligned} \tag{48b}$$

To obtain these, we have used the relation

$$\frac{|V_{dk_F}^\sigma|^2}{\Delta^\sigma} = \frac{4}{\mathcal{N}(E_F)} = \frac{16\pi^2 E_F}{k_F^3} \ .$$

Note that both K_{++} and K_{--} behave independently, each being a function of the position of its own resonance with respect to that of the Fermi level. The coefficient K_{+-} depends upon the relative positions of both resonances. One may state that if both resonances are far from k_F, then they are far from each other so that K_{+-} is much smaller than either K_{++} or K_{--}.

If $R_{\rm av}$ is much smaller than the lesser of $R_c^\pm$, then $|y^\sigma|$ and therefore $|z^\sigma|$ will be small. One may then obtain the coefficients $K_{\sigma\sigma'}$ with the aid of a small argument expansion of $E_1(z)$, or by direct integration. One sees that $K_{\sigma\sigma}$ is given by[8]

$$K_{\sigma\sigma} \simeq \frac{16\pi^2 E_F}{k_F^3} \sin[\eta_2^\sigma(k_F)] \sin[3k_F R_{\rm av} + \eta_2^\sigma(k_F)] \ , \tag{49a}$$

since the term proportional to G_σ in Eq. (37) is negligible, going as $(3k_F R_{\rm av})(k_\Delta^\sigma)^2/(k_F k_r^\sigma)$.

The coefficient $K_{\sigma,\,-\sigma}$ in this case does not have a simple form, but if one makes the additional assumption that the two resonances are near k_F, then an integration of Eq. (38) yields

$$\begin{aligned} K_{\sigma\,-\sigma} \simeq {} & \frac{-(16\pi^2/k_F^3) E_F (\Delta^+\Delta^-)^{1/2}}{[(E_{\rm res}^+ - E_{\rm res}^-)^2 + (\Delta^+ - \Delta^-)^2]} \\ & \times \left\{ (E_{\rm res}^+ - E_{\rm res}^-) \left[\ln \left| \frac{\sin[\eta_2^+(k_F)]}{\sin[\eta_2^-(k_F)]} \right| \sin(3k_F R_{\rm av}) + [\eta_2^+(k_F) - \eta_2^-(k_F)] \cos(3k_F R_{\rm av}) \right] \right. \\ & \left. + (\Delta^+ - \Delta^-) \left[-[\eta_2^+(k_F) - \eta_2^-(k_F)] \sin(3k_F R_{\rm av}) + \ln \left| \frac{\sin[\eta_2^+(k_F)]}{\sin[\eta_2^-(k_F)]} \right| \cos(3k_F R_{\rm av}) \right] \right\} . \end{aligned} \tag{49b}$$

Note that Eq. (49a) is valid for any position of the resonance k_r^σ. Equations (49) demonstrates the fact that in the small $R_{\rm av}$ regime, the DM interaction exhibits the range dependence $(R_A R_B R_{AB})^{-1}$ [see Eq. (33)].

The Dzyaloshinsky-Moriya interaction, Eqs. (33) and (34), may be written in a simple form for two special cases. If $R_{\rm av}$ is much greater than the larger of $R_c^\pm$ and if the two resonances are sufficiently far apart; i.e., if $K_{+-} \ll$ both K_{++} and K_{--}, we obtain from Eq. (48a),

$$\begin{aligned} E_{AB\lambda}^{(3)}[\psi(\eta^\sigma)] = {} & + \frac{135\pi}{32} \frac{\lambda_d \Gamma^2}{E_F^2 k_F^2} \frac{P_1(\hat{\mathbf{R}}_A \cdot \hat{\mathbf{R}}_B)}{R_A R_B R_{AB}(R_A+R_B+R_{AB})} \\ & \times \sum_\sigma \frac{1}{(k_\Delta^\sigma)^2} \sin^2[\eta_2^\sigma(k_F)] \cos[k_F(R_A+R_B+R_{AB}) + 2\eta_2^\sigma(k_F)] (\hat{\mathbf{R}}_A \times \hat{\mathbf{R}}_B) \cdot \hat{\mathbf{S}}_T \, (\mathbf{S}_A \times \mathbf{S}_B) \cdot \hat{\mathbf{S}}_T \ . \end{aligned} \tag{50}$$

The interaction is dominated by the anisotropic coupling term arising from both the magnitude and direction of the magnetic moment of the third impurity. To obtain Eq. (50) we have assumed that the density of states for both spin states σ is the same.

The different structures of Eqs. (49a) and (49b) preclude a general form for the interaction when $R_{\rm av}$ is much less than both R_c^+ and R_c^-. However, if the two resonances approach each other, coalescing at a value k_r not necessarily equal to k_F, the magnetic moment $\mathbf{S}_T$ vanishes so that all three coefficients $K_{\sigma\sigma'}$ become equal to that given by Eq. (37) but with the σ index deleted. Then, the "nonmagnetic" DM interaction is given by[9]

$$E^{(3)}_{AB\lambda}[\psi(\eta)]=-\frac{135\pi}{32}\frac{\lambda_d\Gamma^2}{E_F^2k_F^3}\frac{P_1(\hat{\mathbf{R}}_A\cdot\hat{\mathbf{R}}_B)}{R_AR_BR_{AB}}\{\sin[\eta_2(k_F)]\sin[k_F(R_A+R_B+R_{AB})+\eta_2(k_F)]$$
$$+(R_A+R_B+R_{AB})k_\Delta^2\mathrm{Re}G(R_A+R_B+R_{AB})\}(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot(\mathbf{S}_A\times\mathbf{S}_B)\ , \quad (51a)$$

which is seen to equal the result given earlier[1] *only* if the term in $G(R)$ can be neglected; this is the case when k_r is near k_F. However, if the (single) resonance is far from the Fermi level, one finds a substantial contribution to the interaction arising from electrons scattering out of (into) the occupied (empty) states of the *tail* of the VBS. In these cases, the term in $G(R)$ dominates so that for $R_{\rm av}$ much greater than R_c, Eq. (44), the ternary DM interaction is given by

$$E^{(3)}_{AB\lambda}[\psi(\eta)]=+\frac{135\pi}{16}\frac{\lambda_d\Gamma^2}{E_F^2k_F^2k_\Delta^2}\frac{P_1(\hat{\mathbf{R}}_A\cdot\hat{\mathbf{R}}_B)}{R_AR_BR_{AB}(R_A+R_B+R_{AB})}$$
$$\times\sin^2[\eta_2(k_F)]\cos[k_F(R_A+R_B+R_{AB})+2\eta_2(k_F)](\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot(\mathbf{S}_A\times\mathbf{S}_B)\ . \quad (51b)$$

