CONF-850890-4

CONF-850890--6

DE85 014962

PHONON EFFECT ON THE TEMPERATURE DEPENDENCE
OF SPIN SUSCEPTIBILITY AND MAGNETIZATION IN METALS

D. J. Kim

Materials Science and Technology Division
Argonne National Laboratory,* Argonne, Illinois 60439
and
Physics Department, Aoyama Gakuin University, Tokyo, 157,**

and

Chikako Tanaka[†] and Shuji Ukon^{††}

Physics Department, Aoyama Gakuin University, Tokyo 157

June 1985

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Manuscript submitted to the International Conference on Magnetism,
sponsored by the Int. Union of Pure and Applied Physics, San Francisco, CA,
August 26-30, 1985.

MASTER

*Argonne National Laboratory supported by the U.S. Department of Energy.

**Permanent address.

[†]Present address: Fujitsu Laboratories, Atsugi, Kanagawa, 240-01, Japan.

^{††}Present address: Kishine Sr. High School, Kohoku-ku Yokohama, Japan.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

The submitted manuscript has been authored by a contractor of the U. S. Government under contract No. W-31-109-ENG-38. Accordingly, the U. S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for

PHONON EFFECT ON THE TEMPERATURE DEPENDENCE
OF SPIN SUSCEPTIBILITY AND MAGNETIZATION IN METALS

D. J. Kim

Materials Science and Technology Division
Argonne National Laboratory,^{*} Argonne, Illinois 60439
and
Physics Department, Aoyama Gakuin University, Tokyo, 157,^{**}

and

Chikako Tanaka[†] and Shuji Ukon^{††}

Physics Department, Aoyama Gakuin University, Tokyo 157

Abstract

In many transition metals the paramagnetic spin susceptibility χ increases with increasing temperature much beyond ordinary theories could account for. We demonstrate how the effect of the electron-phonon interactions enable us to understand such temperature dependence of χ .

^{*}Argonne National Laboratory supported by the U.S. Department of Energy.

^{**}Permanent address.

[†]Present address: Fujitsu Laboratories, Atsugi, Kanagawa, 240-01, Japan.

^{††}Present address: Kishine Sr. High School, Kohoku-ku, Yokohama, Japan.

Recently we pointed out the possible importance of the effect of the electron-phonon interaction in itinerant electron magnetism [1]. The basic idea is that in a metal the size of the change in the free energy of phonons, F_p , due to magnetization of conduction electrons can be of the same order as that in the free energy of electrons, F_e . The spin susceptibility, χ , is calculated as

$$\frac{1}{\chi} = \left. \frac{\partial^2 F_e(M)}{\partial M^2} \right|_{M=0} + \left. \frac{\partial^2 F_p(M)}{\partial M^2} \right|_{M=0}, \quad (1)$$

M being the magnetization. What we pointed out is that in the right hand side of Eq. (1) the contribution of the second term can be of the same order as that of the first term, although generally $O(F_e/F_p) \approx O(\epsilon_F/\hbar\omega_D) \approx 10^2$, ϵ_F and ω_D being respectively the Fermi energy of electrons and the phonon Debye frequency. We obtain such conclusion from a detailed considerations on the magnetization dependence of the screening of phonon frequency in a metal.

Thus we obtain the following expression for χ including the effect of the electron phonon interaction

$$\chi = \frac{2\mu_B^2 F(0)}{1 - (\tilde{V} + J_p) F(0)} \quad (2)$$

where $\tilde{V}$ is the exchange interaction between electrons,

$F(0) = -\int d\epsilon N(\epsilon) \partial f(\epsilon)/\partial \epsilon$, $f(\epsilon)$ and $N(\epsilon)$ being respectively the Fermi distribution and the electronic density of states, and

$$\begin{aligned} J_p F(0) &= J_p N(0) \\ &= L P(T/\theta_D) \hbar\omega_D/W \end{aligned} \quad (3)$$

where $N(0)$, the $T \rightarrow 0$ limit of $F(0)$, is the electronic density of states at

the Fermi surface, and

$$L(\epsilon_F, \bar{V}) = \frac{1}{2} \frac{N}{WN(0)} \left(\frac{1}{2} \left\{ \frac{N''(0)}{N(0)} - \left(\frac{N'(0)}{N(0)} \right)^2 \right\} - \bar{V} \frac{1}{1 - \bar{V}} \left(\frac{N'(0)}{N(0)} \right)^2 \right) W^2 \quad (4)$$

where N is the number of atoms in the system, $N'(0)$ and $N''(0)$ are the energy derivatives of $N(\epsilon)$ at the Fermi surface, W is a parameter to represent the width of the electron band and we put $\tilde{V}F(0) = \bar{V} \approx \tilde{V}N(0)$. The function $P(T/\theta_D)$ which determines the main temperature dependence of χ is given as

$$P(x) = \frac{3}{8} + \frac{T}{\theta_D} D\left(\frac{x}{T}\right), \quad (5)$$

where $D(x) = (3/x^3) \int_0^x dy y^3/(e^y - 1)$ is the Debye function. We find easily

that $P(T/\theta_D) = T/\theta_D$ for $T \gtrsim \theta_D/3$ and $3/8$ for $T \ll \theta_D$.

