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Equivalence of the dynamical and total-energy approaches in the calculation of elastic constants of magnetic metals

D. J. Kim,* M. W. Long, and W. Yeung
Department of Physics, Queen Mary College, London E1 4NS

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In calculating the elastic constants of itinerant electron magnets the two apparently different methods, the dynamical response approach and the total-energy differentiation approach, are shown to give the same result within the mean-field approximation. We show quite generally that there is a discontinuous drop in the bulk modulus at a magnetic phase transition induced by a change in volume.

I. INTRODUCTION

The mechanism of the observed close relation between elasticity and magnetism in metals is not yet satisfactorily understood despite its rather long history of studies (for references see Shimizu *et al.*[1]). Such a relation has been noted predominantly in transition metals, but recently it is being noticed among much wider classes of metals such as the heavy-fermion compounds.[2] For instance, elucidating their unusual elastic properties in these strongly exchange-enhanced metals is thought to be an important clue to the total understanding of the heavy-fermion system. We would like to find a practical method of calculating elastic moduli and phonon spectra in metals and investigate the effects of magnetism on these properties.

The usual experimental method used to determine the elastic constant in a metal is to measure the velocity of sound in it. Therefore a natural way of calculating the elastic constant is to calculate the acoustic-phonon frequency ω_q and to obtain the sound velocity, s, directly as

$$\lim_{q \to 0} \omega_q = sq \ . \tag{1.1}$$

Since the calculation of the phonon frequency involves the dynamics of the coupled system of electrons and ions, we shall call such a method of calculating the elastic constant the *dynamical approach.*

In the dynamical approach the screening of the bare ion-ion interaction of the conduction electrons is essential. There, the magnetic properties of a metal are reflected in the screening constant. In this way, as will be briefly reviewed in Sec. II, it was recently shown that the elastic constant or the sound velocity in the paramagnetic state of a metal is very directly related to the exchange-enhanced susceptibility χ, as

$$\left[\frac{s}{s_0} \right]^2 = \xi + \frac{2\mu^2 N(0)}{\chi} \ , \tag{1.2}$$

where

$$s_0 = \left[\frac{V \Omega_{\rm pl}}{8\pi e^2 N(0)} \right]^{1/2} \tag{1.3}$$

is the Bohm-Staver sound velocity, $\Omega_{\rm pl}$ and $N(0)$ being, respectively, the ionic plasma frequency and the electronic density of states per spin at the Fermi surface in the paramagnetic state. The parameter ξ is introduced to represent corrections to the jellium model arising from the nonhomogenous nature of actual charge distributions. In the simplest case this is equivalent to writing

$$\Omega_q^2 - \Omega_{\rm pl}^2 = \xi s_0^2 q^2 \ , \tag{1.4}$$

where Ω_q is the bare-phonon frequency. Similarly for the ferromagnetic state it was shown that

$$\left[\frac{s}{s_0} \right]^2 = \xi + \frac{2N(0)}{\dfrac{N_+(0)}{1 - IN_+(0)} + \dfrac{N_-(0)}{1 - IN_-(0)}} \ , \tag{1.5}$$

where I is the exchange interaction between electrons and $N_\pm(0)$ is the density of states of ± spin electrons at the Fermi surface. In the spin-unsplit state $N_+(0) = N_-(0) = N(0)$.

The interplay between elasticity and magnetism is clearly manifested in the results of Eqs. (1.2) and (1.5). The magnetic properties of a metal in the paramagnetic state are embodied in the magnetic susceptibility χ, and Eq. (1.2) shows how directly the elastic constant of the metal is related to χ. In the ferromagnetic state of a metal, the fundamental quantity to represent its magnetic properties is the magnetization, and Eq. (1.5) shows how the elastic constant is directly related to the spin-split electronic density of states at the Fermi surface, caused by the magnetization. Note that Eq. (1.5) is equivalent to Eq. (1.2) when the spin splitting of the bands vanishes since the Stoner susceptibility (at $T=0$) is given by $\chi = 2\mu^2 N(0)/[1 - IN(0)]$.

There is, however, an entirely different way of calculating elastic constants. If we set the total energy of a metal to be E, the elastic constant (bulk modulus) C is calculated as

$$C = V \frac{\partial^2}{\partial V^2} E \ , \tag{1.6}$$

V being the volume of the system. Then the sound velocity[3] of the system is obtained as

$$s=\left[\frac{C}{D}\right]^{1/2} ,$$

where D is the mass density of the metal. We call this method of calculating elastic constants via Eq. (1.6) the *total-energy approach.*

If the calculations are carried out *exactly,* the above two different approaches, the dynamic and the total energy, are expected to give the same result. However, two of us have shown,[4] with a simple quantum-mechanical model, that this apparently obvious equivalence may not always be correct. The paradox appears to stem from the fact that in the total-energy approach the volume derivatives of the energy are taken with both the number of electrons and the number of ions constant and equal, whereas in the dynamical approach the number of ions is kept constant but the number of electrons is allowed to vary to minimize the energy. However, if the electron-electron interaction is long range the two quantities calculated reduce to the same value. In addition, actual calculations necessarily involve some approximations and there are different kinds of approximation. If some approximation is made in the calculation, the two approaches may produce different results even if the approximations taken are of the same nature. Such situations have been well known for the paramagnetic state of an electron gas, the simplest model of a metal, once the effects of the electron-electron interaction are included.[5] Similar situations are noted also for some more realistic models of a metal in the paramagnetic state.[6]