We wish to emphasize several points. Although we have given expressions, both for the coefficients $K_{\sigma\sigma'}$ and for the DM interaction itself, for average interparticle spacings $R_{\rm av}$ much less than or much greater than the two critical distances $R_c^\pm$, Eq. (44), it must be pointed out that in practical cases K_{++} and K_{--} are independent so that one of these may meet the conditions specified while the other may not. Most importantly, the critical distances $R_c^\pm$ are themselves variable, being dependent on the magnitude of the displacement of the resonances from the Fermi surface as well as on the widths of the resonances themselves.[11] Thus, in real systems, both $R_c^\pm$ may be sufficiently small that the interaction is given by its asymptotic form $1/R^4$ even at the minimum value of $R_{\rm av}$ which is $R_0(2+\sqrt{2})/3$ for the nearest-neighbor triad on an fcc lattice, R_0 being the nearest-neighbor distance and equal to 2.55 Å for *Cu*Mn and 2.88 Å for *Au*Fe. Alternatively, both $R_c^\pm$ may be sufficiently large that the interaction is given by its preasymptotic form $1/R^3$ for any $R_{\rm av}$. Clearly, one coefficient may behave as $1/R^4$ while the other may fall off as $1/R^3$. This feature has great consequences for calculations of macroscopic anisotropy energies. We now discuss our results for *Cu*Mn and *Au*Fe.

IV. DZYALOSHINSKY-MORIYA INTERACTION IN *Cu*Mn AND *Au*Fe

As a practical example, we consider the binary spin glass *Cu*Mn. The simplest way to evaluate the coefficients $K_{\sigma\sigma'}$, Eqs. (37) and (38), is to numerically integrate Eq. (B5) for the diagonal terms:

$$K_{\sigma\sigma}=\frac{16\pi^2E_F}{k_F^3}(\sin[\eta_2^\sigma(k_F)]\sin[3k_FR_{\rm av}+\eta_2^\sigma(k_F)]$$
$$+\tfrac{1}{2}\{\cos[\eta_2^\sigma(0)]-\cos(3k_FR_{\rm av})$$
$$-3R_{\rm av}I^\sigma\})\ , \quad (52)$$

where

$$I^\sigma=\int_0^{k_F}\sin[3kR_{\rm av}+2\eta_2^\sigma(k)]dk\ ,$$

and to evaluate $K_{\sigma-\sigma}$ in the form

$$K_{\sigma-\sigma}=\frac{16\pi^2E_F(\Delta^+\Delta^-)^{1/2}}{(E^+_{\rm res}-E^-_{\rm res})^2+(\Delta^+-\Delta^-)^2}$$
$$\times[(E^-_{\rm res}-E^+_{\rm res})(A^+-A^-)$$
$$-(\Delta^--\Delta^+)(B^+-B^-)]\ , \quad (53)$$

where

$$A^\sigma=\frac{1}{(k_\Delta^\sigma)^2}\left[-\int_0^{k_F}k\cos[3kR_{\rm av}+2\eta_2^\sigma(k)]dk\right.$$
$$\left.+\frac{k_F\sin(3k_FR_{\rm av})}{3R_{\rm av}}+\frac{\cos(3kR_{\rm av})-1}{(3R_{\rm av})^2}\right]$$

and

$$B^\sigma=\frac{1}{(k_\Delta^\sigma)^2}\left[-\int_0^{k_F}k\sin[3kR_{\rm av}+2\eta_2^\sigma(k)]dk\right.$$
$$\left.-\frac{k_F\cos(3k_FR_{\rm av})}{3R_{\rm av}}+\frac{\sin(3k_FR_{\rm av})}{(3R_{\rm av})^2}\right].$$

The parameters Δ^σ and $E^\sigma_{\rm res}$ which appear explicitly in these equations as well as implicitly in the expression for $\eta_2^\sigma(k)$, Eq. (4), are not known precisely. One relationship between them is [Eq. (4)]

$$E^\sigma_{\rm res}=E_F+\frac{\Delta^\sigma}{\tan[\eta_2^\sigma(k_F)]}\ , \quad (54)$$

where $\eta_2^\sigma(k_F)$ is determined by the Friedel sum rule $\eta_2^\sigma(k_F)=(\pi/5)Z_d^\sigma$ where Z_d^σ is the number of electrons in spin state σ, given by $Z_d^++Z_d^-=Z_d$ and $Z_d^+-Z_d^-=\mu/\mu_B$, the magnetic moment in units of a Bohr

magneton.

Both $E_{\rm res}^{\sigma}$ and Δ^{σ} are taken as constants but in fact they are functions of energy. As can be seen from cluster calculations,[4] the approximation of the true shape of the resonance by a Lorentzian introduces an error since the tails of the Lorentzian are much longer than those of the true resonance. Since the interactions we describe arise from electrons scattering in and out of the resonances at the Fermi surface, it is easy to see that the further the resonance is from the Fermi surface, the more important is the density of d states in the tail. However, Jena and Geldart[12] have shown that one can still treat $E_{\rm res}^{\sigma}$ and Δ^{σ} as constants provided the Friedel sum rules are obeyed. Thus, our use of Eq. (54) is justified.

