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A THEORY FOR THE ANISOTROPIC INTERACTION BETWEEN TWO SUBSTITUTIONAL MAGNETIC IMPURITIES AND THE MAGNETIC ANISOTROPIC EFFECT IN DILUTE MAGNETIC ALLOYS *

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ABSTRACT

In this paper, a formalism for studying the anisotropic interaction between two substitutional magnetic impurities and the magnetic anisotropic effect in a dilute noble metal- transition metal magnetic alloy has been developed from relativistic scattering theory. The theoretical development and the computational techniques of this formalism are based on relativistic spin-polarized scattering theory and relativistic band structure frameworks. For studying the magnetic anisotropic effect a convenient 'working' frame of reference with its axes oriented along the fcc crystal axes is set up. This formalism is applied to study the situation for two Fe impurities in para-magnetic Au hosts. For AuFe dilute alloy, the two impurity site interaction as a function of separation is not oscillatory and the anisotropic effect is found to be less than the two site interaction itself only by an order of magnitude. Apart from the anisotropic coupling of the two impurity spins to the separation vector, for the first time, another weak anisotropic coupling to the crystal axes is also contained in the two site interaction. These anisotropic effects are the results of the relativistic spin-orbit interaction which are incorporated into the formalism.

I. INTRODUCTION

The interaction between two impurities is important in studying spin-glass and mangetic properties of dilute alloy. The behaviour of spin glass alloys has been studied with the assumption that each pair of the magnetic impurities in a metallic host interact in an RKKY (Ruderman and Kittel, 1954; Kasuya, 1956; Yoshida, 1957) form. The RKKY interaction is unable to describe any anisotropic coupling between the local magnetic moments and thus is inadequate to describe anisotropy fields in dilute magnetic alloys and spin glass. The relativistically generalized RKKY interaction can contain magnetic anisotropy effects through the relativistic spin-orbit interaction which coupled the spin of an electron to the crystal field. Fert and Levy (1980) and Goldberg and Levy (1986) in their papers have shown how a unidirectional anisotropy field can arise in a spin glass from an additional term, as well as from the RKKY interaction. The latter is of the Dzyaloshinsky-Moriya type (Dzyaloshinsky, 1958; Moriya, 1960), i.e.

$$E_{DM} \propto \hat{R}_{12} \cdot (\hat{S}_1 \times \hat{S}_2) \ .$$

In their approach, they consider the interaction between two magnetic impurities via spin-orbit scattering from a third site. They use perturbation theory in their approach and derive a three site interaction. Staunton et al. (1988) also derive an interaction between two magnetic sites mediated by a relativistic electron scattering between them in a uniform positively charged background. Their relativistic RKKY interaction contains uniaxial anisotropic components through a polynomial dependence upon a squared DM type term and a pseudo-dipolar term $((\hat{R}_{12}\cdot\hat{S}_1)(\hat{R}_{12}\cdot\hat{S}_2))$ apart from being a function of an isotropic $(\hat{S}_1\cdot\hat{S}_2)$ term. In this paper, the relativistic effects of the paramagnetic host are also incorporated realistically into the interaction between two substitutional magnetic impurities.

Temmerman (1982) first reported a formalism for studying the non-relativistic interaction between two substitutional impurities in a realistic host within a scattering theory. In this paper, as a first step, the relativistically generalized integrated density of states for a host system with two substitutional magnetic impurities is subtracted from that of the host system alone within a multiple scattering theory (Lloyd and Smith, 1972). This induced integrated density of states for the two substitutional impurities is used to derive the expression for the relativistic interaction between two magnetic impurities in a realistic host. A relativistic spin-polarized scattering theory (Strange et al., 1984) forms the basis. We consider the relativistic effects due to both host sites and the impurity sites.

Finall, we calculate the relativistic interaction between two Fe impurities in a cubic fcc Au host, its anisotropic components $(E_{12}^{\uparrow\uparrow} - E_{12}^{\leftrightarrow})$, the anisotropic effect with respect to both crystal axes and the separation vector $\underline{R}_{12}$. This introduces qualitatively new features to the form of the magnetic anisotropy of dilute magnetic alloys.