Recently a number of very elaborate calculations have been done on the elastic constants of transition metals with the total-energy approach,[7] but from the observations as above on the discrepancy of the two approaches, such results are viewed to have nothing to do with the general physical picture given in Eqs. (1.2) or (1.5) as obtained from the dynamical approach. This is clearly an unsatisfactory state of affairs—especially since the total-energy method is not feasible for calculating the shear modulus for which the dynamical method is most suited. In this paper we wish to address the problem of, given a particular model and approximation in the total-energy approach, what is the corresponding consistent approximation, if any, in the dynamic approach. Since we intend to show explicitly the equivalence of the dynamical and total-energy approaches we must choose a model which is analytically tractable. Within the jellium model we demonstrate explicitly the equivalence of these two different approaches in calculating the bulk modulus with both Hubbard- and $X\alpha$-type interactions. The explicit demonstration hinges on the volume dependence of the effective interaction constant. We show that the equivalence is valid for any volume dependence provided that the effective interaction parameter satisfies Eq. (A.5) where we can include correlations as well in the quantity E_{ex}.

In fact, an example of such an equivalence was earlier given by Brovman *et al.*[6] for a pseudopotential model of a metal, but in that example the exchange interaction between electrons was not considered explicitly and thus it bears little on the subject of the relationship between elasticity and magnetism. As will be shown in Sec. III, the model we use for a metal is a much simpler but more general one including the exchange interaction between electrons. Our new finding in this paper indicates the general validity of the results of Eqs. (1.2) and (1.5). Such an observation would be useful in many ways in understanding the interplay of magnetism and elasticity in metals. It can be argued that the jellium model is not a very realistic model for magnetic systems such as transition metals. We feel that a demonstration of the equivalence between the total-energy and dynamical approaches is a preliminary and necessary step toward the treatment of the magnetic and elastic properties of magnetic metals since in a more realistic band-structure model certain calculations are only feasible in one or other of the two approaches.

First, in Sec. II we briefly summarize how the results of Eqs. (1.2) and (1.5) were obtained from the dynamical approach. Then in Sec. III we show how the total-energy approach also leads to the same results, for the Hubbard-type constant-exchange-interaction model. The corresponding proof for the $X\alpha$ model is given in the Appendix. Concluding remarks are given Sec. IV.

II. DYNAMICAL CALCULATION OF THE ELASTIC CONSTANTS

Starting from the basic model of a metal whose Hamiltonian consists of four terms—the one-particle energy of the electrons, the Coulomb repulsion between electrons, the bare interaction of the ions, and the electron-phonon interaction—the screening of the phonon frequencies from Ω_q to ω_q is obtained as[8]

$$\omega_q^2=\Omega_q^2-|g(\mathbf{q})|^2\chi_e(\mathbf{q}) . \tag{2.1}$$

Here $g(\mathbf{q})$ is the electron phonon–interaction constant and $\chi_e(\mathbf{q})$ is the electron density-response function. In the present discussion we neglect the lattice structure of the ions (jelliumlike model) and accordingly, we consider only the longitudinal-acoustic phonons. Equation (2.1) is an exact result; approximations are introduced only through the calculation of $\chi_e(\mathbf{q})$.

In the mean-field approximation, including the exchange effects, we obtain the following result for the electron density-response function,[9]

$$\chi_e(\mathbf{q})=\frac{\tilde{F}_+(\mathbf{q})+\tilde{F}_-(\mathbf{q})}{1+v(q)[\tilde{F}_+(\mathbf{q})+\tilde{F}_-(\mathbf{q})]} , \tag{2.2}$$

where $v(q)=4\pi e^2/Vq^2$ is the Fourier transform of the Coulomb repulsion between electrons and

$$\tilde{F}_\pm(\mathbf{q})=\frac{F\pm(\mathbf{q})}{1-IF_\pm(\mathbf{q})} \tag{2.3}$$

is the exchange-enhanced Lindhard response function of ± spin electrons which is given in terms of the ordinary Lindhard function

$$F_\pm(\mathbf{q})=-\sum_{\mathbf{k}} f\frac{(\varepsilon_{\mathbf{k},\pm})-f(\varepsilon_{\mathbf{k+q},\pm})}{\varepsilon_{\mathbf{k},\pm}-\varepsilon_{\mathbf{k+q},\pm}} , \tag{2.4}$$

$\varepsilon_{\mathbf{k}\pm}$ and $f(\varepsilon)$ being, respectively, the one-particle energy of ± spin electrons and the Fermi distribution function.

Note that Eq. (2.2) is valid both for the paramagnetic and ferromagnetic state, and that

$$\lim_{q\to 0} F_\pm(\mathbf{q}) = N_\pm(0) \ . \tag{2.5}$$

Inserting Eq. (2.2) in Eq. (2.1),we obtain[10]

$$\omega_q^2 = \left[\Omega_q^2 - \frac{|g(\mathbf{q})|^2}{v(q)}\right] + \frac{|g(\mathbf{q})|^2/v(q)}{1+v(q)[\tilde{F}_+(\mathbf{q})+\tilde{F}_-(\mathbf{q})]} \ . \tag{2.6}$$