The number of d electrons at the manganese site is debatable. Consequently, we have modeled *Cu*Mn in two different ways. In the first (symmetric) model, we have the following:

*Cu*Mn I:

$$\begin{aligned} &Z_d^+ + Z_d^- = 5 , \\ &Z_d^+ - Z_d^- = 4.06 , \\ &\eta_2^+(k_F) = 2.8463 \text{ rad} , \\ &\eta_2^-(k_F) = 0.2953 \text{ rad} . \end{aligned} \tag{55a}$$

Then reasonable choices consistent with these and the value $E_F = 7$ eV are

$$\begin{aligned} &\Delta^+ = 0.20 \text{ eV}, \quad E_{\rm res}^+ = 6.3425 \text{ eV} , \\ &\Delta^- = 0.40 \text{ eV}, \quad E_{\rm res}^- = 8.3150 \text{ eV} . \end{aligned} \tag{55b}$$

In a second model, we have chosen the following set of values:

*Cu*Mn II:

$$\begin{aligned} &Z_d^+ + Z_d^- = 6 , \\ &Z_d^+ - Z_d^- = 3.6 , \\ &\eta_2^+(k_F) = 3.0159, \quad \eta_2^-(k_F) = 0.7540 , \\ &\Delta^+ = 0.25 \text{ eV}, \quad E_{\rm res}^+ = 5.0215 \text{ eV} , \\ &\Delta^- = 0.70 \text{ eV}, \quad E_{\rm res}^- = 7.7454 \text{ eV} . \end{aligned} \tag{56}$$

The moment $3.6\mu_B$ is a representative value.

Figure (1a) illustrates the behavior of a typical component, K_{++} for model I. It is easily seen that in the nonphysical regime of $R_{\rm av} < R_0$ that K_{++} is given very accurately by its preasymptotic form, Eq. (49a). In the spin-glass regime, one sees that the preasymptotic form is seriously in error and that the asymptotic form, Eq. (48a), is a better estimate. In Fig. (1b), we show the *envelopes* of the amplitudes of K_{++} and its pre- and asymptotic forms in the range from $R_{\rm av} \approx 0$ to $R_{\rm av} \approx 4R_0$. From Eq. (43a) we have

$$\begin{aligned} |z^{\sigma}| &= [(x^{\sigma})^2 + (y^{\sigma})^2]^{1/2} \\ &= 3k_F R_{\rm av}[1 + (\alpha^{\sigma})^2 - 2\alpha^{\sigma}\cos(\phi^{\sigma}/2)]^{1/2} \end{aligned} \tag{57}$$

and by defining the critical values R_c^{σ} as before as the values for which $|z^{\sigma}| = 1$, we obtain the following for the two models:[10]

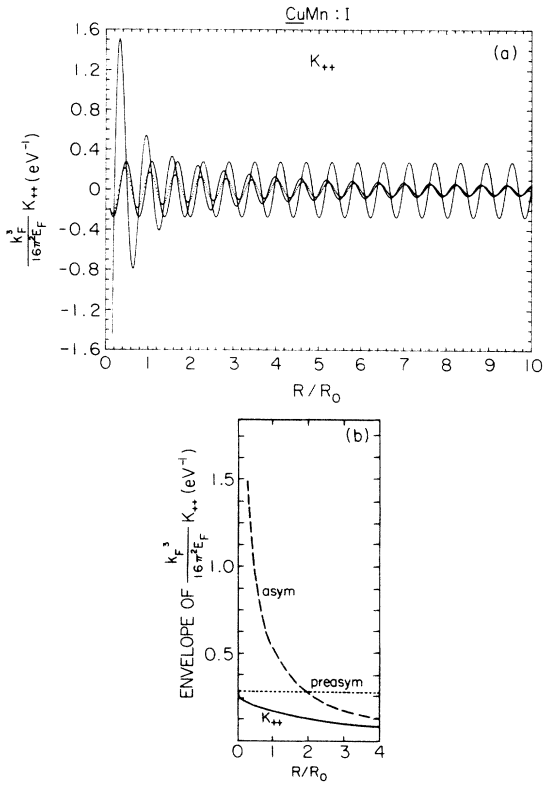

FIG. 1. (a) Coefficient K_{++} and its preasymptotic and asymptotic forms for model I of *Cu*Mn, as functions of the average interparticle spacing, in units of a nearest-neighbor distance $R_0 = a/\sqrt{2}$. The true K_{++} is given by the dotted curve. Its preasymptotic form displays constant amplitude, while its asymptotic form diverges for small R/R_0. (b) Envelopes of the curves in (a).

*Cu*Mn I:

$$\begin{aligned} &R_c^+ = 4.64 \text{ Å} = 1.82R_0 , \\ &R_c^- = 2.69 \text{ Å} = 1.06R_0 , \end{aligned} \tag{58}$$

*Cu*Mn II:

$$\begin{aligned} &R_c^+ = 1.57 \text{ Å} = 0.61R_0 , \\ &R_c^- = 3.56 \text{ Å} = 1.40R_0 , \end{aligned}$$

where the nearest-neighbor distance $R_0 = 2.55$ Å and the average interparticle distance for a nearest-neighbor triad is $R_{\rm min} = 1.14R_0$. Thus, in both models we would expect the integrals K_{++} and K_{--} to begin to show asymptotic behavior [Eq. (48a)] in the range from R_0 to $10R_0$, with K_{--} reaching its asymptotic form earlier than K_{++} in model I, and *vice versa* in model II. These observations are borne out by our results for these coefficients which are displayed in Figs. 2 and 3 in the form of graphs of the envelopes of the oscillations. These graphs also show the effect of the placement of the resonance with respect to the Fermi surface. In model I, $E_{\rm res}^+$ is closer to E_F than is

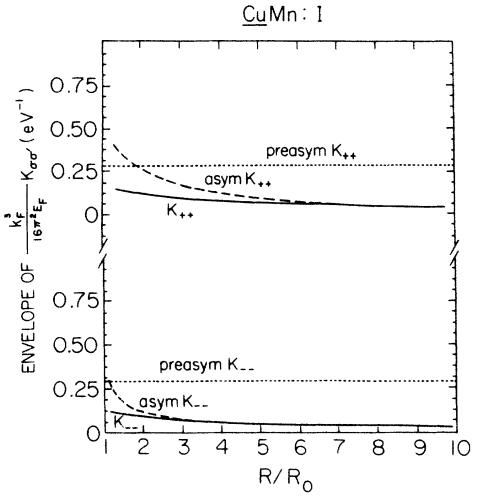

FIG. 2. Envelopes of the coefficients K_{++} and K_{--} and of their preasymptotic and asymptotic forms for model I of *Cu*Mn, as functions of the average interparticle spacing.