II. RELATIVISTIC SPIN POLARIZED SCATTERING THEORY

Kohn and Sham (1965) showed how a one-particle Schrödinger equation can be set up, which includes all the effects of the correlation and exchange among the particles of the system within the unique density functional approach. The relativistic generalization of the theory has been developed by a number of authors (Raman and Rajagopal, 1979; MacDonald and Vosko, 1979). The spin polarized scattering theory for a muffin-tin potential $(v^{ext.})$ has been discussed within this relativistic generalization of the Kohn-Sham one particle Schrödinger equation by Feder et al. (1983) and Strange et al. (1984). This relativistic spin-polarized scattering theory for the magnetic component of the potential oriented along the z-axis has revealed the opportunity to derive a realistic theory for magnetic anisotropy. The mathematics has been described in detail in the papers of Strange et al. (1984) and Staunton et al. (1988) and ended up with the following set of radial differential equation for the magnetic component of the potential oriented along the z-axis appropriate to the local coordinate frame attached to the single site, (in a.u.)

$$\left[-c\frac{\partial}{\partial r} + \frac{(\kappa_2 - c)}{r}\right] f_{\kappa_2\kappa_1}^{m_{j2}m_{j1}}(r) + \left[E - V^{eff.}(r) - \frac{c^2}{r}\right] g_{\kappa_2\kappa_1}^{m_{j2}m_{j1}}(r) + B^{eff.}(r) \sum_{\kappa'}{}' G(\kappa_2, \kappa', m_{j2})\, g_{\kappa'\kappa_1}^{m_{j2}m_{j1}}(r) = 0$$

$$\left[c\frac{\partial}{\partial r} - \frac{(\kappa_2 - c)}{r}\right] g_{\kappa_2\kappa_1}^{m_{j2}m_{j1}}(r) + \left[E - V^{eff.}(r) + \frac{c^2}{2}\right] f_{\kappa_2\kappa_1}^{m_{j2}m_{j1}}(r) - B^{eff.}(r) \sum_{\kappa'}{}' G(-\kappa_2, -\kappa', m_{j2})\, g_{\kappa'\kappa_1}^{m_{j2}m_{j1}}(r) = 0$$

(2.1)

These coupled differential equations can numerically be solved outside the potential $(r > r_m)$ in terms of the transition t-matrix and satisfies

$$t_{\ell m\sigma,\ell' m'\sigma'} = t^{\ell}_{m,\sigma;\, m+\sigma-\sigma',\sigma'}\,\delta_{\ell\ell'}\,\delta_{m,m'-\sigma+\sigma'} \qquad (2.2)$$

To study the magnetic anisotropy, we need to allow the magnetic component be oriented along an arbitrary direction. The arbitrary working frame can be set up by rotating through the Euler angles α,β,γ the 'local' coordinate frame (the frame with its z-axis set up along the magnetic component of the potential).

Now the t-matrix, $t^{\ell,\text{working}}_{m\sigma,m'\sigma'}$ describing scattering from a potential with its magnetic component oriented along z-axis of this arbitrary "working" frame is written in terms of that of the "local" frame $t^{\ell,\text{local}}_{m\sigma,m'\sigma'}$ (Staunton et al., (1988))

$$t^{\ell,\text{working}}_{m\sigma,m'\sigma'} = \sum_{m'',m''',\sigma'',\sigma'''} R^{\ell}_{mm''}(A)\left(R^{1/2}_{\sigma\sigma''}(A)\, t^{\ell,\text{local}}_{m''\sigma'',m'''\sigma'''}\, R^{1/2\,\dagger}_{\sigma'''\sigma''}(A)\right) R^{\ell\,\dagger}_{m'''m'}(A) \qquad (2.3)$$

where R is the rotational matrix operator (Messiah, 1965). Non-relativistically, the t-matrix is dependent only on ℓ through the spherically symmetric potential. But relativistically the t-matrix is also dependent on m, that is it has different values for different components of m corresponding to a particular ℓ, as if a spherically asymmetric potential $V(\underline{r})$ is experienced by the scattering electron. Thus the magnetic anisotropy arises from this m-dependence contrary to the non-relativistic case. In order to derive an expression for the interaction between two magnetic impurities in a host lattice, scattering from many potentials needs to be considered.

The powerful scattering path operator τ^{ij} for multiple scattering problem gives the scattered waves emanating from the site $\underline{R}_j$ operating on the wave incident at $\underline{R}_i$ and includes all the effects in between. The relativistic "on the energy shell" components of the path operator $\tau^{ij}_{\ell m\sigma,\ell' m'\sigma'}(E)$ satisfy the following equation (Györffy and Stocks, 1979)

$$\tau^{ij}_{\ell m\sigma,\ell' m'\sigma'} = t^{i,\ell}_{m\sigma,m'\sigma'}(E)\,\delta_{ij}\,\delta_{\ell\ell'} + \sum_{k\neq i}\sum_{\substack{m''\sigma'' \\ \ell'''\sigma'''}} t^{i,\ell}_{m\sigma,m''\sigma''}\, G_{\ell''m'',\ell'''m'''}(\underline{R}_i-\underline{R}_k,E)\,\tau^{kj}_{\ell'''m'''\sigma'',\ell' m'\sigma'}(E) \qquad (2.4)$$

where the structure constants have been written (Staunton et al., 1980)

$$G_{\ell m\sigma,\ell' m'\sigma'} = G_{\ell m,\ell' m'}\,\delta_{\sigma\sigma'}$$

Eq.(2.4) gives $\tau^{ij}_{\ell m\sigma,\ell' m'\sigma'}$ in terms of the relativistic spin-polarized scattering single site t-matrix, $t_{\ell m\sigma,\ell' m'\sigma'}$.

