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Ruderman-Kittel-Kasuya-Yosida Spin Polarization in a Strongly Perturbed Medium and Applications to Hyperfine Fields

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Hyperfine fields at normal impurities in ferromagnetic metals and alloys vary systematically in sign and magnitude. These results are explained by an extension of Ruderman-Kittel-Kasuya-Yosida spin polarization to the case of an electron gas with a strong local perturbation.

The hyperfine field at *sp* impurities in the ferromagnetic metals has attracted considerable attention since it was shown experimentally that the fields were systematically negative for elements in the first half of an *sp* series and positive for elements in the second half. It has been a bone of contention whether the observed positive fields can be explained by purely conduction-electron effects[1,2] or whether it is necessary to invoke a direct overlap mechanism between host *d* orbitals and *s* states on the impurity.[3,4]

Recently, a number of results have been obtained[5-11] for the hyperfine fields at the *sp* sites *Y* in the Heusler alloys X_2MnY, Table I. Although the results are rather incomplete, it appears that a crossover occurs from negative to positive fields when the element *Y* is in the middle of the *sp* series, as for *sp* impurities in Fe or Ni hosts.[12] For the Heusler compounds the *Y* site has no magnetic nearest neighbors, so any direct overlap would be small; the change in sign of the field appears to be a purely conduction-electron effect.

The results can be compared with the model of Caroli and Blandin[13] which has been widely used in interpreting experimental data. In this model, the conduction-electron band is taken as free-electron-like with an effective number of electrons per atom equal to the average over all sites. A *d* resonance at each Mn site leads to spin-density oscillations, and summing over the contributions from different Mn sites around a given nonmagnetic atom leads to a prediction for the hyperfine field at that site. While predictions for *X* sites are good, fields at *Y* sites are generally expected to be negative and to vary little with the effective charge on the *Y*-site element, in disagreement with experimental results, Table I.

A weakness of the model is that the charge screening at the nonmagnetic site is not included explicitly[14]; this has little importance for nuclei such as Cu on *X* sites, but may be very important for *Y* sites where the effective charge is large. Here we calculate the two-impurity problem in order to show the effect of the charge screening at the nonmagnetic site on the polarization at that site. This calculation is an extension of the Ruderman-Kittel-Kasuya-Yosida (RKKY) approach to an electron gas with a strong perturbation, in the same spirit as the calculation of Daniel and Friedel.[1]

The conduction electrons will be considered as free-electron-like with Fermi wave vector k_F. A normal impurity at the origin has a spin-independent spherical potential $V_0(r)$ [with $V_0(r)=0$ for $r>r_0$] giving rise to phase shifts δ_l. This potential will not be treated within the Born approximation, but its effect will be treated exactly

TABLE I. Hyperfine fields for series of Y-site atoms in Heusler-alloy hosts. The experimental values are the only cases we are aware of in which the fields on more than one element on a Y site have been measured. The calculated hyperfine fields are from Eq. (8), summing over three Mn neighbor shells and normalizing to 300 kG for Sb.

	Experimental H_{eff} (kG)			Calculated H_{eff}
Y-site atom	Cu_2MnIn host	Ni_2MnSb host	Pd_2MnSb host	Cu_2MnIn host
Ag				− 230
Cd	− 147 [a]			− 180
In	− 93 [b]			− 25
Sn	+ 200 [c]	+ 45 [c]	± 30 [d]	+ 185
Sb		+307 [e]	+580 [e]	+ 300
Te				+ 180

[a] Ref. 11.
[b] Ref. 6.
[c] Ref. 8.
[d] Sn in Pd_2MnSn has a field of − 35 kG, see Ref. 8.
[e] Ref. 9.

through considering the phase shifts explicitly. A magnetic impurity at $\vec{R}_0$ interacts with the conduction electrons through the effective s-d exchange $W = -J\delta^3(\vec{r} - \vec{R}_0)\vec{s}\cdot\vec{S}$. The spin-dependent potential will be treated within the Born approximation which is reasonable if we accept the usual estimates for J. Within this approximation and for a polarized impurity spin $\langle S_z\rangle$, the conduction-electron polarization produced *at the origin* is identical to that produced by a potential shell on a sphere of radius R_0:

$$W'(r) = -\tfrac{1}{2}\sigma\epsilon\delta(r - R_0), \tag{1}$$

where $\sigma = \pm 1$ for conduction electron spin $s_z = \pm\frac{1}{2}$ and $\epsilon = J\Omega_0\langle S_z\rangle/4\pi R_0^2$. The hyperfine field at the center site depends only on the spin density at $\vec{r} = 0$ and so only upon s scattering.

With a spherical potential, s-wave functions are

$$\Psi_k = \frac{1}{\sqrt{4\pi}}\frac{y_k(r)}{kr},$$

behaving as

$$\frac{a_k}{\sqrt{4\pi}}\frac{\sin[kr + \delta_0(k)]}{kr}$$

for r in the region $V(r) = 0$. Using Friedel's arguments,[15] renormalizing in a sphere of radius R gives

$$a_k^2 = 2k^2(R + d\delta_0/dk)^{-1}$$

with allowed values of k given by $\sin(kR + \delta_0) = 0$ or $kR + \delta_0 = n\pi$. Consecutive values of k are separated by $\Delta k = \pi/(R + d\delta_0/dk)$.