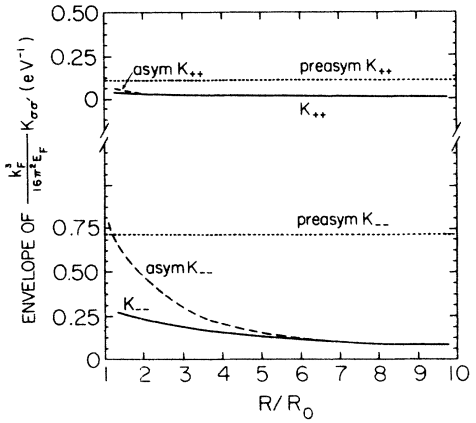

FIG. 3. Envelopes of the coefficients K_{++} and K_{--} and of their preasymptotic and asymptotic forms for model II of *Cu*Mn.

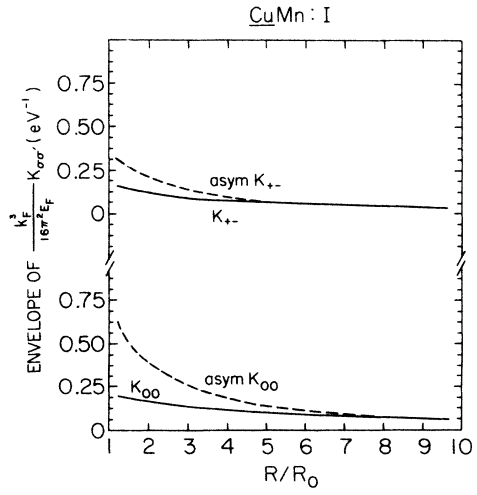

FIG. 4. Envelopes of the interaction coefficients K_{+-} and $K_{00}=\frac{1}{2}(K_{++}+K_{--})-K_{+-}$ and of their asymptotic forms for model I of *Cu*Mn, as functions of the average interparticle spacing. The results for model II are nearly identical.

$E_{\rm res}^-$. Thus preasymptotic corrections are more important to K_{++} than to K_{--}, and the deviation of K_{++} from its asymptotic form exceeds that of K_{--}. The situation is reversed in model II. However, in both models, the sum of K_{++} and K_{--} is roughly constant so that the interaction coefficients K_{+-} and $K_{00}\equiv\frac{1}{2}(K_{++}+K_{--})-K_{+-}$ of Eq. (34) are very similar. Consequently, we display in Fig. 4 K_{+-} and K_{00} for *Cu*Mn I only. The strengths of the two types of Dzyaloshinsky-Moriya terms $(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot(\mathbf{S}_A\times\mathbf{S}_B)$ and $(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot\hat{\mathbf{S}}_T(\mathbf{S}_A\times\mathbf{S}_B)\cdot\hat{\mathbf{S}}_T$ are nearly equal.

A much stronger variation in the interaction coefficients K_{+-} and K_{00} may be seen from our choice of models for *Au*Fe. In our first model, we have used the following values:

*Au*Fe I:

$$\begin{aligned}
&Z_d^+ + Z_d^- = 6\ ,\\
&Z_d^+ - Z_d^- = 2.2\ ,\\
&\eta_2^+(k_F)=2.5761,\quad \eta_2^-(k_F)=1.1938\ ,\\
&\Delta^+ = 0.20\ \text{eV},\quad E_{\rm res}^+ = 5.2148\ \text{eV}\ ,\\
&\Delta^- = 0.40\ \text{eV},\quad E_{\rm res}^- = 5.6884\ \text{eV}\ ,
\end{aligned}\tag{59}$$

and in our second model, we used the following values:

*Au*Fe II:

$$\begin{aligned}
&Z_d^+ + Z_d^- = 7\ ,\\
&Z_d^+ - Z_d^- = 2.83\ ,\\
&\eta_2^+(k_F)=3.0882,\quad \eta_2^-(k_F)=1.3100\ ,\\
&\Delta^+ = 0.10\ \text{eV},\quad E_{\rm res}^+ = 3.6267\ \text{eV}\ ,\\
&\Delta^- = 0.35\ \text{eV},\quad E_{\rm res}^- = 5.6237\ \text{eV}\ ,
\end{aligned}\tag{60}$$

where $E_F=5.53$ eV.

In Figs. 5 and 6 we illustrate our results. Once again we have plotted the envelopes of the amplitudes of K_{+-}

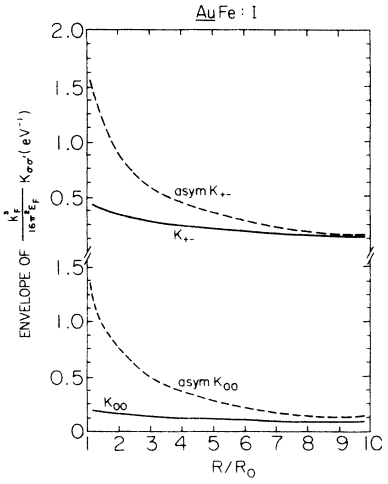

FIG. 5. Envelopes of the interaction coefficients K_{+-} and K_{00} and of their asymptotic forms for model I of *Au*Fe.

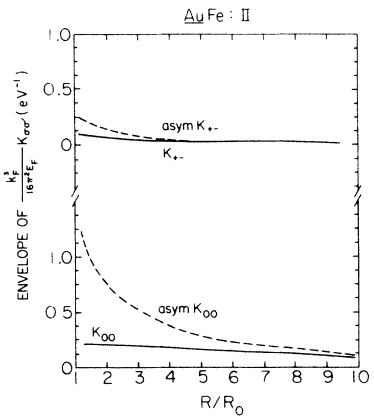

FIG. 6. Envelopes of the interaction coefficients K_{+-} and K_{00} and of their asymptotic forms for model II of *Au*Fe.

and K_{00}, together with their asymptotic forms.