III. THE ANISOTROPIC INTERACTION BETWEEN TWO MAGNETIC IMPURITIES IN A REALISTIC HOST

Following Staunton et al. (1988), the relativistic interaction energy between two magnetic impurities, which contains the magnetic anisotropic effect in it, is

$$\Omega' = -\int_0^{\infty} f(E-\nu)\, N(E)\, dE \qquad (3.1)$$

where N(E) is the integrated density of states induced by two mangetic impurities in a realistic heat. The relativistically generalized integrated density of states of a pure system is (Györffy and Stocks, 1979)

$$N(E) = N_0(E) - \frac{1}{\pi}\,\mathrm{Im}\,\ln\left|\, t^{o\,-1}_{n,\Lambda\Lambda'}(E)\,\delta_{nn'} - G^{o}_{\Lambda\Lambda'}(\underline{R}_n-\underline{R}_{n'},E)\,\delta_{\sigma\sigma'}\,\right| \qquad (3.2)$$

where $N_0(E)$ is the free electron itnegrated density of states and $\Lambda \equiv (\ell,m,\sigma)$. The second term of Eq.(3.2) arises from the multiple scattering effect. Focussing on the second term of Eq.(3.2), using $\mathrm{tr}(M) = \det|M|$ for the site index part of the matrices, the relativistically generalized number of states due to the scattering sites of the host system, containing the two substitutional impurities is written

$$N_I = -\frac{1}{\pi}\,\mathrm{Im}\,\ln\left|\begin{pmatrix} \underline{I}^{-1} & 0 \\ t^{-1}_{n=1,2} & \\ 0 & t^{o\,-1}_{n\neq 1,2} \end{pmatrix} + \begin{pmatrix} 0 & -G^{o} \\ -\tilde{G}_0 & 0 \end{pmatrix}\right|$$

The t-matrices in this expression are expressed in "working" frame i.e. rotated through Euler angles. $t^{I^{-1}}_{n=1,2}$ is a 2x2 diagonal matrix for the two impurity sites, $t^{0^{-1}}_{n\neq 1,2}$ is a (N-2) x (N-2) diagonal matrix for the (N-2) host sites.

The relativistically generalized induced number of states due to two substitutional impurities in a paramagnetic host

$$\Delta N(E) = -\frac{1}{\pi}\,\mathrm{Im}\,\ln\left|\tau^{-1} + \Delta_{n,n'=1,2}\,\delta_{nn'}\right| + \frac{1}{\pi}\,\mathrm{Im}\,\ln\left|\tau^{-1}\right| \tag{3.3}$$

where

$$\Delta_{n,n'=1,2}\,\delta_{nn'} = \begin{pmatrix} t_1^{I^{-1}} - t_1^{0^{-1}} & 0 & 0 & 0 & \cdots \\ 0 & t_2^{I^{-1}} - t_2^{0^{-1}} & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix} \cdots$$

$$= \begin{pmatrix} \Delta_1 & 0 & 0 & 0 & \cdots \\ 0 & \Delta_2 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix} \equiv \Delta_{1,2}$$

$$\Delta N(E) = -\frac{1}{\pi}\,\mathrm{Im}\,\ln\left|1+\tau^{11}\Delta_1\right| - \frac{1}{\pi}\,\mathrm{Im}\ln\left|1+\tau^{22}\Delta_2\right|$$

$$-\frac{1}{\pi}\,\mathrm{Im}\,\ln\left|\tilde{1} + \begin{pmatrix} 0 & (1+\tau^{11}\Delta_1)^{-1}\tau^{12}\Delta_2 & 0 & 0 & \cdots \\ (1+\tau^{22}\Delta_2)^{-1}\tau^{21}\Delta_1 & 0 & 0 & 0 & \cdots \\ 0 & & 0 & 0 & \cdots \\ \vdots & & \vdots & \vdots & \end{pmatrix}\right| \tag{3.4}$$

