New Phonon Effect on Itinerant-Electron Ferromagnetism

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This paper reports a study of the effect of the electron-phonon interaction on the magnetization below the Curie point of an itinerant-electron ferromagnet. From a numerical calculation on a simple model, it is found that the size of the effect can be much larger than the generally assumed value of $\sim\hbar\omega_D/\epsilon_F$ in the units of Bohr magneton per atom, where ω_D and ϵ_F are, respectively, the phonon Debye frequency and the electron Fermi energy.

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It is widely believed that the possible effect of the electron-phonon interaction on the magnetism of a metal is not of quantitative importance.[1] Discussions to justify such a conclusion, however, do not appear convincing enough, and currently controversies are still going on.[2-6] The purpose of this Letter is to present a new, interesting result of a simple model calculation which, contrary to the prevailing view, strongly suggests that in itinerant-electron ferromagnetism the electron-phonon interaction might be playing a role much more important than generally thought. While previous works were concerned about the spin susceptibility of a paramagnetic metal, in this Letter we study the magnetization behavior below the Curie point of an itinerant-electron ferromagnet. In principle, the size of the possible electron-phonon interaction contribution, M_p, to magnetization is expected to be very small, $|M_p| \sim\hbar\omega_D/\epsilon_F \simeq 10^{-2}$ in units of Bohr magneton per atom, where ω_D is the phonon Debye frequency and ϵ_F is the Fermi energy of the electrons. Quite surprisingly, however, the model calculation indicates that M_p can be much larger than that, by a factor of ~10 to ~10^2.

In order to make the discussion simple, in this Letter I treat the situation of zero temperature. The starting point is to note that in a metal the phonon contribution to the energy, E_p, as well as the electron part, E_e, depends on the magnetization M of the conduction electrons of the metal; the phonon frequency is screened by the conduction electrons and the screening behavior changes with the spin splitting of the bands. The equilibrium value of the magnetization is to be obtained by minimizing the total energy with respect to the magnetization M,

$$\partial E_e(M)/\partial M + \partial E_p(M)/\partial M = 0. \tag{1}$$

Usually the second term of Eq. (1) is completely neglected.

As can be seen from Eq. (1), in our discussion it is most essential that we use the same model and approximation in dealing with $E_e(M)$ and $E_p(M)$. Under such requirement the only possible choice at present may be to use the jellium model, with some extension, and the mean-field approximation.

If we put the electronic density of states as $N(\epsilon)$, and the exchange interaction between electrons as $\tilde{V}$, the electron part of the energy in the mean-field approximation is given as

$$E_e(M) = \sum_{\sigma=\pm}\left[\int_0^{\epsilon_{F\sigma}} \epsilon N(\epsilon)d\epsilon - \tfrac{1}{2}\tilde{V} n_\sigma^2\right], \tag{2}$$

where $\epsilon_{F\pm}(M)$ is the Fermi energy of the $\pm$-spin electrons measured from the bottom of each band, and $n_\pm = n(1\pm M)$ is the number of $\pm$-spin electrons in the system. Note that $n_+ + n_- = 2n$ and $M = (n_+ - n_-)/2n$. The Stoner theory of itinerant-electron ferromagnetism is to determine the equilibrium value of magnetization by minimizing $E_e(M)$ alone.

As for the phonon energy, at zero or low temperatures it is represented by the zero-point oscillation contribution,

$$E_p(M) = \tfrac{1}{2}\textstyle\sum_q \hbar\omega_q(M), \tag{3}$$

where ω_q is the phonon frequency with wave number q, and sum over phonon polarization is understood. As mentioned already we adopt essentially the jellium model, and we use the Debye approximation. Then we have only longitudinal acoustic phonons and the phonon frequency is related to the sound velocity $s(M)$ as $\omega_q(M) = s(M)q$.