In model I, K_{+-} is about twice K_{00} so that the strength of the DM term in $(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot(\mathbf{S}_A\times\mathbf{S}_B)$ is about twice that of the term in $(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot\hat{\mathbf{S}}_T(\mathbf{S}_A\times\mathbf{S}_B)\cdot\hat{\mathbf{S}}_T$. In model II, K_{00} is unchanged *vis-à-vis* model I but K_{+-} has been reduced considerably. The anisotropy is dominated by the second type of DM interaction.

These results may be understood in terms of the density of d states $\rho_d^\sigma=(1/\pi\Delta^\sigma)\sin^2\eta_2^\sigma$ at the Fermi level. For both *Cu*Mn I ($\rho_d^+=0.1348$ eV^{-1}, $\rho_d^-=0.0674$ eV^{-1}) and *Cu*Mn II ($\rho_d^+=0.0200$ eV^{-1}, $\rho_d^-=0.2131$ eV^{-1}), one value of ρ_d^σ is noticeably larger than the other but neither turns out to dominate in either model. For *Au*Fe I ($\rho_d^+=0.4570$ eV^{-1}, $\rho_d^-=0.6879$ eV^{-1}) the same may be said. Thus, for these models, we see that both types of DM interaction are important. However, for *Au*Fe II ($\rho_d^+=0.0091$ eV^{-1}, $\rho_d^-=0.8490$ eV^{-1}) the density of states at E_F of the upper resonance is 2 orders of magnitude larger than that of the majority spin state. This leads to a strong suppression of the term in $(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot(\mathbf{S}_A\times\mathbf{S}_B)$ relative to the spin-polarized contribution $(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot\hat{\mathbf{S}}_T(\mathbf{S}_A\times\mathbf{S}_B)\cdot\hat{\mathbf{S}}_T$. It is clear then that there is sufficient variation of the material parameters of *Cu*Mn and *Au*Fe in the literature to preclude a presentation of exact number results.

V. CONCLUSIONS

We have found that in transition-metal binary spin-glass systems there is a second type of Dzyaloshinsky-Moriya coupling which depends upon both the magnitude and direction of the magnetic moment on the third impurity site. The relative values of the density of d states at the Fermi surface of the VBS resonances determine the strength of the coefficient K_{+-} of the "unpolarized" DM term $(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot(\mathbf{S}_A\times\mathbf{S}_B)$ *vis-à-vis* that of the new "polarized" term $(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot\hat{\mathbf{S}}_T(\mathbf{S}_A\times\mathbf{S}_B)\cdot\hat{\mathbf{S}}_T$. For example, if $\rho_d^+\ll\rho_d^-$, the unpolarized term is suppressed. Both densities play a role in determining the strength of the polarized term and we find that the magnitude of its coefficient K_{00} is somewhat model independent as can be seen from Figs. 4–6. Thus, in our model, the primary difference between materials shows up in the prefactor of the DM interaction, the factor $\lambda_d\Gamma^2/E_F^3$ in Eq. (33). If one assumes that both λ_d and Γ are similar for *Cu*Mn and *Au*Fe, the DM interaction in *Au*Fe will be twice as strong as that of *Cu*Mn since the ratio of the cubes of E_F is 2.0. Then the macroscopic anisotropy energy $\sim(E_{\rm DM})^2$ will be 4 times larger. There are additional sources of anisotropy in *Au*Fe which we have not taken into account, the effects of the gold hole and of the orbital contribution to the magnetic moment of iron.

We have also shown that the coefficients of both types of DM interactions exhibit a variable range dependence whose most important determinant is the magnitude of the separation of the VBS resonances from the Fermi surface, $|k_F-k_r^\sigma|$. For hypothetical materials for which this quantity is very small, the interactions $K_{\sigma\sigma'}/R^3$ will fall off as $1/R^3$. In practical cases, the interactions exhibit this behavior only in the nonphysical regime where the average interparticle distance is less than a nearest-neighbor distance. In the spin-glass regime where $R_{\rm av}$ ranges from 1 to 10 lattice constants, the interactions show strong deviations from $1/R^3$ behavior, going over to the form $1/R^4$ for sufficiently large $R_{\rm av}$. However, depending upon the material parameters, "sufficiently large $R_{\rm av}$" can be as small as a lattice constant. In general, the $1/R^4$ forms of the interactions are better approximations but preasymptotic corrections will be important when $|k_F-k_r^\sigma|$ is small. The major consequence of this finding is that previous calculations have lead to serious overestimates of the macroscopic anisotropy energy.

We have refrained from attaching specific numbers to our results. Four parameters are required to determine the magnitudes of the functions K_{+-} and K_{00}: the number of d electrons at the impurity sites, the value of the magnetic moment, and one of the pair Δ^σ and $E_{\rm res}^\sigma$ for each VBS resonance. Three additional parameters are needed to evaluate the interactions: the spin-orbit constant, the strength of the spin-spin coupling constant, and E_F. Generally λ_d and E_F are known but the values of the remaining five parameters are not known with sufficient precision to allow for a good numerical analysis. For example, one of the pair Γ and S (or μ), depending upon which is considered the independent variable, can be measured by the approach of the magnetization to saturation[13] and by NMR.[14] Both experiments probe the first few nearest-neighbor interactions, and previous analyses assume that the impurities are coupled by the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction. However, the latter assumption is questionable. The variable range dependence of the DM interaction is not a characteristic of the DM interaction *per se;* i.e., of the effect of spin-orbit scattering, but is an effect of the resonant scattering. A crude second-order RKKY-type calculation but with the wave function given by $\psi(\eta^\sigma)$ instead of by plane waves shows the same behavior:

$$E^{(2)}\sim\frac{V(R_{AB})}{R_{AB}^2}\mathbf{S}_A\cdot\mathbf{S}_B\ , \tag{61}$$

where $V(R_{AB})/R_{AB}^2$ varies from $1/R_{AB}^2$ to $1/R_{AB}^3$. This particular calculation has been done more precisely by taking into account the variation of Γ with energy, and is

able to explain the variation of the spin-glass temperature with impurity concentration.[6] Thus, it is clear that the experiments probe the region where the interaction is closer to $1/R^2$ than it is to $1/R^3$. Consequently, the values of Γ and/or S derived by assuming the interaction goes as $1/R^3$ are probably incorrect. Thus, before one can accurately calculate macroscopic anisotropic energies, experiments which give the necessary parameters should be reanalyzed with more realistic interactions.