The first and second terms are the relativistic induced number of states for the individual impurity sites 1 and 2, respectively. The third term is the net induced number of states due to the interaction between the two impurity sites via the host. Thus, the relativistic induced number of states due to the interaction between two impurities in a realistic metallic host

$$N(E) = -\frac{1}{\pi}\,\mathrm{Im}\,\ln\left|\left(\tilde{1} - (1+\tau^{11}\Delta_1)^{-1}\tau^{12}\Delta_2\left(1+\tau^{22}\Delta_2\right)^{-1}\tau^{21}\Delta_1\right)\right| \tag{3.5}$$

Expanding the natural logarithm and retaining the first term for two well-separated impurity sites

$$N(E) \simeq \frac{1}{\pi}\,\mathrm{Im}\sum_{\Lambda}\left(\left(1+\tau^{11}\Delta_1\right)^{-1}\tau^{12}\Delta_2\left(1+\tau^{22}\Delta_2\right)^{-1}\tau^{21}\Delta_1\right)_{\Lambda\Lambda}$$

$$= \frac{1}{\pi}\,\mathrm{Im}\sum_{\Lambda} M_{\Lambda\Lambda} \tag{3.6}$$

Thus, for two well-separated magnetic impurities, the relativistic interaction energy between two magnetic impurities in a paramagnetic host is

$$E_{12} \simeq \frac{1}{\pi}\,\mathrm{Im}\int_0^\infty dE\, f(E-\nu)\sum_{\Lambda_1\Lambda_2\Lambda_3\Lambda_4\Lambda_5} M^1_{\Lambda\Lambda_1}\tau^{12}_{\Lambda_1\Lambda_2}\Delta_{2,\Lambda_2\Lambda_3}\times M^2_{\Lambda_3\Lambda_4}\tau^{21}_{\Lambda_4\Lambda_5}\Delta_{1,\Lambda_5\Lambda} \tag{3.7}$$

where

$$M^1_{\Lambda\Lambda_1} = \left(\left(\tilde{1}+\tau^{11}\Delta_1\right)^{-1}\right)_{\Lambda\Lambda_1}$$

$$M^2_{\Lambda\Lambda_1} = \left(\left(\tilde{1}+\tau^{22}\Delta_2\right)^{-1}\right)_{\Lambda\Lambda_1}$$

and for a pure paramagnetic host is

$$\tau^{11}_{\Lambda_1\Lambda_2}(E) = \frac{1}{\Omega_{BZ}} \int_{BZ} d\underline{k} \left(\left(t^{o\,-1} - G^{o}(\underline{k},E) \right)^{-1} \right)_{\Lambda_1\Lambda_2} \qquad (3.8a)$$

and

$$\tau^{12}_{\Lambda_1\Lambda_2}(E) = \frac{1}{\Omega_{BZ}} \int_{BZ} d\underline{k} \left(\left(t^{o\,-1} - G^{o}(\underline{k},E) \right)^{-1} \right)_{\Lambda_1\Lambda_2} e^{i\underline{k}\cdot(\underline{R}_1 - \underline{R}_2)} \qquad (3.8b)$$

where $G^0(\underline{k},E)$ is the lattice Fourier transform of $G^0(\underline{R}_{12},E)$ and Ω_{BZ} is the Brillouin zone volume. A substantial computational task is involved in the calculation of (3.8). Eq.(3.7) is to be calculated in a "working" frame to calculate the relativistic two site interactions and the anisotropic component.

A convenient 'working' frame is set up with its three axes (X,Y,Z) oriented along the crystal axes (a,b,c) of the fcc cubic host system. The local frames at 1 and 2 are defined by the requirement that their z-axes are oriented along the directions $\hat{S}_1$ and $\hat{S}_2$ of the magnetic moments of the two impurities as in Figs.3.1. In these figures (X,Y,Z) are the axes of the convenient "working" frame at two impurity sites 1 and 2, set up by rotating the axes of the "local" coordinate frame through Euler angles $A_1(\alpha_1,\beta_1,\gamma_1)$ at impurity site 1 and $A_2(\alpha_2,\beta_2,\gamma_2)$ at impurity site 2. In Eq.(3.7), in the working frame

$$\Delta_{1,\Lambda\Lambda_1} = \left(R^{\dagger} t_1^{I\,-1} R - t_1^{o\,-1} \right)_{\Lambda\Lambda_1}$$

and

$$\Delta_{2,\Lambda\Lambda_1} = \left(R^{\dagger} t_2^{I\,-1} R - t_2^{o\,-1} \right)_{\Lambda\Lambda_1} \qquad (3.9)$$