In the smeared-out point-charge ion model (pure jellium) the first term on the right-hand side of Eq. (2.6) vanishes since there $(\Omega_q)^2 = (\Omega_{\rm pl})^2$ and

$$\Omega_{\rm pl}^2 = \frac{|g(\mathbf{q})|^2}{v(q)} \ . \tag{2.7}$$

We, however, account for deviations from the pure jellium model by the parameter ξ as in Eq. (1.4). Note that if we assume the pure jellium model (i.e., $\xi=0$) and confine attention to the paramagnetic state $[F_+(\mathbf{q}) = F_-(\mathbf{q}) = F(\mathbf{q})]$ and neglect the effects of the exchange interaction on the electron density response or the screening (i.e., $I=0$), Eq. (2.6) reduces to the familiar result[7]

$$\omega_q^2 = \frac{\Omega_{\rm pl}^2}{1+2V(q)F(\mathbf{q})} \ . \tag{2.8}$$

The Bohm-Staver sound velocity s_0, Eq. (1.3), is obtained from Eq. (2.8) by the procedure of Eq. (1.1) and similarly, the results of Eqs. (1.2) and (1.5) are obtained from Eq. (2.6). Note the Stoner susceptibility at finite temperature is given as $\chi = 2\mu^2 F(0)/[1-IF(0)]$.

III. TOTAL-ENERGY CALCULATION OF THE ELASTIC CONSTANTS

The total energy of a metal at $T=0$ in the Hartree-Fock approximation is given in standard texts on many-body theory.[8,11] Here we shall write it as follows

$$E = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} - \frac{I}{2}(\mathcal{N}_+^2 + \mathcal{N}_-^2) + \tfrac{1}{2}\sum_{i\neq j} U_\xi(i,j)$$
$$\equiv E_0 + E_{\rm ex} + E_\xi \ . \tag{3.1}$$

In the one-particle energy E_0 of electrons $n_{\mathbf{k}\sigma}$, the number of electrons in the state with wave number $\mathbf{k}$ and spin σ (+or−), is 1 or 0 depending on whether $k \le k_{F\sigma}$ or $k > k_{F\sigma}$, $k_{F\sigma}$ being the Fermi wave number of σ-spin electrons. Note that we have chosen to shift the chemical potential instead of shifting the energy.

Under our assumption of the uniform distribution of both the negative electron charge and the positive ion charge, the three kinds of (direct) Coulomb interaction energy—between electron and electron, ion and ion, and electron and ion—cancel each other and do not appear in Eq. (3.1). Note that such a cancellation persists through uniform change in the volume of the system and magnetization of the electrons. The last two terms in Eq. (3.1) are outside of such classical Coulomb interactions.

For the exchange energy $E_{\rm ex}$, we have replaced the relevant matrix element of the Coulomb potential by I, which is the same effective exchange interaction as appeared in Eqs. (1.5) and (2.3). $\mathcal{N}_\sigma = \sum_{\mathbf{k}} n_{\mathbf{k}\sigma}$ is the total number of electrons with spin σ. The last term in Eq. (3.1) represents the energy of ion-ion interaction beyond that of smeared-out point-charge jellium ions.

In calculating the elastic constant from Eq. (3.1) with the prescription of Eq. (1.6), we first treat the paramagnetic as in (3.1) and then in (3.2) we treat the ferromagnetic case.

A. Elastic constant in the paramagnetic state

Let us carry out the required volume differentiation of the total-energy equation (3.1), term by term. First, in the paramagnetic state, since $n_{\mathbf{k}+} = n_{\mathbf{k}-} = n_{\mathbf{k}}$, the one-particle part of the electron energy is written as

$$E_0 = 2\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} n_{\mathbf{k}} \ . \tag{3.2}$$

Now, we are required to know how $\varepsilon_{\mathbf{k}}$ depends on the volume V and there seems to be no simple general answer for realistic electronic levels. In this paper, corresponding to the assumption of the uniform distribution of the ionic charge, we assume the following free-electron-like dispersion,

$$\varepsilon_{\mathbf{k}} = \frac{\hbar^2}{2m}k^2 \ , \tag{3.3}$$

where m is the effective mass of an electron. In this case Eq. (3.2) reduces to

$$E_0 = \tfrac{3}{5}\mathcal{N}\varepsilon_F \ , \tag{3.4}$$

where $\varepsilon_F = \hbar^2 k_F^2/2m$ is the Fermi energy with $k_{F+} = k_{F-} = k_F$ related to the volume as

$$k_F = \left[\frac{3\pi^2\mathcal{N}}{V}\right]^{1/3} , \tag{3.5}$$

$\mathcal{N} = \mathcal{N}_+ + \mathcal{N}_-$ being the total number of electrons.

Note that the entire volume dependence of E_0 comes only through that of k_F given in Eq. (3.5). Thus the elastic constant C_0 originating from E_0 is obtained as

$$C_0 = V\frac{d^2}{dV^2}F_0 = \frac{2}{3}\frac{\mathcal{N}\varepsilon_F}{V} \ . \tag{3.6}$$

The corresponding sound velocity s_0 is obtained from Eq. (1.7) with $D = NM_i/V$, N and M_i being, respectively, the total number and the mass of the ions, as

$$s_0 = \left[\frac{2\mathcal{N}\varepsilon_F}{3NM_i}\right]^{1/2} = \left[\frac{mZ}{3M_i}\right]^{1/2} v_F \ , \tag{3.7}$$

where we set $\mathcal{N} = NZ$ and $v_F = \hbar k_F/m$ is the Fermi velocity of the electrons. This sound velocity coincides with that of Bohm-Staver, Eq. (1.3), as can be checked if we note

$$\Omega_{\rm pl}^2 = \frac{4\pi\mathcal{N}Ze^2}{VM_i} \quad \text{and} \quad N(0) = \frac{Vmk_F}{2\pi^2\hbar^2} \quad \left[= \frac{3\mathcal{N}}{4\varepsilon_F}\right] , \tag{3.8}$$

corresponding to Eq. (3.3).

