Elastic behavior of magnetic systems with a narrow twofold-degenerate band

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The modification of the effect of electron-lattice interaction on the shear modulus $C'=\frac{1}{2}(C_{11}-C_{12})$ in itinerant magnetic systems with the Fermi energy lying on a narrow twofold-degenerate band is investigated on the basis of the Hartree-Fock approximation of the degenerate Hubbard Hamiltonian. The softening of the elastic constant due to the electron-lattice interaction at $T=0$ is more for weakly magnetic (ferro- or antiferromagnetic) systems compared to the case of saturated moment systems. As T approaches T_c (or T_N) the elastic constant C' decreases sharply and the amount of decrease is larger for the saturated ferromagnetic (or antiferromagnetic) system than that for the weakly magnetic system. These results are found to be sensitive functions of the interorbital exchange. In the paramagnetic phase, the electronic contribution to C' depends on the density of states at the Fermi energy and is weakly temperature dependent. These results are discussed in light of the elastic anomalies of C' in bcc iron.

I. INTRODUCTION

It has been established that the electron-lattice interaction in degenerate electronic states plays the dominant role in causing structural transitions in various types of systems, e.g., the high-temperature superconductors like $A15$ compounds,[1] lanthanum chalcogenides,[2] and compounds showing cooperative Jahn-Teller transitions.[3] The softening of elastic constants with temperature is seen as the manifestation of this interaction. Even in the absence of any structural transition, the magnetic interactions between the electrons in the degenerate bands would modify the amount of softening of the elastic constants. There exists a considerable amount of experimental evidence of this effect—partiuclarly of the shear modulus near magnetic transition temperatures—in three-dimensional systems.[4] Recent neutron scattering results on bcc iron[5] showing a 75% drop in the value of the shear modulus C' between room and Curie temperatures and considerable softening of some phonon branches have raised the necessity of undertaking self-consistent calculations of electron-phonon and the magnetic interactions present in such systems. The renormalization of longitudinal sound velocity as a function of magnetic moment has been studied earlier in an itinerant ferromagnet by Kim.[6] Subsequently, a similar study has been made by Yamda for itinerant antiferromagnetic system.[7] But no model calculation of the temperature dependence of the elastic constant has been made by them. Also these calculations have been done for nondegenerate band systems. Recently Hasegawa *et al.*[8] have done an *ab initio* calculation of elastic constants in bcc iron and have included the spin-fluctuation effect which is important near the transition temperature T_c and also the coupling of electrons with the lattice through the hopping integrals. It has been argued that the spin fluctuation affects the shear modulus strongly around T_c. The effect of the electron-lattice interaction (the band Jahn-Teller mechanism in which there is a splitting of the degenerate subbands proportional to the strain[2,9–11]) on the shear modulus in degenerate band systems have not yet been studied systematically in the magnetic phases. Theoretical understanding remains incomplete without such an analysis.

The interplay between the elastic and magnetic interactions in a twofold-degenerate Hubbard band model has recently been studied on the basis of the Hartree-Fock approximation of intrasite Coulomb and interorbital exchange interactions by making Landau expansion of the free energy in terms of two order parameters, namely, tetragonal strain and magnetic moment.[10] It is, therefore, limited to weak ferromagnetic cases. In this paper we report a model calculation on the thermal variation of shear modulus C' in itinerant magnetic systems with twofold-degenerate bands both for ferromagnetic and antiferromagnetic cases without making any Landau-type analysis so that the results are applicable to both strong and weak moment systems. It is shown that the coupling of the lattice with local density of orbitals causes the shear modulus to decrease as T tends to the transition temperature and the interorbital exchange J plays a very crucial role in determining the magnitude of softening. In fact a small increase in the value of J, the exchange parameter, can completely destroy the effect of magnetic ordering on C'—particularly for an antiferromagnetic system with half-filled band. We also consider the effect of different fillings of the band on C' using a simple model density of state (DOS).

The analysis for the ferromagnetic and antiferromagnetic cases are presented in Secs. II and III, respectively. Since for bcc iron the DOS near the Fermi energy E_f arises principally from e_g-type electrons, favorable comparison of our result with that of Hasegawa *et al.*[8] is possible. These and the discussions on our results are given in Sec. IV.