The matrix property $(R^{+}tR)^{-1} = R^{+}t^{-1}R$ is used here. The Euler angle rotation operator, which can transform the "working" frame into some other coordinate frame like the "local" is (Messiah, 1965)

$$R(\alpha,\beta,\gamma) = \begin{pmatrix} \cos\gamma\cos\beta\cos\alpha - \sin\gamma\sin\alpha & -\sin\gamma\cos\beta\cos\alpha - \cos\gamma\sin\alpha & \sin\beta\cos\alpha \\ \cos\gamma\cos\beta\sin\alpha + \sin\gamma\cos\alpha & -\sin\gamma\cos\beta\sin\alpha + \cos\gamma\cos\alpha & \sin\beta\sin\alpha \\ -\cos\gamma\sin\beta & \sin\gamma\sin\beta & \cos\beta \end{pmatrix}$$

Throughout the whole calculation α is kept zero. For site 1, the unit vectors along the axes of the convenient "working" frame $(\hat{X},\hat{Y},\hat{Z})$ can be transformed into the unit vectors of the "local" frame $(\hat{X}_1,\hat{Y}_1,\hat{Z}_1)$ by

$$\begin{pmatrix} \hat{X}_1 \\ \hat{Y}_1 \\ \hat{Z}_1 \end{pmatrix} = R(\alpha,\beta,\gamma) \begin{pmatrix} \hat{X} \\ \hat{Y} \\ \hat{Z} \end{pmatrix}$$

Therefore, for site 1, (cf. Fig.3.1a)

$$\hat{Z}_1\cdot\hat{X} = \hat{S}_1\cdot\hat{X} = -\cos\gamma_1\sin\beta_1$$
$$\hat{Z}_1\cdot\hat{Y} = \hat{S}_1\cdot\hat{Y} = \sin\gamma_1\sin\beta_1$$
$$\hat{Z}_1\cdot\hat{Z} = \hat{S}_1\cdot\hat{Z} = \cos\beta_1$$

where $\hat{Z}_1 = \hat{S}_1$ is the unit vector along the magnetic component of the impurity potential at site 1. Similar relations can also be obtained for site 2. Using these relations, the two spins on the impurity sites can be oriented in various desired directions in the "working" frame. The angle between the two spins is

$$\hat{S}_1 \cdot \hat{S}_2 = \cos\gamma_1 \sin\beta_1 \cos\gamma_2 \sin\beta_2 + \sin\gamma_1 \sin\beta_1 \sin\gamma_2 \sin\beta_2 + \cos\beta_1 \cos\beta_2$$

β and γ are restricted by $0 \leq \beta \leq \pi$, $-\pi \leq \gamma \leq +\pi$. The next stage of this paper is to describe how to compute Eq.(3.7) for various orientations of the spin components on the impurity sites 1 and 2 in the "working" frame.

IV. COMPUTATIONAL PROCEDURE

The matrices τ^{11} and τ^{12} involved in Eq.(3.7), which treat the effect of the host lattice sites realistically, are considered first for computation and for physical reasons τ^{11} and τ^{12} are equal to τ^{22} and τ^{21} respectively. The matrices τ^{11} and τ^{12} involve Brillouin zone integrations via Eqs.(3.8). These fairly complicated Brillouin zone integrations for fcc crystals are evaluated using the special directional methods within the relativistic KKR band theory framework (Stocks et al., 1979). The special directions in $1/48^{th}$ of the irreducible Brillouin zone for fcc crystals are calculated by Bansil's special direction method (Bansil, 1975). The special directions are projected on the 48 irreducible zones using the 48 symmetry oeprations of the cubic group for cubic structures and hence the integration over the whole Brillouin zone done (Satter, 1989). Finally, in evaluating the integration in expression (3.7), it is expressed as a sum over Matsubara frequencies (Fetter and Walecka, 1972). Recalling expression (3.7), the interaction energy between two magnetic impurities is

$$E_{12} = (-2k_B T) \sum_{n=0}^{\infty} \sum_{\Lambda_1\Lambda_2\Lambda_3\Lambda_4\Lambda_5} M^1_{\Lambda\Lambda_1}(\nu + i\omega_n)\, \tau^{12}_{\Lambda_1\Lambda_2}(\nu + i\omega_n)\, \Delta_{2,\Lambda_2\Lambda_3}(\nu + i\omega_n)\, M^2_{\Lambda_3\Lambda_4}(\nu + i\omega_n)\, \tau^{21}_{\Lambda_4\Lambda_5}(\nu + i\omega_n)\, \Delta_{1,\Lambda_5\Lambda}(\nu + i\omega_n)$$

where ν is the chemical potential appropriate to a system and the Matsubara frequency $\omega_n = (2n+1)\pi k_B T$, where $n = 0,1,2,\ldots$ integers. The Matsubara sum is evaluated on a logarithmic mesh for 25 values of the imaginary energy part ω from 0.005 to 1.256 Rydberg instead of the direct sum over many Matsubara frequencies and the results are interpolated to the required Matsubara

frequencies. As the imaginary energy part increases, the contribution to the interaction energy between the two impurities decreases and hence the sum is cut off at $\simeq$ 1.256 Rydberg.