ACKNOWLEDGMENTS

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APPENDIX A: EFFECTIVE HAMILTONIAN

We wish to show that the perturbation about the spin-orbit scattering site can be written as an effective Hamiltonian

$$H_{\rm eff}(\lambda)=\alpha \mathbf{l}\cdot\mathbf{s}+\beta(\mathbf{l}\cdot\hat{\mathbf{S}}_T)(\mathbf{s}\cdot\hat{\mathbf{S}}_T)+\gamma \mathbf{l}\cdot\hat{\mathbf{S}}_T\ , \tag{A1}$$

where $\mathbf{S}_T$ is the magnetic moment at the site of the spin-orbit scattering.

From Eqs. (5) and (7) we may write

$$\begin{aligned} E^{(3)}&\sim \sum_{\sigma,\sigma',\sigma''} \langle\psi(\eta^\sigma)\,|\,\mathbf{S}_A\cdot\mathbf{s}\,|\,\psi(\eta^{\sigma'})\rangle\langle\psi(\eta^{\sigma'})\,|\,\mathbf{l}\cdot\mathbf{s}\,|\,\psi(\eta^{\sigma''})\rangle\langle\psi(\eta^{\sigma''})\,|\,\mathbf{S}_B\cdot\mathbf{s}\,|\,\psi(\eta^\sigma)\rangle \\ &= \sum_{\sigma,\sigma',\sigma''} \langle\psi(\eta^\sigma)\,|\,\mathbf{S}_A\cdot\mathbf{s}\,|\,\sigma'\rangle\langle m_{l'}\sigma'\,|\,H_{\rm eff}(\lambda)\,|\,m_{l''}\sigma''\rangle\langle\sigma''\,|\,\mathbf{S}_B\cdot\mathbf{s}\,|\,\psi(\eta^\sigma)\rangle\ . \end{aligned} \tag{A2}$$

In Eq. (A2) the trace over spin states cannot be taken immediately because the space and spin variables are coupled in the wave function $\psi(\eta^\sigma)$. However, the spin dependence of the spatial part can always be expressed as $|\eta^\sigma\rangle\langle\eta^\sigma| = g + h\mathbf{s}\cdot\hat{\mathbf{u}}$, where $\hat{\mathbf{u}}$ is an axis of quantization. We obtain

$$E^{(3)}\sim\sum_\sigma\langle\sigma\,|\,\mathbf{S}_A\cdot\mathbf{s}(g+h\mathbf{s}\cdot\hat{\mathbf{u}})\mathbf{l}\cdot\mathbf{s}(g'+h'\mathbf{s}\cdot\hat{\mathbf{u}})\mathbf{S}_B\cdot\mathbf{s}\,|\,\sigma\rangle\ , \tag{A3}$$

so that

$$H_{\rm eff}(\lambda)=(g+h\mathbf{s}\cdot\hat{\mathbf{u}})\mathbf{l}\cdot\mathbf{s}(g'+h'\mathbf{s}\cdot\hat{\mathbf{u}})\ . \tag{A4a}$$

By expansion, this is equivalent to

$$\begin{aligned} H_{\rm eff}(\lambda)=&gg'\mathbf{l}\cdot\mathbf{s}+hg'\mathbf{s}\cdot\hat{\mathbf{u}}\,\mathbf{l}\cdot\mathbf{s}+gh'\mathbf{l}\cdot\mathbf{s}\,\mathbf{s}\cdot\hat{\mathbf{u}} \\ &+hh'\mathbf{s}\cdot\hat{\mathbf{u}}\,\mathbf{l}\cdot\mathbf{s}\,\mathbf{s}\cdot\hat{\mathbf{u}}\ . \end{aligned} \tag{A4b}$$

With the use of

$$\mathbf{s}\cdot\mathbf{A}\,\mathbf{s}\cdot\mathbf{B}=\tfrac{1}{4}\mathbf{A}\cdot\mathbf{B}+\tfrac{1}{2}i\mathbf{s}\cdot(\mathbf{A}\times\mathbf{B})\ , \tag{A5}$$

we obtain

$$\begin{aligned} H_{\rm eff}(\lambda)=&\left[gg'-\frac{hh'}{4}\right]\mathbf{l}\cdot\mathbf{s}+\frac{hh'}{2}(\mathbf{l}\cdot\hat{\mathbf{u}})(\mathbf{s}\cdot\hat{\mathbf{u}}) \\ &+\tfrac{1}{4}(hg'+gh')\mathbf{l}\cdot\hat{\mathbf{u}}+\frac{i}{2}(hg'-gh')\mathbf{s}\cdot(\hat{\mathbf{u}}\times\mathbf{l})\ . \end{aligned} \tag{A6}$$

When the principal value integrals indicated in Eq. (5) are performed, the last term on the right-hand side of Eq. (A6) will vanish, since hg' is a function of k',k'' while gh' is the same function of k'',k'. The remaining terms are

$$H_{\rm eff}(\lambda)=(g^2-\tfrac{1}{4}h^2)\mathbf{l}\cdot\mathbf{s}+\frac{h^2}{2}(\mathbf{l}\cdot\hat{\mathbf{u}})(\mathbf{s}\cdot\hat{\mathbf{u}})+\tfrac{1}{2}gh\mathbf{l}\cdot\hat{\mathbf{u}}\ . \tag{A7}$$

This result has been demonstrated for an arbitrary axis of quantization. However, for $\psi(\eta^\sigma)$, Eq. (3), to be an eigenfunction of the zeroth-order Hamiltonian, the axis $\hat{\mathbf{u}}$ must be that of $\mathbf{S}_T$ itself, which proves Eq. (A1).

