SPIN SUSCEPTIBILITY OF CONDUCTION ELECTRONS IN IRON

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Hyperfine field measurements[1] at neighboring sites of nonmagnetic solute atoms in Fe allow, for the first time, an experimental determination of the conduction-electron spin susceptibility function $\chi(q)$. Analysis indicates that $\chi(q)$ has a large maximum at the wave vector $q = 2k_F$, and that indirect exchange interactions between localized $3d$ spins via the $4s$ conduction band are antiferromagnetic for nearest-neighbor and second-neighbor pairs.

The theory of indirect exchange interactions, $J_{ab}(R)\vec{S}_a\cdot\vec{S}_b$, between localized spins $\vec{S}_a$ and $\vec{S}_b$ separated by $\vec{R}$ in a metal, provides an expression for the numerical coefficient, $J_{ab}(R)$:

$$J_{ab}(R) = \text{const}\int\chi(q)F_a(q)F_b(q)\cos\vec{q}\cdot\vec{R}\,d^3q. \quad (1)$$

The usual derivations[2] of $J_{ab}(R)$ are equivalent to using $\chi_0(q)$ for $\chi(q)$, where $\chi_0(q)$ is the spin susceptibility function of a noninteracting electron gas,

$$\chi_0(q) = \chi_p\left[\tfrac{1}{2} + \frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right|\right], \quad (2)$$

χ_p being the Pauli susceptibility and $x = q/2k_F$. A derivation of Eq. (1), which includes the effects of conduction-electron interactions, has been given.[3] One object of this paper is to emphasize the significant difference between $\chi(q)$ and $\chi_0(q)$. They are shown in Fig. 1. The functions $F_a(q)$ and $F_b(q)$ in Eq. (1) are magnetic form factors which correspond to the finite spatial distribution of each localized spin. The hyperfine field measurements determine $J_{ab}(R)$ directly, so $\chi(q)$ can be obtained by Fourier inversion.

Employment of Eq. (1) to interpret experimental results in Fe involves, of course, many oversimplifications. First of all, the result depends on the validity of perturbation theory, which in this case requires that s-d exchange interactions be small relative to the conduction-electron Fermi energy, $h^2k_F^2/2m^*$. This ratio is expected to be ~0.1, which seems sufficiently small. The observed[1] additivity of hyperfine fields arising from several neighbors gives assurance in this regard, since additivity would not apply to higher order corrections. The derivation of (1) is understood to be within the framework of effective mass theory, and the result is appropriate to a single spherical, parabolic, unpolarized conduction band. Finally, the exchange-scattering matrix elements that arise in the theory are functions of $\vec{k}$ and $\vec{k}'$, not merely of $q = |\vec{k}'-\vec{k}|$. The use of the magnetic form factors, e.g., $F_a(q)$, as a pragmatic approximation is to some extent justified by the fact that the exchange-scattering matrix elements reduce to magnetic form factors for short-range interactions, and also by the fact that the results described below are insensitive to $F_a(q)$, reasonably chosen.

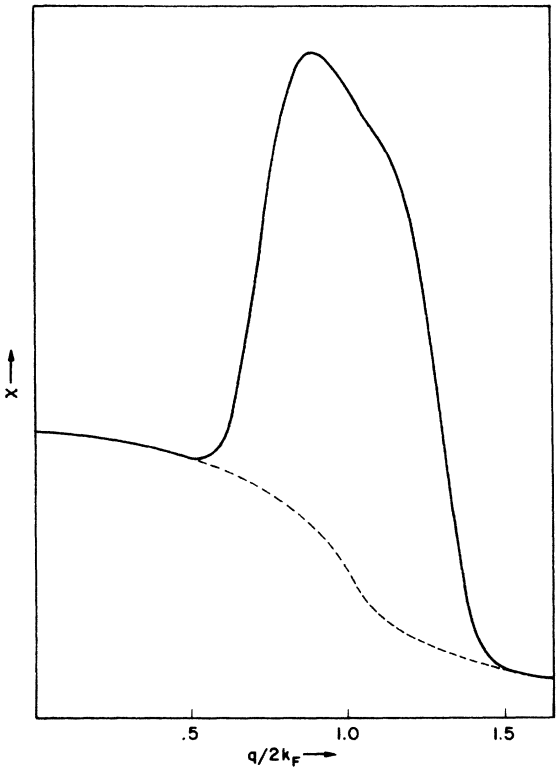

FIG. 1. Spin susceptibility χ vs $q/2k_F$. The dashed curve is χ_0, the susceptibility function of a noninteracting electron gas. The solid curve is $\chi(q)$ according to Eq. (4) of the text, which provides a best fit to the hyperfine field deviation data in Fe.

