IC/84/141
INTERNAL REPORT
(Limited distribution)

International Atomic Energy Agency
and
United Nations Educational Scientific and Cultural Organization

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

MUON ZERO POINT MOTION AND THE HYPERFINE FIELD IN NICKEL *

M.E. Elzain **
International Centre for Theoretical Physics, Trieste, Italy.

ABSTRACT

It is argued that the effect of zero point motion of muons in Ni is to induce local vibrations of the neighbouring Ni atoms. This local vibration reduces the Hubbard correlation and hence decreases the net spin per atom. This acts back to reduce the hyperfine field at the muon site.

MIRAMARE - TRIESTE
September 1984

* To be submitted for publication.

** Permanent address: Department of Physics, Faculty of Science, University of Khartoum, Sudan.

I. INTRODUCTION

In recent years the muon spin rotation (μSR) technique has been applied to determine the internal fields in magnetic materials. These fields are determined from the precession frequency of the decaying spin polarized muons [1]. A muon could be considered as a light proton of mass of order 1/9 proton mass.

The magnetic field B_μ seen by the muon in the limit of zero applied field is

$$B_\mu = B_{hf} + \frac{4\pi}{3}M + B_d \qquad (1)$$

where B_{hf} is the hyperfine field, B_d the field due to the local dipole moments inside a sphere centred on the muon site and $\frac{4\pi}{3}M$ is the Lorentz field [2].

In the fcc Ni the muon occupies an octahedral site and hence B_d and the Lorentz fields are zero because of the cubic symmetry. The muon spends all its lifetime (2.2 μs) on this site [3]. At the non-cubic interstitial tetrahedral or octahedral sites in bcc Fe, the dipolar fields seen by muons are averaged to zero because of the rapid diffusion between crystallographically equivalent but magnetically inequivalent sites [4]. Hence, for both Ni and Fe the net field seen by the muons is B_{hf} if the external field is zero.

In the following we shall give,brief,summaries of the electronic structures of muons and the origin of the hyperfields at muon sites in Secs.II and III respectively. In Sec.IV we will outline the effect of the muon zero point motion on the hyperfine field and conclude in Sec.V.

II. ELECTRONIC STRUCTURE

The electronic structure of muons is rather complicated and a number of theories have been developed. For muons in simple metals non-linear screening has been used in the jellium model [5]. However, for the transition metals the proper band structure needs to be taken into account. Calculations have been performed using the KKR Green function technique [6], embedded cluster models [7] and phenomenological pseudopotential models [8]. The general finding is that the proton forms a deep covalent bonding state with the 3d electrons.

The Hamiltonian of an electron of spin σ in a ferromagnetic metal containing a muon is

$$H = -\frac{1}{2}\nabla^2 + V_\sigma[\underline{r};\underline{R}|\{\underline{R}_m\}] \quad (2)$$

where $\underline{r}$ denotes the position of the electron, $\underline{R}$ that of the muon and $\{\underline{R}_m\}$ that of the ferromagnetic host atoms. The potential contains electron-ion interaction as well as electron-electron repulsion, exchange and correlation terms. In KKR and cluster methods the muon and lattice motions are frozen while in the pseudopotential model [8] these are taken into account. However, in [8] the electron-phonon interaction is not considered. From these calculations the electronic density of states and hence the net spin density at the muon site is determined.

The hyperfine field at the muon site is given by

$$B_{hf} = \frac{8\pi}{3}\mu_B[n^{\downarrow} - n^{\uparrow}] \quad (3)$$

where μ_B is the Bohr magneton and $(n^{\uparrow} - n^{\downarrow})$ the net spin density at the muon site. The hyperfine field is negative indicating that $n^{\downarrow}$ is greater than $n^{\uparrow}$.

The KKR method [6] gave a result for B_{hf} in Ni which agrees with the experimental value. The experimental value for Ni is - 0.07 T. The more ab initio embedded cluster method gave a value of - 0.13 T [7]. The pseudopotential model [8] has parameters that can be varied to obtain a reasonable result. However, in general the pseudopotential model does not work very well for Ni [8].

III. ORIGIN OF THE HYPERFINE FIELD

In the screening theories the hyperfine field is assumed to result from the piling up of the polarized s-electrons in the conduction band [9]. However, the detailed solution has shown that the proton forms a bonding state with the 3d host electrons.

The net negative spin at the muon site is due to the exchange attraction between the majority d-electrons on the neighbouring muon site. The attraction leaves a net spin of opposite direction. In another model [10] it was assumed that the net spin is due to the minority 3d-electrons spreading over the muon site.

The embedded cluster method revealed that there are two contributions to the hyperfine field, B_1 and B_2. B_1 is large and negative and it is attributed to the doubly occupied (spin up, spin down) states of order 2 eV and more below the Fermi level. B_2 is positive and small and it is due to the spin up population of the higher levels.

The magnitude of the hyperfine field increases with the magnetic moment of the host. For Ni the magnetic moment per atom is 0.6 μ_B compared to Co and Fe which are 1.78 μ_B and 2.2 μ_B respectively. The measured hyperfine fields at muon sites for Ni , Co and Fe are - 0.07 T , - 0.58 T and - 1.1 T respectively. Hence a decrease of the magnetic moment per host atom may lead to a decrease in the magnitude of the hyperfine field.