The term in $\mathbf{l}\cdot\hat{\mathbf{S}}_T$ of Eq. (A1) makes no contribution to the energy as we now demonstrate. From Eqs. (A3), (A4a), and (A1), we have

$$\begin{aligned} E^{(3)}&\sim\sum_\sigma\langle\sigma\,|\,\mathbf{S}_A\cdot\mathbf{s}[\alpha\mathbf{l}\cdot\mathbf{s}+\beta(\mathbf{l}\cdot\hat{\mathbf{S}}_T)(\mathbf{s}\cdot\hat{\mathbf{S}}_T)+\gamma\mathbf{l}\cdot\hat{\mathbf{S}}_T]\mathbf{S}_B\cdot\mathbf{s}\,|\,\sigma\rangle \\ &=\alpha'\mathbf{l}\cdot(\mathbf{S}_A\times\mathbf{S}_B)+\beta'\mathbf{l}\cdot\hat{\mathbf{S}}_T(\mathbf{S}_A\times\mathbf{S}_B)\cdot\hat{\mathbf{S}}_T+\gamma'\mathbf{l}\cdot\hat{\mathbf{S}}_T\,\mathbf{S}_A\cdot\mathbf{S}_B \end{aligned} \tag{A8}$$

and after the angular integrations of Eq. (5) have been performed, $\mathbf{l}\rightarrow\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B$ so that the matrix element in Eq. (A2) contributes the term

$$\begin{aligned} E^{(3)}=&\alpha''(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot(\mathbf{S}_A\times\mathbf{S}_B) \\ &+\beta''(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot\hat{\mathbf{S}}_T(\mathbf{S}_A\times\mathbf{S}_B)\cdot\hat{\mathbf{S}}_T \\ &+\gamma''(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot\hat{\mathbf{S}}_T(\mathbf{S}_A\cdot\mathbf{S}_B)\ . \end{aligned} \tag{A9}$$

If one considers the matrix element similar to that in Eq. (A2) but with the order of scatterings changed from $(\mathbf{S}_A\cdot\mathbf{s},\mathbf{l}\cdot\mathbf{s},\mathbf{S}_B\cdot\mathbf{s})$ to $(\mathbf{S}_B\cdot\mathbf{s},\mathbf{l}\cdot\mathbf{s},\mathbf{S}_A\cdot\mathbf{s})$, one obtains the same result as Eq. (A9) but with $(\mathbf{R}_A,\mathbf{S}_A)$ interchanged with $(\mathbf{R}_B,\mathbf{S}_B)$. The first two terms of Eq. (A9) are invariant under this operation but the third term goes into its negative. Thus, when all six contributions to the energy are considered, terms like $(\hat{\mathbf{R}}_A\times\hat{\mathbf{R}}_B)\cdot\hat{\mathbf{S}}_T\,\mathbf{S}_A\cdot\mathbf{S}_B$ pair off and cancel, leaving only two types of anisotropic interaction as we have already shown.

APPENDIX B: INTEGRATION OF $K_{\sigma\sigma'}$

The coefficients of the DM interaction, Eq. (32), are given by

$$K_{\sigma\sigma'}=\frac{V^{\sigma}_{dk_F}V^{-\sigma'}_{k_Fd}}{\Delta^{\sigma}\Delta^{\sigma'}}\int_0^{E_F}dE_k\sin[\eta^{\sigma}(k)]\sin[\eta^{\sigma'}(k)]\sin[kR+\eta^{\sigma}(k)+\eta^{\sigma'}(k)]\ , \tag{B1}$$

where the phase shifts are given by

$$\eta^{\sigma}(k)\equiv\eta_2^{\sigma}(k)=\tan^{-1}\left[\frac{(k_{\Delta}^{\sigma})^2}{(k_r^{\sigma})^2-k^2}\right]\ . \tag{B2}$$

Here, $k_{\Delta}^{\sigma}=(2m\Delta^{\sigma}/\hbar^2)^{1/2}$ and $k_r^{\sigma}=(2mE_{\rm res}^{\sigma}/\hbar^2)^{1/2}$.

By means of the identity

$$\frac{dE_k}{\Delta^{\sigma}}=\frac{d\eta^{\sigma}}{\sin^2\eta^{\sigma}}\ , \tag{B3}$$

we obtain for the diagonal term $K_{\sigma\sigma}$,

$$K_{\sigma\sigma}=\frac{|V^{\sigma}_{dk}|^2}{\Delta^{\sigma}}\int_{\eta(0)}^{\eta^{\sigma}(k_F)}d\eta^{\sigma}\sin(kR+2\eta^{\sigma})\ . \tag{B4}$$

An integration by parts yields

$$K_{\sigma\sigma}=\frac{|V^{\sigma}_{dk}|^2}{\Delta^{\sigma}}(\sin[\eta^{\sigma}(k_F)]\sin[k_FR+\eta^{\sigma}(k_F)]+\tfrac{1}{2}\{\cos[\eta^{\sigma}(0)]-\cos(k_FR)-RI^{\sigma}\})\ , \tag{B5}$$

where

$$I^{\sigma}=\int_0^{k_F}\sin[kR+2\eta^{\sigma}(k)]dk\equiv\mathrm{Im}\int_0^{k_F}e^{ikR}\{\cos[2\eta^{\sigma}(k)]+i\sin[2\eta^{\sigma}(k)]\}dk\ .$$

From Eq. (B2), one finds

$$\cos[2\eta^{\sigma}(k)]+i\sin[2\eta^{\sigma}(k)]=1-\frac{2i(k_{\Delta}^{\sigma})^2}{k^2-(k_r^{\sigma})^2+i(k_{\Delta}^{\sigma})^2}\ . \tag{B6}$$