The interpretation of the hyperfine field deviations[1] surrounding a nonmagnetic solute which we propose is that they arise primarily from the indirect exchange interaction via the s band between an (absent) Fe electron spin ($S \approx 1$) and a

neighboring Fe nuclear spin. Since the latter coupling is of the Fermi contact type, $F_b(q)$, say, is independent of q, and can be removed from the integral in (1) and absorbed into the numerical constant, which includes as well all other unknown multiplicative factors. The hyperfine field deviation data, proportional to $J_{ab}(R)$, for the Fe-Al system are shown in Fig. 2, plotted in percent of the pure Fe hyperfine field, $H = -330$ kG. It is very important to determine the value of $J_{ab}(R)$ for $R = 0$, which is the contribution to H at an Fe nucleus arising from the conduction-electron polarization attributable to the electron spin of that same atom. Fortunately, the allowable range for the value of $J_{ab}(0)$ is relatively small, as shown below.

The major contributions[4] to H in Fe are from the core polarization, $H_c \sim -400$ kG, the unquenched $3d$ orbital contribution, $H_L \sim +70$ kG, and the $4s$ conduction-band polarization, $H_{4s} \sim +100$ kG. Since they do not sum to the observed H, one or more of these estimates need revision. Our present interest is confined to $H_{4s}/|H|$, which is accordingly ~30%. The net $4s$ spin polarization in a given unit cell can be attributed to the sum of $4s$ spin-density contributions in that cell

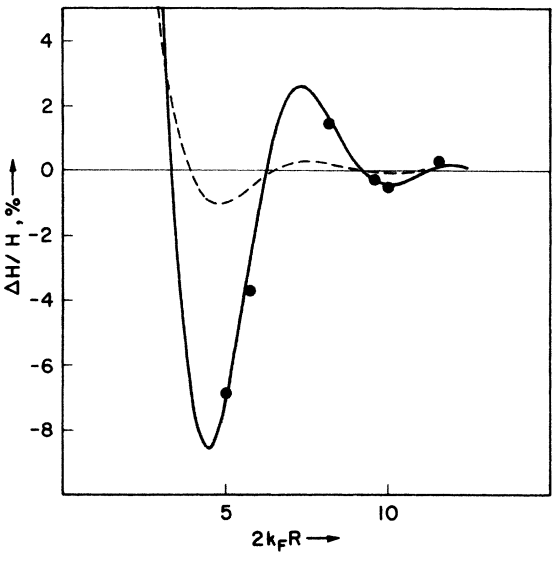

FIG. 2. Indirect exchange interaction between an Fe atomic spin and an Fe nuclear spin vs $2k_FR$. The points are the experimental values, in percent of the pure Fe hyperfine field, for the first six nearest-neighbor distances, from Stearns and Wilson. The dashed curve (abscissa values should be multiplied by 1.2) is the predicted interaction for $\chi = \chi_0$. The solid curve corresponds to the spin susceptibility function, Eq. (4) of the text.

arising from the s-d exchange coupling with each localized Fe spin in the lattice, including the spin of the cell in question. (Van Vleck[5] has shown that interactions arising from the net polarization of the conduction band are included appropriately in the theory of indirect exchange interactions.) The measured hyperfine field deviations arising from first through sixth nearest neighbors sum to −70% of $|H|$, which can be verified from the data in Fig. 2, taking account of the multiplicity (8, 6, 12, 24, 8, 6) of those neighbors. Consequently, the (unmeasured) contribution of the central atom must be taken to be

$$J_{ab}(0)/|H| \approx +100\%, \tag{3}$$

in order that the total $H_{4s}/|H|$ be about 30%. The leverage on this estimate is quite favorable, since the value of (3) would be reduced only to 70% if the total H_{4s} were presumed to be 0.