From the above, for $T \gtrsim \theta_D/3$ the spin susceptibility is rewritten as

$$\chi = \frac{2 \mu_B^2 F(0)}{(1 - \bar{V}) - (Lk_B/W) T} \quad (6)$$

We now obtain the linear T dependence in the denominator of χ which has long been sought for in order to understand the widely observed Curie-Weiss like magnetic susceptibility without invoking the presence of local moments.

The problem on which we are going to apply our new result quantitatively in this paper, for the first time, is the temperature dependence of χ of Cr above T_N [2]. Unlike in insulator magnets, in metals χ does not necessarily

decrease with increasing temperature. In nearly half of the non-ferromagnetic transition metals χ is observed to increase with increasing temperature[3]; Cr is one such example. In spite of its being a most unique feature of itinerant electron system such behavior of χ as in Cr has not been satisfactorily accounted for even with a recent elaborate consideration of spin fluctuation effect by Evangelou, Hasegawa, and Edwards [4].

In order to obtain L for Cr, which determines the sign and size of the phonon effect, first we need is the electronic density of states, $N(\epsilon)$. In Fig. 1 we fit a polynomial to $N(\epsilon)$ of Cr calculated by Lanrent, Wang, and Callaway [5].

For Cr the temperature independent orbital magnetic susceptibility, χ_{orb} , is estimated to be 1.06×10^{-4} emu/mol by Yasui and Shimizu [6], whereas the values of 1.10×10^{-4} and 1.30×10^{-4} emu/mol are adopted by Evangelou et al. [4].

For the given location of the Fermi energy of Fig. 1 we vary the value of χ_{orb} within above range and for each value of χ_{orb} we try to reproduce the observed behavior of χ above T_N by changing the value of $\bar{V}$.

The best fit to the experiment as shown in Fig. 2 is obtained with the following values for these parameters: $N(0)=0.350$ states/(eV, atom, spin), $\bar{V} = 0.395$, $\theta_D = 630$ K[7], $\chi_{orb} = 1.23 \times 10^{-4}$ emu/mol, $L=2.95$ (we put $W = 1$ eV; the final result is independent of W), and $J_p(0)$ (at $T=0$)=0.060. As for the temperature dependence in $F(0)$, we used the following expansion $F(0)=N(0) \{1-\pi^2/6 \{ \langle N'(0)/N(0) \rangle^2 - \langle N''(0)/N(0) \rangle \} (k_B T)^2 \} \equiv N(0) [1-\alpha (k_B T/\epsilon_F)^2]$; we obtain $\alpha(k_B/\epsilon_F)^2 = -2.11 \times 10^{-9}$ from $N(\epsilon)$ of Fig. 1.

Our reproduction of the temperature dependence of χ of Cr is quite satisfactory. For comparison we included in Fig. 2 by the broken line the

result of Evangelou et al.[4] based on the same band calculation result of Laurent et al.[5].

We carried out similar analysis of χ on various other transition metals.

The effect of the electron-phonon interaction can be important also in the temperature dependence of spontaneous magnetization below the Curie temperature of an itinerant electron ferromagnet. The reason may be clear from our discussion on Eq. (1) if we remember that the magnetization is determined from the minimum of $F_e(M) + F_p(M)$. Detailed account of our finding will be published elsewhere.

References

1. D. J. Kim, Phys. Rev. Lett. 47, (1981) 1213; Phys. Rev. B25, (1982) 6919; J. Appl. Phys. 55, (1984) 2347.
2. W. D. Weiss and R. Kohlhaas, Z. Naturf. a19, (1964) 1631.
3. See C. Kittel, Introduction to Solid State Physics, 5th ed. (John Wiley and Sons, New York, 1976) Chap. 14, Fig. 11.
4. S. N. Evangelou, H. Hasegawa, and D. M. Edwards, J. Phys. F: Met. Phys. 12, (1982) 2305.
5. D. G. Laurent, C. S. Wang and J. Callaway, Phys. Rev. B17, (1978) 455.
6. M. Yasui and M. Shimizu, J. Phys. F: Met. Phys. 9 (1979) L227.
7. From Table 1 of Chap. 5 of Ref. 1

Figure Captions

Fig. 1. The electronic density of states for Cr of Laurent et al. (ref. 5) (a) is approximated by polynomial near the Fermi level as in (b).

Fig. 2. Observed χ of Cr (ref. 2) and its analysis with the present electron-phonon interaction effect (real line). The result of Evangelou et al. (ref. 4) is shown by the broken line.

Fig. 1

Fig. 2