V. RESULTS

5.1 Two Fe Impurities in Heavy Paramagnetic Au Host

In Fig.5.1, the relativistic interaction between the two Fe impurities in fcc Au host versus the separation $\underline{R}_{12}$ are plotted for two directions [010] and [110]. Qualitatively these curves are neither of the usual RKKY form nor of the relativistic RKKY form (Staunton et al., 1988). The curve for along [010] direction is critically damped, while for along [110] it is of damped oscillatory type and pulled down. Fig.5.2, the anisotropic component versus separation curves are also plotted for the same two dierctions and the anisotropic effect, which is found to be enhanced, in the two site interaction is oscillatory. The Fe potential constructed self-consistently by Moruzzi et al. (1978) is used throughout the calculations.

The relativistic interaction between two Fe impurities in a Cu host and its anisotropic components are also examined. In this case, although copper (Z = 29) is host of low atomic number, the anisotropic components are still enhanced through smaller than that for AuFe by an order of magnitude. It is also found that in this calculation, the two site interction is changing sign with separation more rapidly than the relativistic two site interaction for AuFe and thus the two site itneraction can be closer to the relativistic RKKY interaction for a host of very low atomic number.

5.2 The Anisotropic Effect with Respect to Both Separation Vector and the and the Crystal Axes

In Fig.5.3, the solid line, which is varying sinusoidally, is plotted for parallel spins 1 and 2 rotating in the XY-plane making angles from 0° to 180° with respect to $\underline{R}_{12}(0,4\pi,0)$. The interaction energies for the cases of the two extreme points are equal and largest. In the same figure, the broken line is plotted for both 1 and 2 parallel and rotating in the XZ-plane making angles 0° to 180° with the crystal axis, while both $\hat{S}_1$ and $\hat{S}_2$ make an angle of 90° with $\underline{R}_{12}(0,4\pi,0)$. The broken line shows a weak growing anisotropy with respect to the crystal axis, however, the solid curve shows a strong growing anisotropy with respect to the separation vector $\underline{R}_{12}$. Thus the spion-orbit interaction couples the spins very weakly to the crystal axes as well as a stronger coupling to the separation vector $\underline{R}_{12}$.

VI. DISCUSSION

The relativistic expression (3.7) for the interaction between two magnetic impurities in a realistic paramagnetic host contains an anisotropic effect. Although from this expression the anisotropic effect is not obvious at once, it is demonstrated through the numerical computation. The Dzyaloshinsky-Moriya term, which appeared in Fert et al. (1980) anisotropic two site interaction, breaks the inversion symmetry of the two site interaction with respect to the mid-point between the two impurity spins and this anisotropic interaction is regarded as the unidirectional anisotropy. The anisotropic interaction found in this paper is termed as a uniaxial anisotropy, because the inversion symmetry for the interaction with respect to the mid-point is found to be preserved in this circumstance.

The relativistic interaction between two Fe impurities in a realistic Au host, as in Fig.5.1, has been found to be a critically damped oscillatory function of separation along [010] and of damped oscillatory type along [110]. These results have ruled out the possibility of existence of a sinusoidal oscillating RKKY and R-RKKY (Staunton et al., 1988) interaction between two magnetic impurities in a heavy paramagnetic host. However, the relativistic interaction has been found to change sign for two Fe impurities in Cu host, as the separation is varied, more rapidly than in AuFe. Thus, still the RKKY or the R-RKKY interaction can exist in shape for magnetic impurities in a paramagnetic host of very low atomic number. In Fig.5.2, the anisotropic components, $(E_{12}^{\uparrow\uparrow}-E_{12}^{\rightarrow\rightarrow})$, have been found to be oscillatory functions of separation R_{12} along both [010] and [110] directions. This suggests that for a random arrangement of magnetic impurities, which is the case of 'ideal' spin glasses, the anisotropic interactions are also random. This new anisotropic frustration caused by random anisotropy can be an essential ingredient in the study of ground state properties of spin glasses. The size of the anisotropic components contained in the relativistic two site interaction in a realistic host has been determined and found to be remarkably enhanced (for AuFe $\sim 10^{-4}$ Rydberg and for CuFe $\sim 10^{-5}$ Rydberg) compared to the results found by Fert et al. (1980) and Staunton et al. (1988) (which for two Fe impurities in a jellium model was of the order of 10^{-6} Rydberg), while the two site interaction itself has been $\sim 10^{-3}$ Rydberg. Thus a realistic treatment of heavy host sites in studying two impurity site interaction has been shown to be crucial and the spin-orbit interaction can no longer be justified as a small perturbation for studying the anisotropic effect in dilute magnetic alloys.