If we call $\varphi_k(r)$ the function behaving as $(4\pi)^{-1/2}\times\sin(kr + \delta_0)/kr$ for large r, then the total density of states per unit k

$$\rho_k(r) = \pi^{-1}(R + d\delta_0/dr)|\Psi_k(r)|^2 = (2k^2/\pi)|\varphi_k(r)|^2. \tag{2}$$

In particular at $r = 0$

$$\rho_r(0) = (2k^2/\pi)|\varphi_k(0)|^2. \tag{3}$$

The variation of the normalizing factor cancels the variation of the density of states with k (cf. the Van Laue theorem[15]).

With the spin-dependent potential

$$V_0(r) \mp \tfrac{1}{2}\epsilon\delta(r - R_0),$$

the wave function $\varphi_k{}^\sigma$ will behave as

$$(\sqrt{4\pi}\,kr)^{-1}\sin(kr + \delta_0 + \varphi_\sigma) \text{ for } r > R_0$$

and as

$$(1 + b_\sigma)[(\sqrt{4\pi}\,kr)^{-1}\sin(kr + \delta_0)] \text{ for } r < R_0.$$

From continuity of the wave function and the discontinuity of its first derivative (due to the δ-type potential) at R_0, we obtain

$$(1 + b_\sigma)\sin x = \sin(x + \varphi_\sigma),$$

$$k(1 + b_\sigma)\cos x = k\cos(x + \varphi_\sigma) + \sigma\epsilon\sin(x + \varphi_\sigma),$$

respectively, where $x = kR_0 + \delta_0$. For small ϵ,

$$b_\sigma = (\sigma\epsilon/2k)\sin(2kR_0 + 2\delta_0).$$

Hence the spin density per unit k at $r = 0$ is

$$\rho_k{}^\sigma(r = 0) = (2k^2/\pi)|\varphi_k{}^\sigma(0)|^2 = (2k^2/\pi)|\varphi_k(0)|^2(1 + b_\sigma)^2. \tag{4}$$

The total spin density at $r=0$ is for small ϵ

$$m_{R_0}(r=0)=\int_0^{k_F}(\rho_k{}^{+}-\rho_k)$$
$$=\frac{4\epsilon}{\pi}\int_0^{k_F}|\varphi_k(0)|^2\sin(2kR_0+2\delta_0)k\,dk. \quad (5)$$

This result is exact for R_0 greater than r_0, the range of the potential $V_0(r)$; it represents an extension of the RKKY spin polarization for a perturbed medium. When $V_0(r)=0$ everywhere, then $\delta_0=0$ and $\varphi_k(0)=1/\sqrt{4\pi}$, and the expression reduces to the usual RKKY result. It should be noted that the exact result (5) depends only on the s wave function $\varphi_k(r)$ and the s phase shift $\delta_0(k)$. One can in principle calculate numerically $m(r=0)$ for given $V_0(r)$. For the present discussion we will simply keep the leading term in powers of $R_0{}^{-1}$, obtained by integration by parts:

$$m_{R_0}(r=0)=-\frac{k_F}{2\pi^2}J\Omega_0\langle S_z\rangle|\varphi_{k_F}(0)|^2$$
$$\times\cos(2k_FR_0+2\delta_0{}^F)/R_0{}^3. \quad (6)$$

Equations (5) and (6) are the main results of this paper; they show that for fixed R_0 the polarization at the center site $m(r=0)$ will oscillate with phase $2\delta_0{}^F$. Going across a series of sp impurities in any given host, $2\delta_0{}^F$ will change giving negative and positive hyperfine fields. The crossing point as a function of Z will depend on the host, but the change in sign should be a general feature.

The hyperfine field will be the sum of contributions over neighboring magnetic sites,

$$H_{\rm eff}=\tfrac{1}{3}8\pi\mu_B\sum_i m_{R_0{}^i}(r=0). \quad (7)$$

For the same impurity in a similar host where there are no magnetic sites, the Knight shift is

$$K=\tfrac{1}{3}8\pi\mu_B{}^2(4k_F/\pi)|\varphi_{k_F}(0)|^2.$$

So the hyperfine field in the magnetic alloy can be related to K by

$$H_{\rm eff}\simeq-\frac{J\Omega_0K}{8\pi\mu_B}$$
$$\times\left(\sum_i\langle S_z(R_0{}^i)\rangle\frac{\cos(2k_FR_0{}^i+2\delta_0{}^F)}{(R_0{}^i)^3}\right). \quad (8)$$