Thus, for the electron-gas model of a metal with Eq.

(3.3), we have confirmed that the elastic constant in the paramagnetic state calculated without considering the exchange interaction ($I=0$) or deviations from the smeared-out point-charge jellium model ($\xi=0$ or $E_\xi=0$), using two different methods, the dynamic and total-energy approaches, give the same answer. This result is well known. However, it is only up to here that the equivalence of the two different approaches has been demonstrated explicitly.

Let us now proceed to calculate the effect of the exchange energy on the elastic constant. In the paramagnetic state the exchange energy given by Eq. (3.1) is rewritten as

$$E_{\text{ex}} = -\tfrac{1}{4} I \mathcal{N}^2 \ . \tag{3.9}$$

Obviously the total number of electrons, $\mathcal{N}$, is independent of the volume of the system. As for the effective exchange interaction I, the volume dependence depends on the approximation used for the effective exchange. In this section we consider a Hubbard-type short-range interaction employed in magnetism, whereas in the Appendix we consider a density-dependent exchange interaction used in the $X\alpha$ or local-density approaches. We first note that it is the Fourier transform of the distance-dependent exchange interaction $I(\mathbf{r})$,

$$I(\mathbf{q}) = \frac{1}{V} \int_V I(\mathbf{r}) e^{i\mathbf{r}\cdot\mathbf{q}} d\mathbf{r} \ . \tag{3.10}$$

If $I(\mathbf{r})$ is short ranged the integral would not depend on V and, further, on $\mathbf{q}$, as in the case of the Hubbard model. Thus, $I(\mathbf{q}) = I \propto 1/V$, or

$$\frac{d}{dV} I = -\frac{1}{V} I, \quad \frac{d^2}{dV^2} I = \frac{2}{V^2} I \ . \tag{3.11}$$

With the relation of Eq. (3.11), we obtain, from Eq. (3.9),

$$V \frac{d^2}{dV^2} E_{\text{ex}} = -\frac{I}{8V} \mathcal{N}^2 = -\frac{2}{3} \frac{\mathcal{N} \varepsilon_F}{V} I N(0) \ , \tag{3.12}$$

where we have used the relationships of Eqs. (3.5) and (3.8). Adding this contribution to Eq. (3.6) we arrive at

$$V \frac{d^2}{dV^2} (E_0 + E_{\text{ex}}) = \frac{2}{3} \frac{\mathcal{N} \varepsilon_F}{V} [1 - I N(0)] \ . \tag{3.13}$$

It is obvious that this result reproduces the dynamical approach result of Eq. (1.2) with $\xi=0$.

Finally, let us consider the effect of E_ξ on the elastic constant. If we write the effective non-Coulombic ion-ion interaction as $U_\xi(\mathbf{R}_i - \mathbf{R}_j)$, $\mathbf{R}_i$ being the position of the ith ion, the corresponding energy is given as

$$\begin{aligned} E_\xi &= \frac{1}{2} \sum_{i \neq j} U_\xi(\mathbf{R}_i - \mathbf{R}_j) \\ &= \tfrac{1}{2} \int U_\xi(\mathbf{R} - \mathbf{R}') N(\mathbf{R}) N(\mathbf{R}') d\mathbf{R}\, d\mathbf{R}' \ , \\ &= \tfrac{1}{2} \sum_q \tilde{U}_\xi(\mathbf{q}) N(\mathbf{q}) N(-\mathbf{q}) \ , \end{aligned} \tag{3.14}$$

where $N(\mathbf{R})$ is the density of ions, $N(\mathbf{q})$ is its Fourier transform,

$$N(\mathbf{q}) = \int_V N(\mathbf{r}) e^{i\mathbf{r}\cdot\mathbf{q}} d\mathbf{r} \ , \tag{3.15}$$

and the Fourier transform of U_ξ is defined similarly to Eq. (3.10) with the same V dependence as in Eq. (3.11). Extracting the N dependence from the Fourier transform $N(q)$, we obtain

$$E_\xi = \tfrac{1}{2} N^2 \tilde{U}_\xi(\mathbf{Q}) \ , \tag{3.16}$$

where $\mathbf{Q}$ is a representative wave vector. It corresponds to the inverse of the dominant range of the non-Coulombic interactions. In a real lattice this may entail a sum over the reciprocal lattice. Accordingly,

$$V \frac{d^2}{dV^2} E_\xi = \frac{N^2}{V} \tilde{U}_\xi(\mathbf{Q}) \ . \tag{3.17}$$

If we include this contribution to Eq. (3.13), we obtain

$$V \frac{d^2}{dV^2} (E_0 + E_{\text{ex}} + E_\xi) = \frac{2}{3} \frac{\mathcal{N} \varepsilon_F}{V} [1 - I N(0) + \xi] \ , \tag{3.18}$$

with ξ defined as

$$\xi s_0^2 = \frac{N}{M_i} \tilde{U}_\xi(\mathbf{Q}) \ . \tag{3.19}$$

It is obvious that the result of Eq. (3.18) reproduces that of Eq. (1.2). That the definition of ξ as given by Eq. (3.19) is equivalent to that of Eq. (1.4) can be checked from the general formulation relating the ion-ion interaction to the phonon frequency.[8]