The unidirectional anisotropy and the relativistic two site interaction, which has been studied in this paper, are good starting points from which to study the remanent magnetization and other spin glass properties of dilute

magnetic alloys, like AuFe and CuMn, because of the incorporation of the full effect of the host sites into the interaction between two magnetic impurities. The inversion symmetry of this relativistic two site interaction would be broken if the interaction had been derived by considering a third impurity site in the realistic host and the resulting anisotropy would be then have been unidirection. Then the effect of the concentration of the third non-magnetic impurities on the remanent magnetization can also be investigated by studying the anisotropic effect on the relativistic two site interaction moving a thrid non-magnetic impurity gradually (Prejean et al., 1980).

Ultimately, the more complicated theory for the relativistic interaction between many magnetic impurities in a realistic host can also be studied within this framework and consequently, a new insight for dilute magnetic alloys can be evolved and a better understanding on the origin of magnetic anisotropy for such alloy can be achieved.

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FIGURE CAPTIONS

Fig.3.1a Working frame and local frame at impurity site 1.

Fig.3.1b Working frame and local frame at impurity site 2.

Fig.5.1 Relativistic interaction between two Fe impurities in a Au host as a function of separation. The solid line shows the interaction between two Fe spins which are both perpendicular to $\underline{R}_{12}$ along the [110] direction, while the broken line is for $\underline{R}_{12}$ along [010]. The dotted line is for the relativistic RKKY interaction calculated by Staunton et al. (1988).

Fig.5.2 The anisotropic component $(E_{12}^{\uparrow\uparrow}-E_{12}^{\rightarrow\rightarrow})$ versus separation curves for two Fe impurities in Au host. The solid line is drawn for the anisotropic component along the [110] direction, while the broken line is for along the [010] direction (left vertical axis). The dotted curve shows the anisotropic component versus separation calculated by Staunton et al. (1988) (right vertical axis).

Fig.5.3 Relativistic interaction versus angle of rotation of the impurity spin. a) The solid line is drawn for spins 1 and 2 rotating simultaneously in the XY-plane making an angle with $\underline{R}_{12} = (0,4\pi,0)$. b) The broken line is drawn for spins 1 and 2 rotating simultaneously in the XZ-plane making an angle with the crystal axis.