Thus,

$$I^{\sigma}=-\frac{1}{R}[\cos(k_FR)-1]-2(k_{\Delta}^{\sigma})^2\mathrm{Re}\int_0^{k_F}e^{ikR}\frac{1}{k^2-(k_r^{\sigma})^2+i(k_{\Delta}^{\sigma})^2}dk\ , \tag{B7}$$

from which

$$K_{\sigma\sigma}=\frac{|V^{\sigma}_{dk}|^2}{\Delta^{\sigma}}\{\sin[\eta^{\sigma}(k_F)]\sin[k_FR+\eta^{\sigma}(k_F)]-\sin^2[\eta^{\sigma}(0)]+R(k_{\Delta}^{\sigma})^2\ \mathrm{Re}G_{\sigma}(R)\}\ , \tag{B8}$$

where

$$G_{\sigma}(R)=\int_0^{k_F}e^{ikR}\frac{1}{k^2-(k_r^{\sigma})^2+i(k_{\Delta}^{\sigma})^2}dk\ .$$

This is Eq. (37) of the text.

The off-diagonal coefficient $K_{\sigma-\sigma}$ may be obtained in a similar way. It may be written as ($K_{+-}=K_{-+}$)

$$K_{\sigma-\sigma}=\frac{\hbar^2}{2m}\frac{V^{\sigma}_{dk_F}V^{-\sigma}_{k_Fd}}{\Delta^{+}\Delta^{-}}\mathrm{Im}\int_0^{k_F}dk\,k\,e^{ikR}\varepsilon^{i\eta^{+}}\sin\eta^{+}\varepsilon^{i\eta^{-}}\sin\eta^{-}\ , \tag{B9}$$

and by means of

$$\varepsilon^{i\eta^{\sigma}}\sin\eta^{\sigma}=\frac{(k_{\Delta}^{\sigma})^2}{(k_r^{\sigma})^2-k^2-i(k_{\Delta}^{\sigma})^2} \tag{B10}$$

and the use of partial fractions as

$$K_{\sigma-\sigma}=2V^{\sigma}_{dk_F}V^{-\sigma}_{k_Fd}\mathrm{Im}\left[\frac{\Delta[H_{\sigma}(R)]}{(E_{\rm res}^{-}-E_{\rm res}^{+})-i(\Delta^{-}-\Delta^{+})}\right]\ , \tag{B11}$$

where

$$H_\sigma(R)=\int_0^{k_F} dk\, k\, \frac{e^{ikR}}{(k_r^\sigma)^2-k^2-i(k_\Delta^\sigma)^2}$$

and

$$\Delta[H_\sigma(R)]\equiv H_+(R)-H_-(R)\ .$$

Since $H_\sigma=id/dRG_\sigma$, this yields Eq. (38) of the text. There remains only the integral $G_\sigma(R)$ to be determined.

By defining $\mu=kR$, $G_\sigma(R)$ may be cast into the form

$$G_\sigma(R)=\frac{R}{\mu_-^\sigma-\mu_+^\sigma}\int_0^{k_F} d\mu\, e^{i\mu}\left[\frac{1}{\mu-\mu_-^\sigma}-\frac{1}{\mu-\mu_+^\sigma}\right], \tag{B12}$$

where $\mu_\pm^\sigma$ are the roots of the equation $(\mu^\sigma)^2=(\mu_r^\sigma)^2-i(\mu_\Delta^\sigma)^2$. Therefore,

$$\mu_\pm^\sigma=\pm\alpha^\sigma e^{i\phi^\sigma/2}\ , \tag{B13}$$

where

$$\alpha^\sigma=[(k_r^\sigma)^4+(k_\Delta^\sigma)^4]^{1/4}/k_F$$

and

$$\tan\phi^\sigma=-\left[\frac{k_\Delta^\sigma}{k_r^\sigma}\right]^2 .$$

Then a change of variables $\mu=it+\mu_\pm^\sigma$ in Eq. (B12) leads to

$$\int_0^{\mu_F} e^{i\mu}\frac{1}{\mu-\mu_\pm^\sigma}d\mu=e^{i\mu_\pm^\sigma}\int_{i\mu_\pm^\sigma}^{-i\mu_F+i\mu_\pm^\sigma} dt\frac{e^{-t}}{t}$$
$$=e^{i\mu_\pm^\sigma}[E_1(i\mu_\pm)-E_1(-i\mu_F+i\mu_\pm)]\ , \tag{B14}$$

where $E_1(z)$ is the exponential integral function. This completes the integration of $G_\sigma(R)$, Eq. (39).[9]

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[7]For the special case of $l=1$, the $\hat{\varepsilon}_m$ are called spherical unit vectors, $\hat{\varepsilon}_{\pm1}=\mp(1/\sqrt{2})(\hat{x}\pm i\hat{y})$, $\hat{\varepsilon}_0=\hat{z}$. See, e.g., A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University, Princeton, N.J., 1957), p. 82. For general properties of the Clebsch-Gordan coefficients, see Chap. 3. In the notation of Edmonds, our symbol $(lm,l'm'\,|\,l''m'')$ would be written as $(lm,l'm'\,|\,ll'l''m'')$. Note that the spin operators have the properties $s_0\,|\,\pm\rangle=\pm\frac{1}{2}\,|\,\pm\rangle$, $s_{+1}\,|\,-\rangle=-(1/\sqrt{2})\,|\,+\rangle$, and $s_{-1}\,|\,+\rangle=(1/\sqrt{2})\,|\,-\rangle$.

[8]See A. R. Edmonds, Ref. 7. His Eq. (5.1.8) has the wrong sign, which may be seen by calculating his component $T(1\ 0)$.

[9]The factor $\sin^2[\eta_2(k)]$ for $k=0$ is always small and may be deleted.

[10]Q. Zhang (unpublished). The observation of the importance of $|k_F-k_r^\sigma|$ is due to him.

[11]That the values of R_c^σ depend upon Δ^σ as well as on $|k_F-k_r^\sigma|$ may be seen by setting $|z^\sigma|$, Eq. (43a), equal to 1. Equation (44) is a simplified version for purposes of discussion.

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