B. Elastic constant in the ferromagnetic state

In dealing with the ferromagnetic state of a metal we define the relative magnetization as

$$M = \frac{\mathcal{N}_+ - \mathcal{N}_-}{\mathcal{N}} = \frac{\mathcal{N}_+ - \mathcal{N}_-}{\mathcal{N}_+ + \mathcal{N}_-} \ , \tag{3.20}$$

which is determined from the condition of the total-energy minimum

$$\frac{\partial E}{\partial M} = 0 \tag{3.21}$$

and

$$\frac{\partial^2 E}{\partial^2 M} > 0 \ . \tag{3.22}$$

For the total energy of Eq. (3.1) the condition of Eq. (3.21) gives

$$\varepsilon_{F+} - \varepsilon_{F-} = I \mathcal{N} M \ , \tag{3.23}$$

where $\varepsilon_{F\sigma}$ is the Fermi energy of the σ-spin electrons measured from the bottom of each spin band. For the present free-electron-like energy dispersion of Eq. (3.3), $\varepsilon_{F\sigma} = \hbar^2 k_{F\sigma}^2 / 2m$ with

$$\mathcal{N}_\pm = \frac{V k_{F\pm}^3}{6\pi^2} = \frac{\mathcal{N}}{2} (1 \pm M) \ . \tag{3.24}$$

Thus Eqs. (3.21) and (3.23) become

$$\frac{\partial E}{\partial M} = \frac{\mathcal{N}}{2} \varepsilon_F [(1+M)^{2/3} - (1-M)^{2/3}] - \tfrac{1}{2} I \mathcal{N}^2 M = 0 \ , \tag{3.21'}$$

$$[(1+M)^{2/3}-(1-M)^{2/3}]=\frac{I\mathcal{N}}{\varepsilon_F}M=\tfrac{4}{3}IN(0)M\ . \tag{3.23'}$$

Since ε_F and I change with volume by the relations of Eqs. (3.5) and (3.11), Eq. (3.23') reminds us that changes in V induce changes in M: $dM/dV\neq 0$. Because of this, for the elastic constant in the ferromagnetic state we are required to calculate

$$V\frac{d^2E}{dV^2}=V\frac{\partial^2E}{\partial V^2}+V\frac{\partial^2E}{\partial M^2}\left[\frac{dM}{dV}\right]^2+2V\frac{\partial^2E}{\partial V\,\partial M}\left[\frac{dM}{dV}\right]\ . \tag{3.25}$$

The last two terms do not appear in the paramagnetic state.

If we note that in the ferromagnetic state the energy of Eq. (3.1) is rewritten as

$$E=\tfrac{3}{5}(\mathcal{N}_+\varepsilon_{F+}+\mathcal{N}_-\varepsilon_{F-})-\frac{I}{4}\mathcal{N}^2(1+M^2)+E_\xi\ , \tag{3.26}$$

the first term on the right-hand side of Eq. (3.25) is calculated as

$$V\frac{\partial^2E}{\partial V^2}=\frac{2}{3}\frac{\mathcal{N}\varepsilon_F}{V}\left\{\tfrac{1}{2}[(1+M)^{5/3}+(1-M)^{5/3}]-IN(0)(1+M^2)+\xi\right\}\ . \tag{3.27}$$

As mentioned already, E_ξ is independent of magnetization. Obviously if we set $M=0$ in Eq. (3.27) it reduces to Eq. (3.18).

In calculating the two remaining terms in Eq. (3.25), from Eq. (3.23') first we obtain

$$\frac{dM}{dV}=\frac{\frac{2}{3V}IM}{[(1/N_+(0)+1/N_-(0))]-2I}\ , \tag{3.27'}$$

where we used

$$N_\sigma(0)=\frac{Vmk_{F\sigma}}{2\pi^2\hbar^2} \tag{3.28}$$

together with Eq. (3.24).

The other necessary two derivatives are obtained from Eq. (3.21'),

$$\frac{\partial^2E}{\partial M^2}=\frac{\mathcal{N}^2\mu^2}{\chi_{\mathrm{HF}}}=\frac{\mathcal{N}^2}{4}\left[\frac{1}{N_+(0)}+\frac{1}{N_-(0)}-2I\right]\ , \tag{3.29}$$

$$\frac{\partial^2E}{\partial V\,\partial M}=\frac{-1}{6V}I\mathcal{N}^2M\ , \tag{3.30}$$

where χ_{HF} is what is the so-called high-field susceptibility, the condition of Eq. (3.22) being equivalent to requiring $\chi_{\mathrm{HF}}>0$, and in Eq. (3.30) the relation of (3.23') was used. Combining these results in Eq. (3.25), we finally obtain the elastic constant (bulk modulus) or the sound velocity in the ferromagnetic state

$$\left[\frac{s}{s_0}\right]^2=\tfrac{1}{2}[(1+M)^{5/3}+(1-M)^{5/3}]-IN(0)(1+M^2)+\xi-\tfrac{2}{9}IN(0)\frac{IM^2}{[(1/N_+(0)+1/N_-(0)-2I)]}\ . \tag{3.31}$$

The result of Eq. (3.31) which is obtained by the present total-energy calculation looks quite different from that of Eq. (1.5), which is obtained by the dynamical approach, except the case of $M=1$, where the last term vanishes in Eq. (3.31). (As for the case of $M=0$, see discussion below.) Quite pleasingly, however, we can show the equivalence of Eq. (3.31) and Eq. (1.5) for general values of M. A procedure to prove this equivalence is to rewrite the quantities M and $IN(0)$ appearing in both of these results in terms of $\zeta_\pm$ which is defined by

$$N_\pm(0)=N(0)(1\pm M)^{1/3}=N(0)\zeta_\pm$$

and using the following relations:

$$M=\tfrac{1}{2}(\zeta_+^3-\zeta_-^3)=\tfrac{1}{2}(\zeta_+-\zeta_-)(\zeta_+^2+\zeta_+\zeta_-+\zeta_-^2)\ , \tag{3.32}$$

$$IN(0)=\frac{3}{2}\frac{\zeta_++\zeta_-}{\zeta_+^2+\zeta_+\zeta_-+\zeta_-^2}\ . \tag{3.33}$$

