

curate values, as we have verified, for instance, on the calculation of the ground-state energy of the anharmonic oscillator where, for an intermediate coupling, the accuracy is, for six terms of the perturbation series, of the order of 10^{-2} for the Padé method, 10^{-3} for the Padé-Borel method, and 3×10^{-4} for our method. Second, to improve efficiently the rate of convergence of a series by means of the Padé-Borel method, the perturbation series has to alternate in sign. This condition is not crucial in our approach. This is particularly important in the calculation of critical exponents from ϕ^4 field theory in three dimensions, where Baker *et al.*⁵ only used $1/\gamma(g)$ and $\eta_2(g) \equiv W(g)(d/dg)\ln[Z_{(2)}(g)]$, whose series alternate in sign, the other critical exponents being obtained by scaling relations. With our method, we could calculate all exponents independently.

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Ultrasonic Propagation and Structural Instabilities in Itinerant-Electron Ferromagnets

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An itinerant-electron model for ultrasonic propagation in a ferromagnetic metal, for both above and below the Curie temperature T_C , is developed within the mean-field approximation. The attenuation maxima of the longitudinal acoustic wave are shown to occur at slightly below T_C in agreement with the experimental observation on Ni. In addition, new possibilities of magnetically driven structural instabilities in metals are pointed out.

The ultrasonic method has been used extensively in studying ferromagnetic substances.¹ Most of the previous theoretical treatments² of the ultrasonic propagation, however, are based on the localized-spin model for ferromagnetism. In this Letter I develop a simple itinerant-electron mod-

el for the ultrasonic behavior of a ferromagnetic metal.

In discussing the lattice vibrations of a metal, either magnetic or nonmagnetic, it is most important to consider the screening of the ion-ion interaction by the conduction electrons.³ I pursue

how the screening behavior and, accordingly, the velocity and attenuation of ultrasound change with the magnetic properties in an itinerant-electron ferromagnet. In this way it was found⁴ recently that in the paramagnetic state of the jellium model the ultrasonic attenuation is directly proportional to the spin susceptibility. Thus it was concluded that the observed maxima of ultrasonic attenuation near the ferromagnetic Curie point T_C are caused by the divergence of the paramagnetic spin susceptibility at T_C .

In the present Letter I extend an earlier study⁴ (1) beyond the jellium model and (2) into the ferromagnetic state below T_C . With these extensions I find, quite surprisingly, that the origin of the attenuation maxima is entirely different from what was anticipated in Ref. 4. What is responsible for the attenuation maxima is the sensitive magnetization dependence of the dynamic screening behavior below T_C ; the maxima occur slightly below T_C , not at T_C , in agreement with the observation on Ni.⁵ Further, in addition to the structural instability in the paramagnetic state noticed earlier,⁴ another new structural instability in the ferromagnetic state is found.

In this Letter I concentrate on the longitudinal acoustic wave of a ferromagnetic metal. With the mean-field approximation, including the effect of the exchange interaction between electrons, the phonon frequency ω_q with wave number q , both above and below the Curie point T_C , is obtained from the following relation⁴:

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

where Ω_q is the bare phonon frequency, $g(q)$ is the electron-phonon interaction,³ $V(q)$ ($= 4\pi e^2/q^2$, for plane-wave states) is the Coulomb repulsion between electrons, and $\tilde{F}_\pm(q, \omega) = F_\pm(q, \omega)/[1 - \tilde{V}(q) \times F_\pm(q, \omega)]$ are the exchange-enhanced Lindhard response functions³ of plus or minus spin electrons with $\tilde{V}(q)$ the effective exchange interaction between electrons.⁶ Note that in the paramagnetic state $F_+(q, \omega) = F_-(q, \omega) = F(q, \omega)$, and that the familiar exchange-enhanced paramagnetic spin susceptibility is given as $\chi_m(q, \omega) = 2F(q, \omega)/[1 - \tilde{V}(q)F(q, \omega)]$ (with $\mu_B^2 = 1$).