To compare explicitly with the experiments in Heusler alloys we will assume as in Ref. 13 that k_F is fixed by the overall average number of electrons per atom; the Y-site effective charge is the difference relative to this background (e.g., for In in Cu_2MnIn, $Z_{\rm eff}=3-\frac{6}{4}=1.5$). We will also assume $\delta_1=\delta_0$ so that $2\delta_0=\pi Z_{\rm eff}/4$. Using experimental Knight shift values for sp impurities in Cu, Ag, and Au[16] as a guide and normalizing to 300 kG for the field on Sb (which leads to a reasonable value for J), we give estimated hyperfine fields for the impurities at Y sites in Cu_2MnIn, Table I. The calculated values show the same general behavior as the experimental results, with the oscillating dependence of $H_{\rm eff}$ on $Z_{\rm eff}$. For different Heusler-alloy hosts the phase and amplitude of the oscillation will change somewhat, but the overall sinusoidal form should be observed in each case. The model predicts essentially the general form of the results which can be expected for a series of impurities in a given host rather than accurate values for single systems, as the parameters of the model, particularly k_F, are phenomenological. Thus if we estimate that in Ni_2MnSb and Pd_2MnSb the Sb contributes 5 electrons and the Pd or Ni 0.5 electrons to the conduction band, the predictions for the Y-site fields in these two hosts would be identical to those in Cu_2MnIn. That the observed fields are not precisely the same is not surprising, particularly as an estimate of the effective number of conduction electrons from a transition-metal site (Pd or Ni) is very approximate.

In Fe and Ni hosts the hyperfine fields on sp impurities clearly follow a similar pattern; we suggest that this is because the conduction-electron polarization mechanism again dominates. It should be possible to analyze hyperfine fields in rare-earth compounds with normal metals in the same manner. More detailed calculations and comparisons with experiment will be published elsewhere.

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Measurement and Miscroscopic Analysis of the Reactions ^{6}Li(^{6}Li, ^{6}Li*(3.56))^{6}Li*(3.56) and ^{6}Li(^{6}Li, ^{6}He)^{6}Be†

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Angular distributions and an excitation function have been measured for the reactions ^{6}Li(^{6}Li, ^{6}Li*(3.56))^{6}Li*(3.56) and ^{6}Li(^{6}Li, ^{6}He)^{6}Be at laboratory bombarding energies between 28 and 36 MeV. A microscopic distorted-wave Born-approximation analysis which includes the tensor interaction and exchange gives good agreement with the data, except at forward angles, and predicts the correct magnitude of the cross sections. Estimates of the strengths of the effective Majorana and spin-tensor isospin interactions are given.

The reactions ^{6}Li(^{6}Li,^{6}Li*)^{6}Li* and ^{6}Li(^{6}Li, ^{6}He)^{6}Be proceed to three members of the same $T=1$ isospin multiplet. Naive charge independence would predict identical differential cross sections, but Coulomb distortions and other effects produce significant differences. (Here ^{6}Li* indicates the $T=1$, $J^\pi=0^+$ state at 3.56 MeV excitation in ^{6}Li.) The wave functions[1] of the isomultiplet states have a configuration which is nearly identical to the ^{6}Li ground state except for a different spin-isospin coupling of the $1p$-shell nucleons, and it is expected that these reactions are quasielastic.[2-4] Thus such reactions can be analyzed microscopically to obtain information on the spin-isospin–dependent effective nucleon-nucleon interaction in finite nuclei, in the same spirit as similar analyses of inelastic and charge-exchange reactions such as (p,p'), (p,n), and $(^3\mathrm{He}, t)$.[5] In the present work we have studied these Li + Li induced reactions, measuring angular distributions and excitation functions at laboratory bombarding energies between 28 and 36 MeV, and have analyzed the data with distorted-wave Born-approximation (DWBA) calculations employing microscopic form factors, as will be discussed below.[2]

The experiment was performed using ^{6}Li^{+++} beams from the FN tandem Van de Graaff incident upon self-supporting targets of 80–300 μg/cm^2 thickness. The two reactions were measured simultaneously by observing both ^{6}He and ^{6}Li in the same ΔE-E detector telescope. The ^{6}Li*, which is detected after it undergoes photon decay, is required to be in fast coincidence with the recoil ^{6}Li* detected in a recoil counter. To assure a high coincidence efficiency, a major problem at forward angles, the recoil-detector solid angle was chosen as large as 0.045 sr which was up to 1000 times the telescope solid angle. Before and after each measurement the coincidence efficiency for the elastic scattering was measured at the same recoil energy as in the measurement of ^{6}Li(^{6}Li,^{6}Li*)^{6}Li*; the recoil energies were chosen to be equal so that we could accurately monitor the multiple scattering of the recoil ^{6}Li in the target. This was important for recoil energies less than 3 MeV. We then did a series of calculations using our measured elastic coincidence efficiency to determine our inelastic coincidence efficiency. The differences between the two efficiencies arose solely from kinematics and the decay of each ^{6}Li* which were known exactly. The calculated inelastic efficiencies varied between 70% and 99.9% and were greater than 90% at nearly all angles greater than $\theta_{\mathrm{c.m.}} = 20°$. The absolute cross sections were obtained by normal-