Equation (3.33) is derived from Eq. (3.23'). In this way we finally see that both Eqs. (1.5) and (3.31) reduce to the following same expression:

$$\left[\frac{s}{s_0}\right]^2=\xi-\frac{1}{2}\frac{(2\zeta_++\zeta_-)(2\zeta_-+\zeta_+)}{(\zeta_++\zeta_-)(\zeta_+^2+\zeta_+\zeta_-+\zeta_-^2)}=\xi-\frac{N(0)}{2}\frac{[2N_+(0)+N_-(0)][2N_-(0)+N_+(0)]}{[N_+(0)+N_-(0)][N_+(0)^2+N_+(0)N_-(0)+N_-(0)^2]}\ . \tag{3.34}$$

Discontinuity. One important point to note about Eq. (3.34) is that it does not reduce to Eq. (1.2) for $M=0$. If we set $N_+(0)=N_-(0)=N(0)$ corresponding to $M=0$ in Eq. (3.34), we obtain $(s/s_0)^2=\xi-\frac{3}{4}$. On the other hand, if we set $IN(0)=1$ corresponding to $M=0$ in Eq. (1.2), we obtain $(s/s_0)^2=\xi$. Since Eq. (3.34) is equivalent to Eq. (1.5), this implies that for $M\rightarrow 0$ Eq. (1.5) does not continuously reduce to Eq. (1.2). Such a jump in the elastic constant of an itinerant-electron ferromagnet at $M=0$ was earlier noted from the dynamical approach[12] and our present findings show that the jump is not due to any inadequacy inherent only in the dynamical approach. Note that such a jump in the longitudinal elastic constant persists even in a more elaborate treatment of electron energy.[13]

We can get a physical picture of the origin of the jump in the bulk modulus across the magnetic phase transition as follows. Consider the critical region where the system becomes ferromagnetic upon varying the volume. We may expand the energy in a Landau fashion:

$$E(V,M)=E_p(V)+A(V)M^2+B(V)M^4+\cdots\ .$$

We may replace $A(V)$ by $\alpha(V-V_0)$ and $B(V)$ by $B(V_0)$, where V_0 is the volume at which the system becomes ferromagnetic. Differentiating with respect to volume we have

$$V\frac{d^2E}{dV^2}-V\frac{d^2E_p}{dV^2}=-V\frac{\partial^2E}{\partial M^2}\left[\frac{dM}{dV}\right]^2 .$$

Thus the discontinuity arises from the fact that M^2 is nonzero in the magnetic phase and has nonzero slope, whereas M^2 vanishes identically in the paramagnetic phase and therefore its slope also vanishes identically. This is similar to the λ discontinuity in the specific heat in second-order phase transitions. There the abruptness comes from extra entropy due to magnetic degrees of freedom.

Since E is a function[14] of M^2 (denoted here by z), one can show quite generally that

$$\begin{aligned} V\frac{d^2E}{dV^2}-V\frac{d^2E_p}{dV^2} &=(-1)\frac{n^2}{V}\frac{\partial^2E}{\partial n\,\partial z}\left[\frac{\partial^2E}{\partial z^2}\right]^{-1}\frac{\partial^2E}{\partial z\,\partial n} \\ &=-V\frac{\partial^2E}{\partial z^2}\left[\frac{dz}{dV}\right]^2 , \end{aligned} \tag{3.35}$$

the discontinuity then arises from nonzero $\partial^2E/\partial z^2$. One can convince oneself that this quantity corresponds to the change in the effective Hamiltonian or force with magnetization and hence the discontinuity is seen to be a truly magnetoelastic effect.

Furthermore, thermodynamic stability requires that this quantity is positive definite and hence the discontinuity is always negative. In the dynamical approach, this is understood as the overscreening of the ion-ion interaction by the negative screening constant of electrons. Now we have seen how the total-energy approach also leads to the same result.

IV. CONCLUDING REMARKS

The dynamical response approach gives us the compact and transparent expressions of Eqs. (1.2) and (1.5) for the longitudinal sound velocity or bulk modulus. Indeed it can be generalized to obtain not only other elastic constants but also the dynamical matrix.[15] Our present paper demonstrated how such results of the dynamical approach can be reproduced from the total-energy approach with the standard mean-field approximation. In other words, we explained which kind of approximation in the total-energy approach corresponds to the results of the dynamical approach. Such a correspondence between these two approaches is not obvious at all. For instance, at no time in the dynamical calculation did we need the volume dependence of the effective exchange interaction explicitly, but in the total-energy approach it was essential to invoke the correct volume dependence of the effective exchange [e.g., (3.11) or (A2)] to obtain the same results of Eqs. (1.2) and (1.5).