One may now take any assumed functional form for $\chi(q)$, compute $J_{ab}(R)$, using (1), normalize the result in conformity with (3), and adjust the scale of R to give the best fit to the experimental data. We have carried out this program for an extensive set of $\chi(q)$, employing the measured[6] $3d$ form factor of Fe for $F_a(q)$. The computed $J_{ab}(R)$ corresponding to the noninteracting electron gas $\chi_0(q)$, Eq. (2), is shown by the dashed curve in Fig. 2. The amplitude of this curve at the observed R is too small by a factor of 7. (Renormalizing the curve by such a factor would require, in accordance with the argument given above, that $H_{4s} = +2\times10^6$ G, 20 times larger than the upper limit quoted above.) Wolff[7] has shown that $\chi(q)$ for an electron gas with δ-function interactions is given by $\chi_0(q)/[1-\gamma\chi_0(q)]$, where γ is proportional to the strength of the interaction. The computed $J_{ab}(R)$ for this functional form, with values of γ between 0 and χ_p^{-1}, manifests an even greater discrepancy with experiment.

It has been shown[8] that $\chi(q)$, computed in Hartree-Fock approximation, for Coulomb interactions has a sharp maximum at $q = 2k_F$. Consequently, we carried out the above analysis for $\chi(q) = \chi_0(q) +$ (a bell-shaped function centered at $x \equiv q/2k_F = 1$). Lorentzian or Gaussian forms did not permit as good a fit as that given by

$$\chi(q) \sim \chi_0(q) + \alpha\chi_p \exp[-\beta^4(x-1)^4]. \tag{4}$$

The solid curves in Figs. 1 and 2, which fit the data relatively well, are those given by (4) with $\alpha = 1.7$, $\beta = 3.25$. The Fermi radius, k_F, is accurately determined by the scale adjustment in

R, and is

$$k_F = 1.01\times10^8 \text{ cm}^{-1}, \quad (5)$$

which yields a value 0.41 for the 4s conduction electron/atom ratio. The appreciable width of the bell-shaped term in (4) is surprising, and may possibly be attributed to the nonsphericity of the conduction-electron Fermi surface or to inaccuracies of the underlying theoretical model, employed in the analysis. A number of other functional forms for $\chi(q)$ were tried. We are convinced that the essential features of the solution presented here are implied by the data.

A striking conclusion that must be drawn from the form of the derived $\chi(q)$ is that indirect exchange interactions in Fe via the 4s conduction band are strongly antiferromagnetic. (This feature is actually directly apparent from the ΔH data for nearest and next-nearest neighbors, which, being negative, imply a 4s polarization opposite to that of the central atom. It can be established quantitatively by employing Eq. (9) of reference 3.) The origin of ferromagnetism in Fe must be sought elsewhere. A promising solution to this puzzle has been found and will be presented later.

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SEARCH FOR NEUTRAL LEPTONIC CURRENTS IN K^+ DECAY*

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A basic assumption of most present models of the weak interaction is that primitive neutral leptonic currents, to first order in the weak coupling constant, do not exist.[1] However, some models propose the existence of neutral nonleptonic currents in order to explain the $|\Delta T| = \frac{1}{2}$ rule.[2] Recently it has been suggested that primitive neutral leptonic currents of strength comparable to that of charged currents might exist, but some reactions where they would appear could be inhibited by selection rules among the strongly interacting particles.[3] Even if primitive neutral currents do not exist, the combined effects of weak and electromagnetic interactions can cause induced neutral currents which may be observable.[4,5]

In order to look for evidence of neutral currents in strangeness-changing interactions, the possible decay mode

$$K^+ \to \pi^+ + e^+ + e^- \quad (1)$$

has been searched for in a sample of 1.7×10^6 stopped-K^+ decays. The K^+ mesons were stopped in the Lawrence Radiation Laboratory 30-inch heavy-liquid chamber filled with C_3F_8. No unambiguous events have been found corresponding to decay mode (1).

The detection procedure consisted of initially scanning for three-track decays that were not examples of the ordinary τ decay of the K^+. About two thirds of the film was scanned twice. Each event was then carefully looked at again on the scanning table and was classified in one of the following three categories: (a) ordinary Dalitz pair with obvious missing momentum; (b) apparent momentum-conserving event; (c) electron pairs which converted very near the K^+ decay.

The events in categories (a) and (b) were used to compute the absolute scanning efficiency from the number of Dalitz decays expected. About