IV. MUON ZERO POINT MOTION

The observation that the muon does not diffuse at low temperatures in Ni while it does in Fe [3] leads us to conclude that the effect of the muon zero point motion on the surroundings is different in the two systems. In Ni we assume the muon to be trapped in a potential well of finite extent. This will lead to a large muon momentum. While in Fe, the extension of the trapping potential is large and hence the muon momentum is low.

The vigorous oscillation of the muon in the octahedral site in Ni will make the surrounding Ni atoms vibrate. Let the amplitude of vibration at the j^{th} site be x_j and the number operator of the Ni 3d electrons be $n_{j\sigma}$. The interaction term between 3d electrons and the atomic vibrations is

$$H_{int} = \sum_j \lambda_j x_j (n_{j\uparrow} + n_{j\downarrow}) \quad (4)$$

where λ_j is the coupling constant. The Hamiltonian for the atomic vibrations is

$$H_a = \sum_j \left\{\frac{1}{2}M\dot{x}_j^2 + \frac{1}{2}M\omega_j^2 x_j^2\right\} \quad (5)$$

where M is the mass per atom and ω_j some characteristic frequency.

The rigid lattice Hamiltonian for 3d electrons expressed via the Hubbard model is

$$H_e = \sum_{j\sigma} \epsilon_j^{(0)} n_{j\sigma} + \sum_{j} U_j^{(0)} n_{j\uparrow} n_{j\downarrow} + \sum_{i\neq j\,\sigma} T_{ij}^{(0)} C_{i\sigma}^{\dagger} C_{j\sigma} \qquad (6)$$

where $\epsilon_j^{(0)}$ are site energies which are constant for regular lattices, $U_j^{(0)}$ are the Coulomb repulsion at j^{th} site and $T_{ij}^{(0)}$ the overlap matrix.

The total Hamiltonian is then

$$H = H_e + H_a + H_{int} \qquad (7)$$

suppose that the atomic oscillations are slow compared to the characteristic vibration so that we can ignore the kinetic term in H_a. Then we eliminate x_j from the total Hamiltonian to get

$$H = \sum_{j\sigma} \epsilon_j n_{j\sigma} + \sum_{j} U_j n_{j\uparrow} n_{j\downarrow} + \sum_{i\neq j\,\sigma} T_{ij} C_{i\sigma}^{\dagger} C_{j\sigma} \qquad (8)$$

where

$$\epsilon_j = \epsilon_j^{(0)} - \frac{1}{2} \lambda_j^2/[M\omega_j^2]$$

and

$$U_j = U_j^{(0)} - \lambda_j^2/[M\omega_j^2]$$

The effect of the lattice vibrations on the j^{th} site is to introduce an attractive interaction between electrons of opposite spin at that site. However, the net interaction is still repulsive but lower that the bare Coulomb repulsion. The reduction of the repulsive interaction will reduce the exchange splitting between the majority and minority bands:

$$\Delta_j = (n_{j\uparrow} - n_{j\downarrow}) U_j \qquad (9)$$

Hence, the filling of the bands will change leading to a local decrease of the net spin per atom and thus to the decrease of the magnetic moment per atom. Kim [11] has shown that the electron-phonon interaction may lead up to one Bohr magneton decrease of magnetic moment per atom.

Since the polarization of the electrons at the muon site depends on the net spin of the 3d electrons,the aforementioned change will lead to the lowering

of this polarization. This will lead to less negative hyperfine fields at the muon site.

V. CONCLUSIONS

It is argued that the effect of moun zero point motion in Ni would be to induce local vibrations of neighbouring atoms. This local vibration, through electron-phonon interaction reduces the repulsive Coulomb interaction on those sites resulting in the decrease of the net spin per site. The polarization of the electrons at the muon site will then be reduced and hence the hyperfine field.

This effect would be the missing element in the treatment by Estreicher and Meier [12]. Inclusion of electron-phonon interaction may lead to reasonable values of the hyperfine field and its temperature dependence.

Estimation of the electron-phonon effect could be worked out by reducing the repulsive Coulomb term in (2) by a site dependent term and using the embedded cluster method to calculate B_{hf}. This is currently under consideration.

ACKNOWLEDGMENTS

The author would like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste.

REFERENCES

[1] B.D. Patterson, Physics of Transition Metals, 55 (1980) p.645.

[2] A. Schenck, Nuclear and Particle Physics at Intermediate Energies, Nato (1975) Ed. J.B. Warren, p. [illegible].

[3] T. Yamazaki, Physica B+C, 86-88 (1977) 1053.

[4] M.B. Stearn, Phys. Lett. 47A (1974) 397.

[5] A.K. Gupta, P. Jena and K.S. Singwi, Phys. Rev. B18 (1978) 2712.

[6] H. Katamaya, K. Terakura and J. Kanamori, Sol. Stat. Comm. 29 (1979) 431.

[7] B. Lindgren and D.E. Ellis, Phys. Rev. B26 (1982) 636.

[8] S. Estreicher and P.F. Meier, Phys. Rev. B25 (1982) 297.

[9] P. Jena, Sol. Stat. Comm. 19 (1976) 45.

[10] K.G. Petzinger and R. Munjal, Phys. Rev. B15 (1977) 1560.

[11] D.J. Kim, J. Appl. Phys. 55 (1984) 2347.

[12] S. Estreicher and P.F. Meier, Hyperfine Interact. 17-19 (1984) 327.