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Determination through symmetry arguments of the various contributions to the self polarisation field at rare earth nuclei in cubic compounds

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Résumé. — La R.M.N. des noyaux de terre rare dans les composés cubiques TR-X₂ a montré que le champ de self polarisation, Hₛₛ, contribue notablement au champ total hyperfin au niveau des noyaux. Les interactions d'échange anisotropes entre les moments magnétiques ordonnés des terres rares et les électrons de conduction donnent lieu à des polarisations à la fois orbitales et de spin des bandes de conduction. Ces polarisations se reflètent ensuite dans Hₛₛ par l'intermédiaire des interactions hyperfines orbitales, dipôle-dipôle magnétique et de contact ou de polarisation de cœur. Vu la complexité du problème, on utilise des arguments de symétrie pour déterminer les paramètres indépendants du problème.

Abstract. — NMR of the rare earth nuclei in cubic RE-X₂ compounds has shown that the self polarisation field, Hₛₛ, gives an important contribution to the total hyperfine field at the RE nuclei. Both orbital and spin polarisations of the conduction bands arise through anisotropic exchange interaction between the ordered magnetic moments of the rare earth and the conduction electrons. These polarisations are further reflected through orbital, magnetic dipole dipole and contact or core polarisation terms in Hₛₛ. Due to the complexity of the problem, group symmetry arguments are used to determine the independant parameters of the problem for cubic compounds.

In a recent publication [1], we studied the nuclear magnetic resonance of RE nuclei in RE Al₃ compounds. The hyperfine field at the nucleus of a RE ion in this ordered system is usually assumed composed of three terms

\[ H_N = H_{4f} + H_{sp} + H_{nn} \]  

where \( H_{4f} \) represents the field created by the 4f electrons and is proportional to the magnetic moment of the 4f shell; \( H_{4f} \) is of the order of several Mega Oe. \( H_{nn} \) is the transferred hyperfine field at the nucleus under study arising from polarisation of the conduction electrons by other magnetic ions; it is usually small, of the order of 10 kOe. We focus our attention here on \( H_{sp} \), the self polarisation field arising from polarisation by 4f electron-conduction electron exchange which reflects itself through hyperfine interaction of these conduction electrons with the RE nucleus. It was found that \( H_{sp} \) varies from 200 kG for GdAl₃ to 1 000 kG for ErAl₂.

The first attempts to understand the experimental results have shown [1] that \( H_{sp} \) could not be interpreted through spin polarisation only and that one must include orbital polarisation effects. The orbital polarisation of the 5d band at the RE site is considerable. A phenomenological and crude approach including these effects led us to try to fit the experiments with a self polarisation field given by [1], [2]

\[ H_{sp} = a \langle S_z \rangle + b \langle L_z \rangle \]  

where \( \langle S_z \rangle \) and \( \langle L_z \rangle \) are the average values of the total spin and angular momentum of the RE ion. These two terms result from the spin polarisation of the 5d and 6s conduction electrons and from the orbital polarisation of 5d electrons respectively.

Although great improvement is obtained by including the \( \langle L_z \rangle \) term, the agreement is not perfect and some difficulties arise with the light RE (PrAl₂, NdAl₂).

A more sophisticated model taking into account correctly the microscopic form of the exchange interactions between the 4f and the conduction electrons, a calculation of the spin and orbital polarisation of the conduction bands and a detailed analysis of the hyperfine interactions between the conduction electrons and the RE nucleus is thus necessary. Quite generally, \( H_{sp} \) may be written [3], [4] as

\[ H_{sp} = A \langle L_z \rangle - \sqrt{10} (s \times c)^1_o \rangle_d + B \langle s_z \rangle_d + C \langle s_z \rangle_s \]  