In the present model and approximation the phonon frequency in the ferromagnetic state is obtained as[7]

$$\omega_q^2 = \Omega_q^2 - |g(q)|^2 \frac{\tilde{F}_+(q) + \tilde{F}_-(q)}{1 + V(q)[\tilde{F}_+(q) + \tilde{F}_-(q)]}, \tag{4}$$

where Ω_q is the bare phonon frequency, $g(q)$ is the electron-phonon interaction constant, $V(q)$

$= 4\pi e^2/q^2$ is the Coulomb repulsion between electrons, and $\tilde{F}_\pm(q) = F_\pm(q)/[1 - \tilde{V}F_\pm(q)]$ are the exchange-enhanced Lindhard functions of $\pm$-spin electrons. Without the exchange effect in the screening ($\tilde{V} = 0$) and in the paramagnetic state [$F_+(q) = F_-(q)$], the result of Eq. (4) reduces to the familiar one. The sound velocity $s(M)$ as a function of magnetization is obtained by taking the limit $q \to 0$ in Eq. (4) as[8] $\omega_q(M) = s(M)q$ with

$$\left(\frac{s(M)}{s_0}\right)^2 = \xi + 2N(0)\left[\frac{N_+(M)}{1 - \tilde{V}N_+(M)} + \frac{N_-(M)}{1 - \tilde{V}N_-(M)}\right]^{-1}. \quad (5)$$

In the above, $N_\pm(M)$ [$= \lim_{q\to 0} F_\pm(q)$] are the density of states of $\pm$-spin electrons at the Fermi surface under magnetization M,[9] $N(0)$ is the density of states at the Fermi surface in the paramagnetic state, $s_0 = \Omega_{\rm pl}/[8\pi e^2 N(0)]^{1/2}$ is the Bohm-Staver sound velocity, $\Omega_{\rm pl}$ being the ionic plasma frequency, and ξ is introduced as $\Omega_q^2 - |g(q)|^2/V(q) = \xi s_0^2 q^2$. The parameter ξ represents deviations from the pure jellium model; for the jellium model $\xi = 0$ since there $|g(q)|^2/V(q) = \Omega_{\rm pl}^2 = \Omega_q^2$; if $\xi > 0$ ($\xi < 0$) the phonon is harder (softer) than in the jellium model.

Thus, the phonon part of the energy is given as

$$E_p(M)/NW = \tfrac{3}{8}(\hbar s_0 q m/W)[s(M)/s_0] \equiv a[s(M)/s_0], \quad (6)$$

where N is the total number of atoms in the system, W is the width of the electron band, q_m is the Debye-cutoff wave number ($N = q_m^3/3\pi^2$), and $s(M)/s_0$ is given by Eq. (5). As for the coefficient a of Eq. (6), note that $a \simeq \hbar\omega_D/W \simeq 10^{-2}$.

At first glance, since $E_p(M)/NW \sim 10^{-2}$, whereas $E_e(M)/NW \sim 1$, the electron-phonon interaction effect may appear totally neglegible if we are to determine the equilibrium magnetization only within an error of $\sim 1\%$. As our later numerical example will demonstrate clearly, however, such reasoning is not warranted. Suppose the minimum of $E_e(M)$ alone is located at $M = M_e$. The problem is how far the location of the energy minimum would shift from M_e if we include $E_p(M)$ into consideration. Here note that generally the variation of $E_e(M)$ becomes small in the neighborhood of the stationary point of M, M_e; near M_e the size of variation in $E_e(M)$ may not necessarily be much larger than that of $E_p(M)$.

We are now ready to carry out numerical computation on $E_e(M)$ and $E_p(M)$. In the present Letter we use the following form of density of states:

$$N(\epsilon) = (6N/W^3)\epsilon(W - \epsilon). \quad (7)$$

The shape of $N(\epsilon)$ is illustrated by the lower part of Fig. 2. As for a in Eq. (6), we assume $a = 10^{-2}$.

The result of the numerical calculation is given in Figs. 1 and 2. In Fig. 1 is shown how $E_e(M)$, $E_p(M)$, and $E_e + E_p(M)$ change with M/M_0 for the case $\epsilon_F/W = 0.5$, where M_0 is the maximum possible magnetization. All of the three energies E_e, E_p, and $E_e + E_p$ are plotted with the same en-