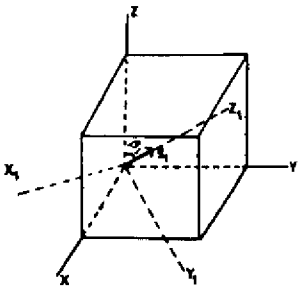

Fig.3.1a

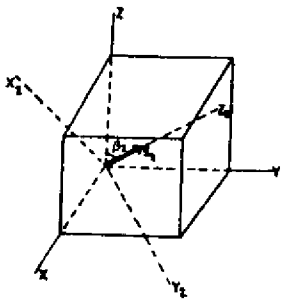

Fig.3.1b

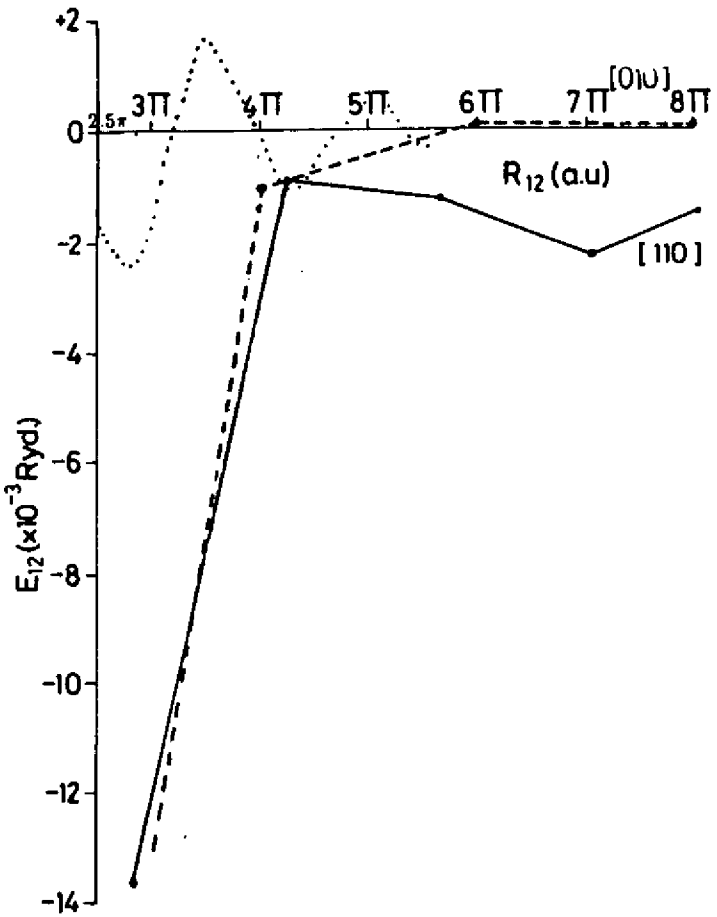

Fig.5.1

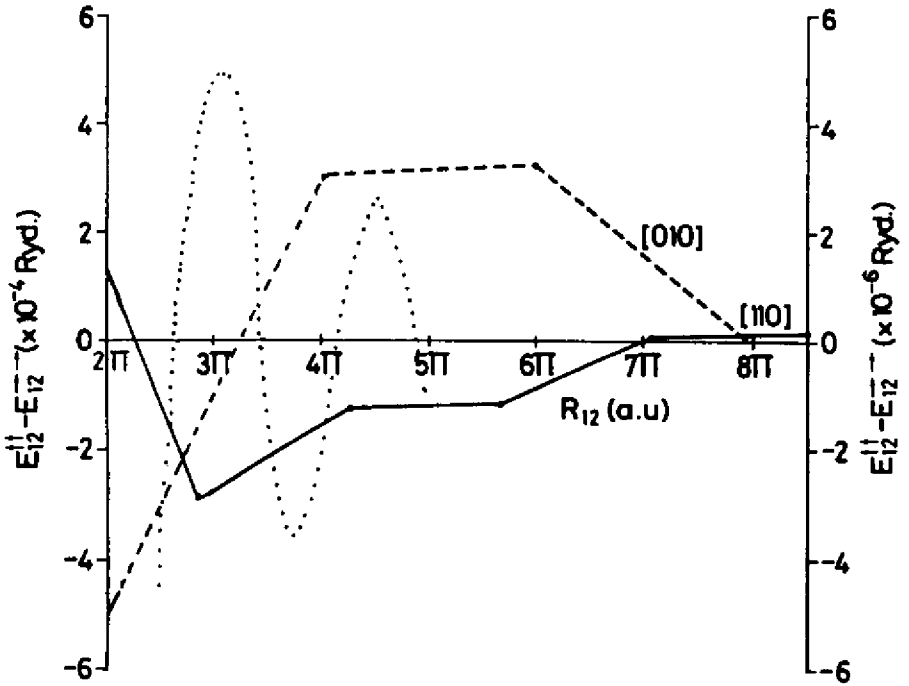
6
4
2
0
-2
-4
-6
2π
3π
4π
5π
6π
7π
8π
[010]
[110]
R_{12} (a.u)
$E_{12}^{\perp\perp}-E_{12}^{\perp\perp}$ (×10⁻⁴ Ryd.)
$E_{12}^{\perp\perp}-E_{12}^{\perp\perp}$ (×10⁻⁶ Ryd.)

Fig.5.2

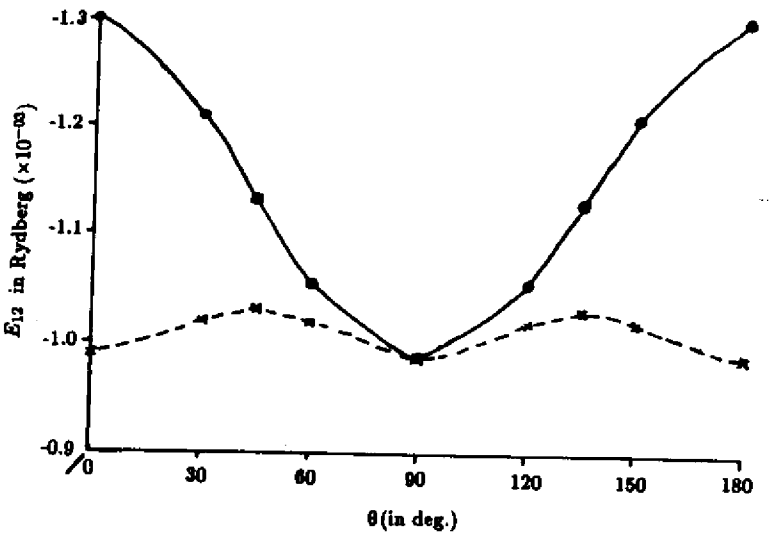
-1.3
-1.2
-1.1
-1.0
-0.9
0
30
60
90
120
150
180
θ(in deg.)
E_{12} in Rydberg (×10⁻⁰³)

Fig.5.3

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