From our present study we learn the importance of referring to both approaches in understanding the various contributions to the elastic constants. One such example is the above volume dependence of the effective exchange interaction. A second example is the correction due to the nonhomogenous or nonjellium nature of actual materials. The discussion in Sec. III around Eq. (3.14) gives a general introduction to the correction ξ in Eq. (1.2). For a more detailed discussion one needs to go to the dynamical approach. According to Ami, Cade, and Young[15] we have two terms to the effective ion-ion interaction, (i) the bare ion-ion interaction and (ii) that mediated by the electrons which depends on the (dielectric) susceptibility. A closer analysis shows that, in an actual metal, besides the exchange enhancement given by Eq. (2.3) and the renormalization by the long-range Coulomb $v(q)$ in Eq. (2.2), there is also a renormalization due the short-range components of the Coulomb potential. In fact, the contribution to ξ from this source is $\approx 2N(0)\sum_{\mathbf{G}}\tilde{v}(\mathbf{G})$, where $\tilde{v}(\mathbf{G})$ is the Fourier transform of the Coulomb interaction (suitably modified by the appropriate from factors) at the reciprocal-lattice vectors $\mathbf{G}$.

In the paragraph titled *Discontinuity* we show quite generally that, in a magnetic phase transition induced by changes in volume, there is a discontinuous drop in the bulk modulus or sound velocity. The origin of this discontinuity is the onset of an effective interaction induced by the magnetization. This is reminiscent of the λ discontinuity in the specific heat in a second-order phase transition. Note, however, that in a complete discussion of the elastic constants it is necessary to include that of ξ discussed previously. Since ξ represents the short-range part, outside of the long-range Coulomb part, of the effective ion-ion interaction, it may also be sensitive to the thermal expansion of the metal.

The total-energy approach necessarily involves the calculation of the electronic density of states, which is required in the dynamical approach. Our present work demonstrates the usefulness of referring to the dynamical approach results [such as Eqs. (1.2) and (1.5)] even when carrying out a total-energy calculation.

Our discussion in this paper is based on a simplified model of a metal as given by Eq. (3.1) with the free-electron-like dispersion of Eq. (2.3). It is an interesting problem to extend the present discussion explicitly to more realistic situations with a periodic ionic lattice. Another interesting problem would be to extend our discussion to antiferromagnetic metals where currently quite different results are obtained by the two approaches.[16]

APPENDIX

In the appendix we give another model for which both the total-energy and dynamic approaches give the same result for the bulk modulus. In this model the exchange energy is taken to be *precisely* that given by the Hartree-Fock approximation. The exchange energy may still be written in a form similar to Eq. (3.1), viz.,

$$E_{\mathrm{ex}}=-\tfrac{9}{4}(\tilde{I}_+\mathcal{N}_+^2+\tilde{I}_-\mathcal{N}_-^2) , \tag{A1}$$

where

$$\tilde{I}_\pm=\frac{\pi e^2}{3V}(6\pi^2)^{1/3}\left[\frac{V}{\mathcal{N}_\pm}\right]^{2/3}=\bar{I}\left[\frac{\mathcal{N}}{2\mathcal{N}_\pm}\right]^{2/3} . \tag{A2}$$

We note that the effective interaction depends on the spin and that the volume dependence is now $V^{-1/3}$ (instead of $1/V$ as in the Hubbard case).

In the paramagnetic case we have an exchange energy

$$E_{\mathrm{ex}}=-\tfrac{9}{8}\bar{I}\mathcal{N}^2\ . \tag{A3}$$

Comparing this to Eq. (3.9) we have an extra factor of $\frac{9}{2}$. However, this factor is cancelled precisely by those arising from the two volume differentiations of $\bar{I}$ with the result that we again obtain Eqs. (3.12) and (3.13) with $\bar{I}$ replacing I.

For the spin-polarized case the sound velocity is given by the following generalization of Eq. (1.5),

$$\left[\frac{s}{s_0}\right]^2=\frac{2N(0)}{N_+(0)/[1-\tilde{I}_+N_+(0)]+N_-(0)/[1-\tilde{I}_-N_-(0)]}\ , \tag{A4}$$

where, as noted above, the effective exchange interaction depends on spin. We note that although Eq. (A4) is an obvious generalization of Eq. (1.5), Eq. (A1) is not obtained from Eq. (3.1) by splitting the I into I_+ and I_-. This is because, to satisfy conservation requirements[17] we must have, for the effective electron-hole interaction[18]

$$I_\pm=(-1)\frac{\partial^2E_{\mathrm{ex}}}{\partial\mathcal{N}_\pm^2}\ . \tag{A5}$$

The total energy corresponding to Eq. (3.26) is

$$\begin{aligned}E=&\frac{3\mathcal{N}\varepsilon_F}{10}[(1+M)^{5/3}+(1-M)^{5/3}]\\&-\frac{3\mathcal{N}\varepsilon_F}{4}\bar{I}N(0)[(1+M)^{4/3}+(1-M)^{4/3}]\ .\end{aligned} \tag{A6}$$

The equilibrium magnetization is then determined by the vanishing of the quantity

$$\begin{aligned}\frac{\partial E}{\partial M}=&\frac{\mathcal{N}\varepsilon_F}{2}\{(1+M)^{2/3}-(1-M)^{2/3}\\&-2\bar{I}N(0)[(1+M)^{1/3}-(1-M)^{1/3}]\}\ .\end{aligned} \tag{A7}$$