How I derive the basic result of Eq. (1)⁴ may be evident from the following: If one notes that in the jellium model³ $\Omega_q^2 = |g(q)|^2/V(q) = \Omega_p^2$, where

Ω_p is the ionic plasma frequency, the first term on the right-hand side of Eq. (1) can be naturally identified as the contribution of the deviation from the simple Coulombic ion-ion interaction. The second term, on the other hand, gives the contribution of the Coulombic part of the ion-ion interaction; the denominator represents the dynamical screening processes by the electrons. If the exchange interaction between electrons is not considered, the screening constant will take the familiar form of $1 + V(q)[F_+(q, \omega) + F_-(q, \omega)]$. Inclusion of the exchange effect replaces the Lindhard functions $F_\pm(q, \omega)$ by the exchange-enhanced ones $\tilde{F}_\pm(q, \omega)$. Note that for the paramagnetic state and without the exchange effect Eq. (1) reduces to the familiar result.³

Starting with Eq. (1) the discussion of the ultrasonic behavior is quite straightforward: The phonon frequency to be obtained from Eq. (1) is a complex quantity, $\omega_q = \bar{\omega}_q - i\gamma_q$, and the velocity s and (energy) attenuation constant α are given, respectively, as $\bar{\omega}_q = s \cdot q$ and $\alpha = z\gamma_q/s$.

Although Eq. (1) can be used for more realistic electronic states, in the following I assume plane-wave states for the electrons. Furthermore, by assuming $\gamma_q/\omega_q \ll 1$ as well as $q/k_F \ll 1$, k_F being the Fermi wave number, Eq. (1) is approximately

$$(\bar{\omega}_q - i\gamma_q)^2 = \frac{s_a^2 q^2 + \Omega_p^2}{\tilde{F}_+(q, \bar{\omega}_q - i0^+) + \tilde{F}_-(q, \bar{\omega}_q - i0^+)}, \quad (2)$$

where $\Omega_q^2 - |g(q)|^2/V(q) \equiv s_a^2 q^2$.³ Note that in the jellium model $s_a^2 = 0$. If $s_a^2 > 0$ the phonon will be harder than in the jellium model, while if $s_a^2 < 0$ the phonon will be softer. Solving Eq. (2) for $\bar{\omega}_q$ and γ_q , one obtains

$$(s/s_0)^2 = \frac{1}{2}[(A + \xi) + [(A + \xi)^2 + B^2]^{1/2}], \quad (3)$$

$$\gamma_q = \frac{1}{2}\bar{\omega}_q B (s_0/s)^2, \quad (4)$$

with

$$\frac{2N(\epsilon_F)}{\tilde{F}_+(q, \bar{\omega}_q - i0^+) + \tilde{F}_-(q, \bar{\omega}_q - i0^+)} \equiv A - iB, \quad (5)$$

where $\xi = s_a^2/s_0^2$, $s_0 = \Omega_p/[8\pi e^2 N(\epsilon_F)]^{1/2}$ is the Bohm-Staver sound velocity,³ and $N(\epsilon_F)$ is the electronic density of states at the Fermi surface.

Thus, for the paramagnetic state one obtains

$$s/s_0 = [\xi + \chi_0/\chi_m]^{1/2}, \quad \alpha/\alpha_0 = (s_0/s)^2, \quad (6)$$

where $\chi_0 = 2N(\epsilon_F)$ is the Pauli spin susceptibility, $\chi_m = \chi_m(0, 0)$ is the exchange-enhanced spin susceptibility, and $\alpha_0 = \pi\bar{\omega}_q/2v_F$ is the attenuation constant in the jellium model without the exchange

effect,³ v_F being the Fermi velocity. The result of Eqs. (6) is valid for a paramagnetic metal as well as for $T > T_C$ in a ferromagnetic metal.

The velocity and attenuation of sound are related to the paramagnetic spin susceptibility in a very direct way. This relation comes from the fact that the exchange interaction between electrons effectively reduces the Coulomb repulsion between electrons⁷ and thus enhances the screening of the ion-ion interaction. Note, however, that since in Eqs. (6) χ_0/χ_m can vary only within the range 0~1, the size of the temperature dependence of s and α depends very crucially on the magnitude of ξ . The absence of significant temperature dependence in the phonon frequency of Pd which has large and strongly temperature dependent χ_m , for instance, can be understood by assuming a large ξ .