II. FERROMAGNETIC CASE

The model Hamiltonian for e_g electrons in the presence of magnetic interactions and tetragonal-type elastic mode e can be written as

$$\begin{aligned} H=&\sum_{i,j,\sigma} t_{ij}(C^{\dagger}_{i1\sigma}C_{j1\sigma}+C^{\dagger}_{i2\sigma}C_{j2\sigma}) \\ &+U\sum_{i}(\hat{n}_{i1\uparrow}\hat{n}_{i1\downarrow}+\hat{n}_{i2\uparrow}\hat{n}_{i2\downarrow}) \\ &+U'\sum_{i,\sigma,\sigma^1}\hat{n}_{i1\sigma}\hat{n}_{i2\sigma^1}-J\sum_{i,\sigma}\hat{n}_{i1\sigma}\hat{n}_{i2\sigma} \\ &+Ge\sum_{i,\sigma}(\hat{n}_{i1\sigma}-\hat{n}_{i2\sigma})+\tfrac{3}{2}NC_0e^2 , \end{aligned} \tag{1}$$

where N is the number of atoms, 1 and 2 denote the two e_g orbitals, U and U' are the intra-atomic intraorbital and interorbital Coulomb terms, J is the interorbital exchange interaction, G is the magnitude of coupling between e_g-type electrons and strain modes, and $C_0=\frac{1}{2}(C_{11}-C_{12})$ is the shear elastic constant arising from electrons other than the e_g ones. Under the Hartree-Fock approximation and for the ferromagnetic case, this Hamiltonian reduces to the following form,

$$\begin{aligned} H^{\mathrm{HF}}=&\sum_{\mathbf{k},\gamma,\sigma}E_{\mathbf{k}\gamma\sigma}\hat{n}_{\mathbf{k}\gamma\sigma}+\tfrac{3}{2}NC_0e^2-NU(n_{1g}n_{1\downarrow}+n_{2g}n_{2\downarrow}) \\ &-NU'\sum_{\sigma,\sigma'}n_{1\sigma}n_{2\sigma'}+NJ\sum_{\sigma}n_{1\sigma}n_{2\sigma} , \end{aligned} \tag{2}$$

where $\langle n_{i\gamma\sigma}\rangle=n_{i\gamma\sigma}=n_{\gamma\sigma}$ for the ferromagnetic case, γ being the band index, the energies $E_{\mathbf{k}\gamma\sigma}$ are given by

$$E_{\mathbf{k}\gamma\sigma}=\varepsilon_{\mathbf{k}}+\gamma\left[Ge+\frac{A}{4}\delta n\right]-\sigma\frac{Bm}{4}+\sigma\gamma\frac{D}{4}\delta m , \tag{3}$$

where $\sigma=\mp 1$ for the up and down spins respectively, $\gamma=\pm 1$ for the orbitals 1 and 2, $A=2U'-U-J$, $B=U+J$. The population excess $\delta n=n_2-n_1$ arises from the lifting of the degeneracies due to the tetragonal strain. This produces different magnetization for two bands, and this difference of magnetization $\delta m=(n_{2\uparrow}-n_{2\downarrow})-(n_{1\uparrow}-n_{1\downarrow})$ will contribute to elastic constant due to its nonzero variation with strain in the limit of $e\to 0$. The magnetic moment is given by $m=n_{\uparrow}-n_{\downarrow}$ in units of μ_B. Also, $n=\sum_{\gamma,\sigma}n_{\gamma\sigma}$, the total number of electrons per atom. The free energy calculated from the Hartree-Fock Hamiltonian given by Eq. (2) leads to the following expression for the total shear elastic constant C's,

$$C'(T)=C_0-\frac{G}{3}\left[\frac{\partial(\delta n)}{\partial e}\right]_{e\to 0} , \tag{4}$$

where

$$\delta n=n_2-n_1=\sum_{\mathbf{k},\sigma}[f(E_{\mathbf{k}2\sigma})-f(E_{\mathbf{k}1\sigma})] , \tag{5}$$