where in the right side of (3), the first term represents the magnetic orbital and dipole-dipole interaction between the 5d conduction electrons and the RE nucleus, the second term arises from the core polarisation due to the same 5d electrons and the third term comes from the contact interaction of the 6s conduction electrons. In (3) only the \( z \) component of the conduction electron operators is involved because the self-polarisation hyperfine interaction may be consi-
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where the \( \varphi_i \) (\( i = 1, \ldots, 5 \)) are the \( t_{2g} \) or \( e_g \) orbital 5d states considered \([5]\) as band states and \( m_l \) refer to the spin state of the d electron (in the particular case of \( 5 \)) we have necessarily \( i = j \). \( S(\varphi_i, \varphi_j) \) is a generalized susceptibility \([5] \). For d electrons in cubic symmetry we have only three independent terms \( S(t, t), S(t, e) \) and \( S(e, e) \). These susceptibilities depend on the bandwidth and on the splitting between the \( t_{2g} \) and the \( e_g \) states. They will be considered as independent of the RE in a given series.

As \( s \) transforms like \( \Gamma_d \), only the combinations of \( \langle Y^*_m(L) S \rangle \) transforming themselves according to the same representation are involved. Furthermore only invariant combinations of \( Y^*_m(l) \) must occur.

Then when the magnetization direction of the RE ion is along a fourfold axis of the cube, we obtain:

\[
\langle s_z \rangle_d = \frac{a_0 b_0}{\sqrt{5}} \left[ 3 S(t, t) + 2 S(e, e) \right] + \frac{a_4 b_4}{2} \left[ \left( \frac{7}{10} Y_{40}(L) + \frac{1}{2} Y_{44}(L) \right) \langle \sigma_{x4} \rangle \right] + \frac{1}{2} \left[ \langle Y_{4-4}(L) \rangle S_{z} \right] \left[ S(t, t) - S(e, e) \right].
\]

Using the same kind of arguments, the average values of \( \langle \langle \langle l_z \rangle_d, \langle s_z \rangle_d \rangle \) and \( \langle \langle s \times C^2 \rangle_d \rangle \) have been derived both when the magnetisation direction of the RE is along a fourfold (\( \text{PrAl}_2, \text{NdAl}_2, \text{DyAl}_2 \)) or a threefold (\( \text{ErAl}_2, \text{TbAl}_2 \)) direction of the local cube.

It is then necessary to project the operators \( Y^*_m(L) S_{z} \) on to the \( Y_{40}(L) \) operators. From (6) we obtain for example

\[
\langle s_z \rangle_d = \frac{a_0 b_0}{\sqrt{5}} \left[ 3 S(t, t) + 2 S(e, e) \right] \langle Y_{10}(J) \rangle + a_4 b_4 \left[ S(t, t) - S(e, e) \right] \times \left\{ \frac{2}{3} \sqrt{7} N_3 \left\langle Y_{30}(J) \right\rangle + \frac{1}{3} \sqrt{7} N_5 \left\langle Y_{50}(J) \right\rangle + \frac{1}{2} \sqrt{5} N_5 \left( \left\langle Y_{54}(J) + Y_{5-4}(J) \right\rangle \right) \right\}.
\]

In (7) the average values are taken over the single ion ground state. \( N_1, N_3 \) and \( N_5 \) are numerical recoupling factors depending on \( L, S, J \) defined in ref. \([5]\).

The presence of terms like \( \langle Y_{10}(J) \rangle, \langle Y_{30}(J) \rangle \), etc., is easily predictable through group symmetry arguments. The same procedure was performed for evaluating \( \langle l_z \rangle_d \) and \( \langle s \times C^2 \rangle_d \) for both possible directions of the magnetisation.

Assuming that the exchange parameters \( a_4 \) do not vary significantly across the rare earth series, we are thus able to calculate \( H_{sp} \) for all rare earths using 6 independent parameters \( A, B, C \) and \( S(t, t), S(t, e) \) and \( S(e, e) \). The fit with the series (\( \text{RE Al}_2 \)) and (\( \text{RE Zn} \)), where important orbital effects appears to be present \([1]\), is under investigation. We are also studying the variation of \( H_{sp} \) versus temperature in order to estimate the magnitude of anisotropic exchange which leads to terms proportional to \( J^3_{z} \) and \( J^5_{z} \).