According to Eqs. (6), for structural stability at and above T_C one requires that $\xi \geq 0$. If $\xi < 0$ and χ_m increases with lowering temperatures, there will be a structural instability at a temperature where $\xi + \chi_0/\chi_m = 0$. This instability will be observed as vanishing of sound velocity and divergence of attenuation. This kind of mechanism might be responsible for the structural transformations observed in the A15 compounds.⁸

In Fig. 1 I illustrate the above ultrasonic behavior by a numerical example. I assumed $\chi_m/\chi_0 = T_C/(T - T_C)$ in Eqs. (6). Note that, according

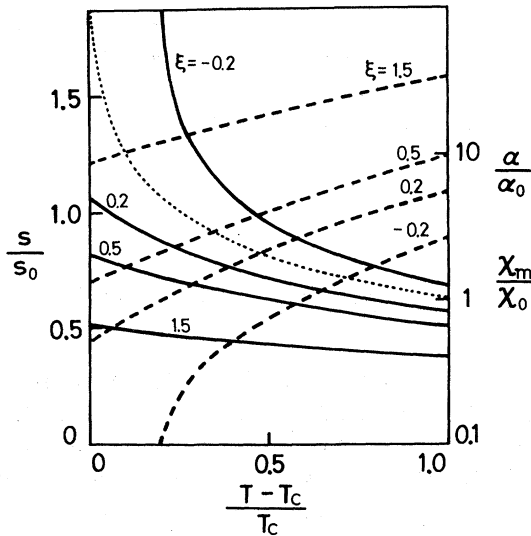


FIG. 1. The attenuation α (solid lines) and velocity s (dashed lines) of longitudinal acoustic waves in the paramagnetic state for different values of ξ . The paramagnetic spin susceptibility (dotted line) is assumed as $\chi_m/\chi_0 = T_C/(T - T_C)$.

to Eqs. (6), the magnitude of ξ can be determined if measurements of the temperature dependence of ultrasonic propagation and paramagnetic spin susceptibility are made simultaneously.

Now let us consider ultrasonic propagation in the ferromagnetic state. Near T_C , by putting^{3,9} $F_{\pm}(q, \bar{\omega}_q - i0^+) \approx R_{\pm}(0, 0) + \frac{1}{2}i\pi N(\epsilon_F)s/v_F$ in Eq. (5), one obtains

$$A \approx -\bar{V}(\beta^2 + \delta^2)^2[(\beta^2 + \delta^2)^2 + \beta^2]^{-1}, \quad (7a)$$

$$B \approx \bar{V}\beta(\beta^2 + \delta^2)[(\beta^2 + \delta^2)^2 + \beta^2]^{-1}, \quad (7b)$$

where $\bar{V}(0)N(\epsilon_F) \equiv \bar{V}$, and

$$1 - \bar{V}(0)R_{\pm}(0, 0) \equiv \mp \delta, \quad (8)$$

$$\frac{1}{2}\pi\bar{V}s/v_F \equiv \beta. \quad (9)$$

Note that $0 \leq \delta \ll 1$ and $0 < \beta \ll 1$ in the present temperature region and that since δ is proportional to the magnetization M of the electrons, in the mean-field approximation,

$$\delta^2 = d(T_C - T)/T_C, \quad (10)$$

where d is a positive constant of order unity.

Actual solution of Eq. (3) with A and B given by Eqs. (7) requires a numerical method. Before the numerical analysis, let us discuss the expected features of the solution. The dynamic screening behavior depends very sensitively on the magnetization near T_C . We may divide the temperatures into the following three regions: (i) $0 \leq (T_C - T)/T_C \ll (s_0/v_F)^2$; (ii) $(s_0/v_F)^2 < (T_C - T)/T_C < (s_0/v_F)$; (iii) $(s_0/v_F) < (T_C - T)/T_C \ll 1$. In region (i) very close to T_C , where $\delta^2 \ll \beta^2$, Eqs. (7) reduce to $A \approx -\bar{V}\beta^2$ and $B \approx \bar{V}\beta$, and, accordingly,

$$s/s_0 \approx \sqrt{\xi}, \quad \alpha/\alpha_0 = (s_0/s)^2. \quad (11)$$

Comparing with the result of Eqs. (6) we find that at $T = T_C$ both the velocity and attenuation of longitudinal acoustic waves are continuous and do not have either minimum or maximum. This result agrees with the experimental observation on Ni.⁵

