Self-consistent fluctuation-phonon approach to the theory of ferromagnetism

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A thermodynamic approach which leads to a self-consistent description of the effect of magnetization on the spectrum of lattice vibrations and of the effect of lattice fluctuations on a spontaneous magnetization is formulated.

The role played by phonon fluctuations in the theory of ferromagnets with collectivized mobile electrons was studied in Ref. 1. A temperature dependence of the magnetization arises because the phonon component (δF_{ph}) of the free energy, treated as a function of the magnetization M, the volume V, and the temperature T,

$$F(V, T, M) = F(V, M) + \delta F_{ph}(V, T, M)$$

$[F(V,M) = F(V,0,M)]$, turns out to depend on the magnetization because the corresponding dependence of the sound velocity is taken into account. In Ref. 1, this point was taken into account not on the basis of the thermodynamics but on the basis of a dynamic approach. It is not difficult to see, however, that the dynamic approach actually gives the bulk modulus K_B at a constant magnetic induction, not a constant magnetization. This circumstance is the reason why the approach of Ref. 1 is not systematic and leads to some paradoxical consequences. In the present letter, in contrast with Ref. 1, we report the results of a self-consistent approach, which makes use of the bulk modulus at constant magnetization, $K_M = V[\partial^2 F(V,M)/\partial V^2]_M$. The thermodynamics thus becomes systematic. The results found here differ qualitatively from those of Ref. 1 and also from the predictions of the Stoner model at $T \neq 0$.

To simplify the analysis, we consider a weak ferromagnet with collectivized mobile electrons, for which Stoner's theory reasonably predicts[2] a temperature-independent description. We can thus write the electron free energy in the form

$$F_e(V, M) = F_e(V) + A(V)M^2 + B(V)M^4,$$

where $A(V) = (1 + 2\psi\nu)V/4\beta^2\nu$, $B(V) = -V(\nu'/\nu^3)'/192\beta^4\nu$, ψ is the exchange interaction constant, ν is the density of electron energy states at the Fermi level, the prime means the derivative with respect to the energy ϵ_F, and β is the magnetic moment of the electron. We are completely ignoring the temperature dependence which stems from the blurring of the Fermi level; that point is traditionally taken into account for the Stoner theory.

We attribute the entire dependence on the temperature T to the lattice part of the free energy, for which we use the expression

$$F_{ph}(V, T, M) = F_{ph}(V) + \mathcal{F}(V, T) + M^2 \mathcal{P}(V, T). \qquad (1)$$

Here $\mathscr{F}(V,T)$ is the ordinary temperature increment in the lattice free energy, which can be illustrated by the following formulas in some simple cases[3]:

$$\mathscr{F}(V,T) = -V\frac{\pi^2(\kappa T)^4}{30(\hbar\bar{u})^3}, \quad T < T_D; \qquad \mathscr{F}(V,T) = N_A C\kappa T \ln\frac{\hbar\bar{\omega}}{\kappa T}, \quad T > T_D, \tag{2}$$

where T_D is the Debye temperature, C is the specific heat per cell, N_A is the number of cells in the lattice, and $\bar{u}$ and $\bar{\omega}$ are the average sound velocity and average vibration frequency of the lattice. Since the magnetization dependence of the sound velocity is known to be $\bar{u}(M^2) = \bar{u}(0) + \bar{u}'(0)M^2$ for ferromagnets, it is natural to regard the term $\mathscr{F}$ as resulting from the incorporation of $\bar{u}(0)$ [and, correspondingly, $\bar{\omega}(0)$] and to regard the coefficient $\mathscr{P}(V,T)$ as arising in an expansion in M^2. Consequently, in accordance with (2), we use

$$\mathscr{P}(V,T) = V\frac{\pi^2(\kappa T)^4}{10[\hbar\bar{u}(0)]^3}\,\frac{\bar{u}'(0)}{\bar{u}(0)}, \quad T < T_D; \quad \mathscr{P}(V,T) = N_A C\kappa T\frac{\bar{\omega}'(0)}{\bar{\omega}(0)}, \quad T > T_D. \tag{3}$$

Correspondingly, we have $\bar{u} \to \bar{u}(0)$ and $\bar{\omega} \to \bar{\omega}(0)$ in (2). Accordingly, for a self-consistent fluctuation-phonon approach to the theory of ferromagnetism we use the free energy in the form

$$F(V,T,M^2) = F_0(V) + \mathscr{F}(V,T) + M^2[A(V) + \mathscr{P}(V,T)] + M^4B(V). \tag{4}$$