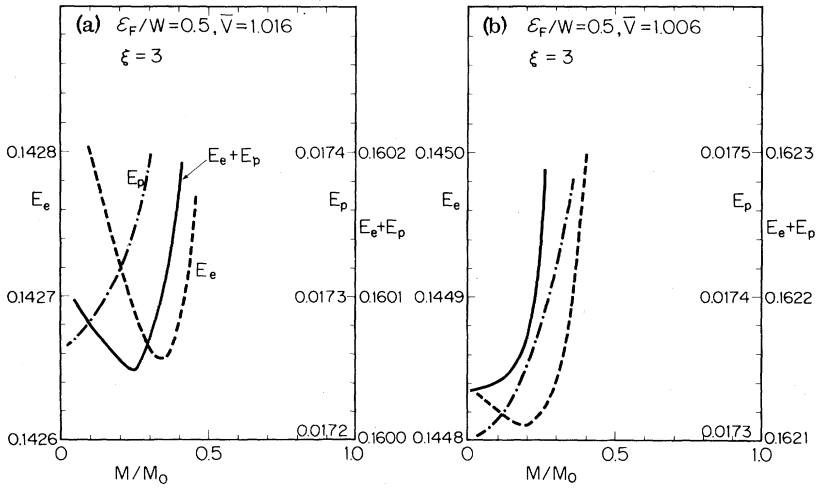

FIG. 1. The magnetization dependence of $E_e(M)$, $E_p(M)$, and $E_e(M) + E_p(M)$ for the case of $\epsilon_F/W = 0.5$ in the electronic density of states of Eq. (7) shown in the lower part of Fig. 2. All the energies are measured in the same unit of NW, although from different origins. M_0 is the maximum magnetization and $\bar{V} = \tilde{V}N(0)$. Note M_0 is different for different ϵ_F/W.

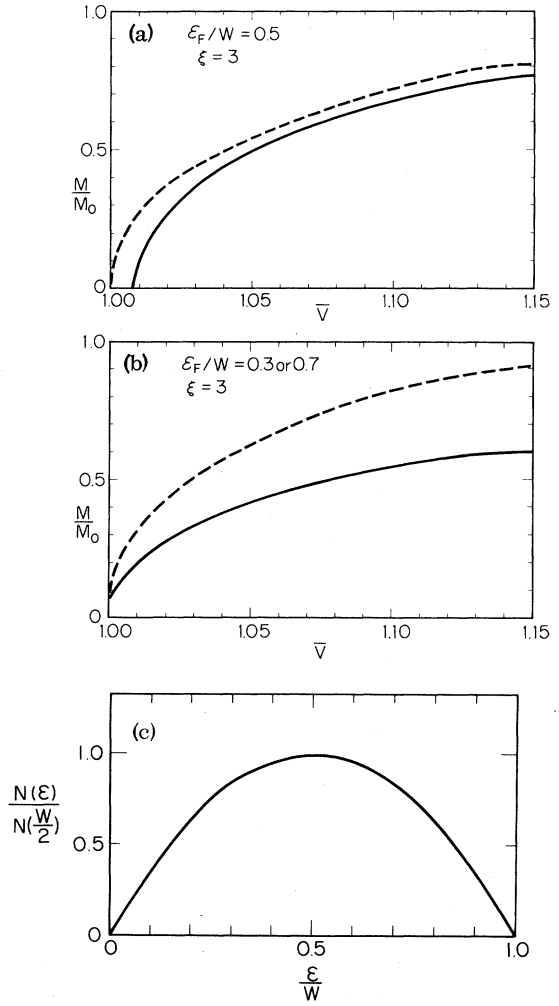

FIG. 2. The equilibrium magnetization with (real lines) and without (broken lines) the phonon effect, as a function of $\bar{V} = \tilde{V}N(0)$, for two different locations of the Fermi energy in the density of states of Eq. (7) shown in the lower part.

ergy scale in the unit of NW, although from different origins. As anticipated, near the stationary point of $E_e(M)$ the size of the M dependence of $E_p(M)$ can be as large as that of $E_e(M)$; the location of the minimum of $E_e(M)+E_p(M)$ shifts appreciably from that of $E_e(M)$ alone. A typical situation is shown in Fig. 1(a); by the phonon effect the magnetization is reduced by as much as ~ 30%, from $M/M_0 = 0.35$ to ~0.25. In the case of the smaller exchange interaction, $\bar{V} = \tilde{V}N(0) = 1.006$ [Fig. 1(b)], the Stoner magnetization of $M/M_0 \simeq 0.2$ is totally destroyed.

In Fig. 2 I show how differently the magnetization would be modified for two different occupations of the electron band. Note that with Eq. (7) the cases of $\epsilon_F/W = x$ and $1 - x$ are equivalent.

I carried out similar calculations for several different values of $\epsilon_F/W = 0.1$ (0.9), 0.2 (0.8), and 0.4 (0.6) with the same density of states of Eq. (7) and the result is found to be qualitatively similar to that of Fig. 2(b).