In region (ii) where $\beta^2 < \delta^2 < \beta$, we obtain $A \approx -\bar{V}\delta^4/\beta^2$ and $B \approx \bar{V}\beta(\delta^2/\beta^2)$. Since α is proportional to B , α is enhanced by a factor $\delta^2/\beta^2 = (v_F/s_0)^2 M^2$ from that of region (i). Note the large factor $(v_F/s_0)^2$ as well as the temperature dependence in M^2 .

Similarly in region (iii) where $\beta < \delta^2 \ll 1$, we obtain $A \approx -\bar{V} + \bar{V}\beta^2/\delta^4$, $B \approx \bar{V}\beta/\delta^2$, and, accordingly,

$$s/s_0 \approx \{(\xi - 1) + [\frac{1}{4}\bar{V}^2 + \bar{V}(\xi - 1)]b^2/\delta^4\}^{1/2}, \quad (12a)$$

$$\alpha/\alpha_0 \approx \bar{V}(s_0/s)^2/\delta^2, \quad (12b)$$

where $\frac{1}{2}\pi\bar{V}s_0/v_F = b$. Firstly, as can be seen from Eq. (12a), if $\xi < 1$, s becomes imaginary in

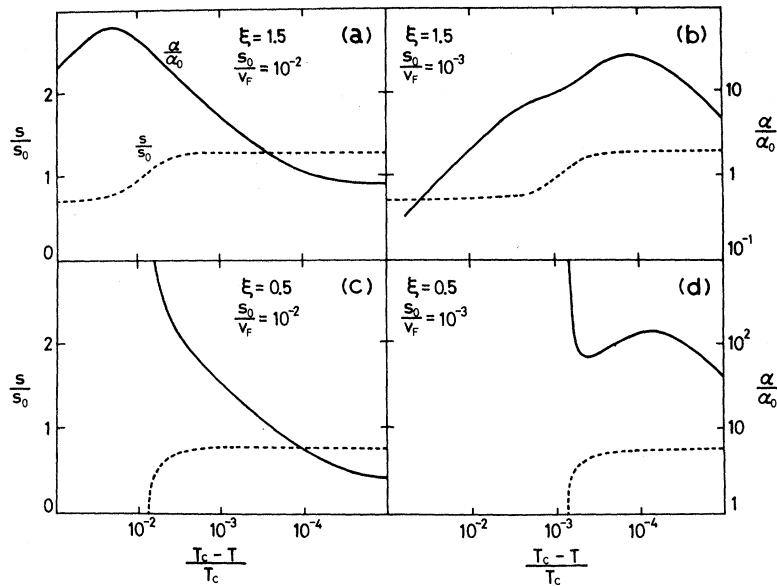


FIG. 2. The attenuation α and velocity s of longitudinal acoustic waves in the ferromagnetic state for different values of ξ and s_0/v_F .

the present temperature region. That is, if $0 < \xi < 1$ an itinerant-electron ferromagnet will have a structural instability at a temperature T_m in region (ii) or (iii), producing a softening of sound velocity and an increase of attenuation. Secondly, as is shown in Eq. (12b), in the present temperature region α is enhanced by a factor $1/\delta^2 \approx 1/M^2$. Thus α decreases, after it increased in region (ii), as one lowers the temperature near T_C . Accordingly a maximum of α is expected to occur between regions (ii) and (iii), without involving a structural instability. Finally, in the case of $0 < \xi < 1$, if it happens $T_m < T_0$ one may observe two maxima in α , one at T_0 and the other at T_m .

In the above, note that T_0 and/or T_m are very close to T_C , lying within the range $(s_0/v_F)^2 < (T_C - T)/T_C < (s_0/v_F)$. Actually for Ni,⁵ since $(T_C - T_0) \approx 0.1$ K whereas $T_C = 630$ K, $(T_C - T_0)/T_C \approx 10^{-4}$. Note that generally $s_0/v_F = 10^{-3} - 10^{-2}$.