In particular, we then find $M^2 = -[A(V)/2B(V)]\{1 + \mathscr{P}(V,T)/A(V)\}$ for the equilibrium spontaneous magnetization. An even more important point is that expression (4) makes it possible to determine the compressibility as a function of M^2 in a self-consistent way, so that it becomes possible to determine the effect of the magnetization on $\bar{u}$ and $\bar{\omega}$ in a self-consistent way. For the bulk modulus, expression (4) gives us $K = V(\partial^2F/\partial V^2)_{TM} = K_0 + V(\partial^2\mathscr{F}/\partial V^2)_T + M^2V(d^2A/dV^2)$. Here we have allowed for the fact that, in contrast with the small quantity A, the quantity $A'' = d^2A/dV^2$ is not small. We can thus conclude that we have $\bar{u}'(0)/\bar{u}(0) = C_u(V/K_0)A''$ and $\bar{\omega}'(0)/\bar{\omega}(0) = C_\omega(V/K_0)A''$, where C_u and C_ω are positive constants on the order of unity.

If we supplement (4) by taking into account the contribution from the magnetic inductions $\mathscr{B}$, then we can write a Belov-Arrott equation corresponding to the stability of the ferromagnet:

$$M^2(\mathscr{B},T) + \frac{2\chi_0 M^2(0,0)\mathscr{B}}{M(\mathscr{B},T)} = M^2(0,0)[1 - f(T)]. \tag{5}$$

The left side of this equation is of the standard form, $M^2(0,0) = -A(V)/2B(V)$, in accordance with the Stoner theory. The new physics stems from the function

$$f(T) = -(VA''/A)d\mathscr{F}/dK_0.$$

If we restrict the discussion to the effect of the magnetization on exclusively the longitudinal sound velocity u_l, then we find

$$\frac{d\mathcal{F}}{dK_0} = V\frac{\pi^2(\kappa T)^4}{60\,K_0(\hbar u_l)^3}, \quad T < T_D; \qquad \frac{d\mathcal{F}}{dK_0} = \frac{N_A C\kappa T}{2K_0}, \qquad T > T_D \tag{6}$$

We can draw some conclusions from this analysis. First, for ferromagnets which exist at $T_c < T_D$ we have the following expression for the Curie temperature:

$$\kappa T_c \sim \left(\frac{\kappa T_D}{\epsilon_F}\right)^{3/4} \epsilon_F \,|\, 1 + 2\psi\nu \,|^{1/4} \tag{7}$$

Second, if $T_c > T_D$, then

$$\kappa T_c \sim \epsilon_F \,|\, 1 + 2\psi\nu \,| \,. \tag{8}$$

Expressions (7) and (8) are strongly influenced by the lattice properties. Third, for the ratio of baric derivatives $\xi = [d\ln M(0,0)/dP]/(d\ln T_c/dP)$ we have $\xi = 2$ at $T_c < T_D$ and $\xi = 1/2$ at $T_c > T_D$. In the Stoner approach, the value is $\xi = 1$. If we take Kim's approach,[1] we find $\xi = 1/4$ at $T_c > T_D$, while in the case $T_c < T_D$, which has not been studied in Kim's approach, the value should be $\xi = 1$. On the other hand, there are (for example) well-known ferromagnets such as $Zr(Fe_{0.3}Co_{0.7})_2$ and $Fe_{0.65}Ni_{0.35}$ for which the values of the ratio are close to the values predicted by us, $\xi = 2.27$ and $\xi = 0.59$, respectively, for the relations between T_c and T_D corresponding to our theory.[4] Finally, we note that expression (7) implies $d\ln T_c/d\ln m_i = -3/8$, where m_i is the mass of the lattice atoms. This result does not contradict experimental data.[5] Another possibility for a larger isotopic effect, according to Ref. 6, stems from a renormalization of the exchange interaction constant ψ due to zero-point vibrations. That possibility is apparently not supported by experiment.[5] The actual temperature dependence of the magnetization may differ from that described by (6) to the extent that (for example) the temperature dependence of the thermal expansion of the volume of the ferromagnet differs from the T^4 and T laws. To the same extent, there will be changes in expressions (7) and (8), the values of ξ corresponding to them, and also in the isotopic effect.

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