An important point in the result of Fig. 2 is that how M_p changes with $\bar{V}$ is quite different for different locations of ϵ_F in the density of states: While in Fig. 2(b) the phonon effect is generally large and increases with increasing $\bar{V}$, in Fig. 2(a) the phonon effect is generally small and decreases with increasing $\bar{V}$. With this result let us see how we can understand the drastic difference between the magnetization behaviors of FeNi alloys and Ni (or Fe).[10] In a very crude view, these two systems have nearly the same form of the density of states but different locations of ϵ_F.

It is well known that in FeNi alloys the temperature dependence of magnetization is anomalous[10]; with increasing temperature the magnetization decreases much faster than, say, in pure Ni. Since in these alloys $\bar{V}$ is considered rather large such magnetization behavior implies that these systems belong to the case of Fig. 2(b); ϵ_F is not located at or very near the maximum of $N(\epsilon)$. Note that the same conclusion on the location of ϵ_F was required[8] to account for the observed large magnetization dependence of elastic constant.[11]

In Ni the phonon effect on magnetization appears much smaller.[10] Since $\bar{V}$ is considered to be not small in Ni, it should belong to the case of Fig. 2(a); ϵ_F is at or very near the maximum of the density of states. Earlier[8] I reached the same conclusion on the location of ϵ_F to explain why the magnetization dependence of the elastic constants is much smaller than and opposite to the case of FeNi alloys.[11] Note that the size of M_p can be changed by changing the parameters a and ξ; smaller a and larger ξ make the phonon effect weaker.

There is an additional support to the above analysis on the difference between FeNi and Ni. It is concerned with the magnetic field dependence of sound velocity in the ferromagnetic state of a metal. Let us put $\Delta s(H)/s(0) = A(\mu_B H/W)$, where $s(H) = s(0) + \Delta s(H)$ is the sound velocity under a magnetic field H, and $M_p = B(\hbar\omega_D/W)$. Then, from a perturbational treatment of Eq. (1),[12] it is straightforward to obtain the relation $A \simeq -B$. If $B \simeq -10^2$ for the FeNi alloys as we propose, on the sound velocity we should observe a large positive magnetic field effect corresponding to $A \simeq 10^2$. Actually such a large and positive magnetic field

effect was observed in the FeNi alloys, while in pure Ni the magnetic field effect was not appreciable.[11]

Finally, note that in Fig. 2 we varied M/M_0 by varying $\bar{V}$ for $T=0$. In reinterpreting the result of Fig. 2 by appropriately translating the role of $\bar{V}$ to that of T we should note that the phonon effect on magnetization is enhanced by the thermal excitation of phonons. With such enhancement effect,[6] which is proportional to $\sim T/\Theta$ and starts from $T\sim\Theta/5$, Θ being the Debye temperature, the size of phonon effect can be larger for higher temperatures (smaller M) than for lower temperatures (larger M) even in the situation of Fig. 2(b).

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Observation of Zero-Point Fluctuations in a Resistively Shunted Josephson Tunnel Junction

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The spectral density of the voltage noise has been measured in current-biased resistively shunted Josephson junctions in which quantum corrections to the noise are expected to be important. The experimental data are in excellent agreement with theoretical pretions, demonstrating clearly the contribution of zero-point fluctuations that are generated in the shunt at frequencies near the Josephson frequency and mixed down to the measurement frequency.

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In a recent Letter, we[1] considered the effects of quantum corrections on the voltage noise in a current-biased resistively shunted Josephson junction. For measurement frequencies much less than the Josephson frequency and for a heavily overdamped junction we predicted a spectral density for the voltage noise $S_v(0)$:

$$\frac{S_v(0)}{R_D^2}=\frac{4k_BT}{R}+\frac{2eV}{R}\left(\frac{I_0}{I}\right)^2\coth\left(\frac{eV}{k_BT}\right). \quad (1)$$

Here, I_0 and R are the critical current and shunt resistance of the junction, I and V are the current and voltage, and R_D is the dynamic resistance. Equation (1) is based on the assumption that the noise arises from equilibrium noise currents in the shunt resistor with a spectral density

$$S_I(\nu)=(2h\nu/R)\coth(h\nu/2k_BT)$$
$$=(4h\nu/R)\{[\exp(h\nu/k_BT)-1]^{-1}+\tfrac{1}{2}\} \quad (2)$$

at frequency ν. The first term on the right-hand side of Eq. (1) represents noise from the resistor at the measurement frequency, while the second term arises from noise mixed down from frequencies near the Josephson frequency. In the limit $eV\gg k_BT$, the latter term represents zero-point