In Fig. 2 I show examples of my numerical analysis based on the full expressions of Eqs. (7). I assumed $\bar{V} = 1$ and $d = 1$. Qualitatively the experimental observation on Ni⁵ is similar to the behavior shown in (a) and (b) of Fig. 2 with $\xi = 1.5$. One maximum in α below T_C is obtained without structural instability. According to my experience, the size of the maximum of α is very sensitive to the value of ξ and can be changed significantly by adjusting ξ within a rather narrow range.

For $\xi = 0.5$, Figs. 2(c) and 2(d), as anticipated,

show structural instabilities associated with softening of sound velocity. Especially for the case of $(s_0/v_F) = 10^{-3}$, one can observe two maxima in α , one smaller and broader at $T = T_0$ and the other larger and sharper at $T = T_m$ ($T_0 < T_C$). Note that a very similar behavior of α is reported¹⁰ in MnP in a magnetic field. It would be interesting to examine whether a structural transformation is induced actually in MnP near T_C .

In this Letter I presented a study only of the longitudinal acoustic phonon which is related to the elastic constant C_{11} . In actuality, however, as in the A15 compounds,⁸ the observed structural instabilities are often associated with softening of the transverse phonon for which the collapse of $C_{11} - C_{12}$ is responsible. Obviously, if $C_{12} > 0$, the collapse of $C_{11} - C_{12}$ comes before that of C_{11} . Thus the possible softening of C_{11} will be arrested by the structural transformation associated with the collapse of $C_{11} - C_{12}$.

I have also formulated here an itinerant-electron-model theory for ultrasonic propagation in a ferromagnetic metal within the simple mean-field approximation. Note, however, that the mean-field-approximation consequences, such as presented here, were not explored before. It is needless to remark that in order to make the discussion more quantitative one has to consider many additional mechanisms² such as the transverse spin fluctuation effects.¹¹ The present Letter is intended to be a starting basis for such

further studies. Also, the concept will be useful for rare-earth metals where it is important to consider the screening of the ionic interaction by conduction electrons.¹²

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Resistivity in Amorphous and Disordered Crystalline Alloys

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The Evans modification of Ziman liquid-metal theory is extended to apply to amorphous and disordered crystalline alloys. In particular, the theory is shown to explain such common behavior of these systems as the change in sign of the temperature coefficient of resistivity with alloy composition, the quadratic temperature dependence of resistivity at low temperature, and the linear temperature dependence of resistivity at high temperatures.

The anomalous temperature and composition dependence of electrical resistivity of amorphous and of many crystalline alloys has been the subject of considerable recent work.¹⁻¹⁴ The behavior of these systems is characterized by (i) temperature coefficients of resistivity which change sign as alloy composition changes, (ii) changes in resistivity which vary as T^2 at low temperature and as T at higher temperatures, and (iii) a generally S-shaped curve of resistivity versus temperature. These common characteristics strongly suggest a common origin. Among the suggested explanations for these effects are localized spin-fluctuation scattering,^{1,2} d -band effects,^{3,4} the Ziman liquid-metal theory,^{5,6} and the Evans, Greenwood, and Lloyd modification of the Ziman theory.⁷⁻¹² We will demonstrate that the modified Ziman theory correctly predicts the observed T^2 and T temperature dependences and explains the effects of composition changes. Furthermore, we present a unified description of the behavior common to amorphous and disordered crystalline metals.

The resistivity of pure metals is given in the modified Ziman theory as

$$\rho = \frac{12\pi\Omega_0}{e^2\hbar V_F^2} \int_0^1 \frac{dq}{2k_F} \left(\frac{q}{2k_F} \right)^3 \bar{S}(q) |t(k, k')|^2, \quad (1)$$

where Ω_0 is the atomic volume, V_F is the Fermi velocity, k_F is the corresponding wave vector, and $\bar{S}(q)$ may be written in terms of the dynamic structure factor as

$$\bar{S}(q) = \int_{-\infty}^{\infty} S(q, \omega) \frac{\hbar\omega}{k_B T} \left[\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1 \right]^{-1} d\omega.$$