To calculate s we require the three derivatives corresponding to Eqs. (3.27), (3.29), and (3.30), viz.,

$$\begin{aligned}V\frac{\partial^2E}{\partial V^2}=&\frac{\mathcal{N}\varepsilon_F}{3V}\{(1+M)^{5/3}+(1-M)^{5/3}\\&-\bar{I}N(0)[(1+M)^{4/3}+(1-M)^{4/3}]\}\ ,\end{aligned} \tag{A8}$$

$$\begin{aligned}\frac{\partial^2E}{\partial M^2}=&\frac{\mathcal{N}\varepsilon_F}{3}\{(1+M)^{-1/3}+(1-M)^{-1/3}\\&-\bar{I}N(0)[(1+M)^{-2/3}+(1-M)^{-2/3}]\}\\=&\frac{\mathcal{N}^2}{4}\left[\frac{1}{N_+(0)}+\frac{1}{N_-(0)}-\tilde{I}_+-\tilde{I}_-\right]\ ,\end{aligned} \tag{A9}$$

and

$$\frac{\partial^2E}{\partial V\,\partial M}=\frac{\mathcal{N}\varepsilon_F}{3V}\bar{I}N(0)[(1+M)^{1/3}-(1-M)^{1/3}]\ . \tag{A10}$$

Using the above we may evaluate dM/dV to give

$$\begin{aligned}\frac{dM}{dV}&=(-1)\frac{\partial^2E}{\partial V\,\partial M}\left[\frac{\partial^2E}{\partial M^2}\right]^{-1}\\&=(-1)\frac{\bar{I}}{V}\frac{(1+M)^{1/3}-(1-M)^{1/3}}{[1/N_+(0)+1/N_-(0)-\tilde{I}_+-\tilde{I}_-]}\ .\end{aligned} \tag{A11}$$

Substituting these into Eq. (3.25) we obtain for the bulk modulus

$$\begin{aligned}\left[\frac{s}{s_0}\right]^2=&\tfrac{1}{2}[(1+M)^{5/3}+(1-M)^{5/3}]\\&-\bar{I}N(0)[(1+M)^{4/3}+(1-M)^{4/3}]\\&-\tfrac{1}{2}\bar{I}N(0)\frac{\bar{I}[(1+M)^{1/3}-(1-M)^{1/3}]^2}{[1/N_+(0)+1/N_-(0)-\tilde{I}_+-\tilde{I}_-]}\ .\end{aligned} \tag{A12}$$

To prove the equivalence of this and Eq. (A4) we recall the definitions $\zeta_\pm$ given above Eq. (3.32) and note that

$$\tilde{I}_\sigma\zeta_\sigma^2=\bar{I},\quad \bar{I}N(0)=\tfrac{1}{2}(\zeta_++\zeta_-)\ . \tag{A13}$$

We find

$$\left[\frac{s}{s_0}\right]^2=\frac{1}{\zeta_++\zeta_-}\ . \tag{A14}$$

We again obtain a jump $(=\frac{1}{2})$ in the bulk modulus. Since this is equivalent to Eq. (3.35), the positive value indicates that $\partial^2E/\partial z^2<0$ and the magnetized state is unstable. This is a well-known result for the Hartree-Fock state.

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*Present address: Department of Physics, Aoyama Gakuin University, Chitosedai, Setagaya-ku, Tokyo 157, Japan.

[1] M. Shimizu, Y. Nakamura, and J. J. M. Franse, Proceedings of the International Symposium on Magnetoelasticity in Transition Metals and Alloys, Nagoya, 1982 [Physica **119B**, Nos. 1 and 2 (1983)].

[2] See, for instance, J. Zieglowski, H. L. Hafner, and D. Wohlleben, Phys. Rev. Lett. **56**, 193 (1986).

[3] Note that in the jellium model treated here there is only the bulk modulus and, therefore, the sound velocity is the longitudinal one.

[4] M. W. Long and W. Yeung, J. Phys. C **19**, 5077 (1986).

[5] For references see G. D. Mahan, *Many Particle Physics* (Plenum, New York, 1981), p. 451.

[6] E. G. Brovman, Yu Kagan, and A. Kholas, Zh. Eksp. Teor. Fiz. **57**, 1635 (1969) [Sov. Phys.—JETP **30**, 883 (1970)].

[7] V. L. Moruzzi, A. R. Williams, and J. F. Janak, Phys. Rev. B **15**, 2854 (1977).

[8] See, for instance, D. Pines, *Elementary Excitations in Solids* (Benjamin, New York, 1964).

[9] D. J. Kim, B. B. Schwartz, and H. C. Praddaude, Phys. Rev. B **7**, 205 (1973).

[10] D. J. Kim, J. Phys. Soc. Jpn. **40**, 1244 1250 (1976); Solid State Commun. **30**, 249 (1979).

[11] A. L. Fetter and J. D. Walecka, *Quantum Theory of Many Particle Systems* (McGraw-Hill, New York, 1971).

[12] D. J. Kim, Phys. Rev. Lett. **39**, 98 (1977).

[13] H. Hasegawa, M. W. Finnis, and D. G. Pettifor, J. Phys. F. **15**, 19 (1985).

[14] See, e.g., V. L. Moruzzi, Phys. Rev. Lett. **57**, 2211 (1986), where it is pointed out that this functional dependence leads to $M \sim (V-V_0)^{1/2}$. We show here that this also leads to a discontinuity in the bulk modulus.

[15] S. Ami, N. A. Cade, and W. Young, J. Magn. Magn. Mater. **31-34**, 59 (1983).

[16] M. W. Long, Ph.D. thesis, Queen Mary College, University of London, 1985.

[17] L. P. Kadanoff and G. Baym, Phys. Rev. **124**, 287 (1961).

[18] N. A. Cade and W. Young, J. Magn. Magn. Mater. **15-18**, 269 (1980).