with $f(E)$ as the Fermi function. In order to derive the second term in the right-hand side of Eq. (4), it is necessary to expand δn. Assuming e, δn, and δm to be small and keeping m arbitrary, we obtain the following expression for $n_{\gamma\sigma}$,

$$\begin{aligned} n_{\gamma\sigma}=&\sum_{\mathbf{k}}f(E_{\mathbf{k}\sigma}) \\ &+\sum_{\mathbf{k}}f'(E_{\mathbf{k}\sigma})\left[\gamma\left[Ge+\frac{A}{4}\delta n\right]+\sigma\lambda\frac{D}{4}\delta m\right] , \end{aligned} \tag{6}$$

where $f'(E_{\mathbf{k}\sigma})$ is the first derivative of $f(E_{\mathbf{k}\sigma})$ with respect to $E_{\mathbf{k}\sigma}=\varepsilon_{\mathbf{k}}-\sigma Bm/4$. Equation (6) then gives us

$$\delta n=F_+\left[-2Ge-\frac{A}{2}\delta n\right]+F_-\left[-\frac{D}{2}\delta m\right] \tag{7}$$

and

$$\delta m=F_+\left[-\frac{D}{2}\delta m\right]+F_-\left[-2Ge-\frac{A}{2}\delta n\right] , \tag{8}$$

where

$$F_{\pm}=\int\rho(\varepsilon)d\varepsilon\left[\frac{\partial f}{\partial\varepsilon}(E_{\downarrow})\pm\frac{\partial f}{\partial\varepsilon}(E_{\downarrow})\right] . \tag{9}$$

In deriving Eqs. (7) and (8) we have neglected the variation of hopping due to strain. In the calculation done by Hasegawa *et al.*[8] the strain dependence of the free energy comes from the variation of hopping. From Eqs. (7) and (8), we now get

$$\delta n=-\frac{2Ge\left[F_+-\frac{D}{2}\frac{F_-^2}{1+\frac{D}{2}F_+}\right]}{1+\frac{A}{2}\left[F_+-\frac{D}{2}\frac{F_-^2}{1+\frac{D}{2}F_+}\right]} . \tag{10}$$

Equation (4), therefore, gives

$$C'(T)=C_0+\tfrac{2}{3}G^2\frac{F_1}{F_2} \tag{11}$$

with

$$\begin{aligned} F_1=&F_+-\frac{D}{2}\frac{F_-^2}{1+\frac{D}{2}F_+} , \\ F_2=&1+\frac{A}{2}F_1 . \end{aligned} \tag{12}$$

Hence

$$\Delta C=\tfrac{2}{3}G^2\frac{F_1}{F_2} , \tag{13}$$

where $\Delta C=C'-C_0$. The temperature dependence of the contribution of e_g electrons to the shear constant then arises from that of F_1 and F_2 through the integrals involv-

ing derivatives of the Fermi functions for the up- and down-spin subbands. These can be evaluated only for specific form of the DOS of the e_g electrons. Only at $T=0$ these integrals can be expressed as

$$F_{\pm} = -(\rho_{\uparrow} \pm \rho_{\downarrow}) , \tag{14}$$

where $\rho_{\uparrow,\downarrow}$ are the values of the DOS at the Fermi energies for the two spin subbands. At $T=0$ we therefore obtain

$$F_1 = -\left[(\rho_{\uparrow}+\rho_{\downarrow}) - \frac{D}{2}\rho_{\uparrow}\rho_{\downarrow}\right] \Big/ \left[1 - \frac{D}{2}(\rho_{\uparrow}+\rho_{\downarrow})\right] ,$$
$$F_2 = 1 + \frac{A}{2}F_1 . \tag{15}$$

The coupling of the lattice with the local electron density in the degenerate band reduces the elastic constant and this reduction is enhanced due to the intrasite Coulomb and exchange interactions. The role of $A=U-5J$ in the paramagnetic state (for e_g-electrons $U'=U-2J$) is important in determining ΔC. In the ferromagnetic state the magnetic contribution to C' depends on the saturation magnetic moment. In an extreme limit ($n_{\uparrow}=n, n_{\downarrow}=0$) the contribution to ΔC is zero. But it can be appreciable for a system with small saturation moment. We note that the part of F_1 namely proportional to D comes from the variation of moment due to unequal population of subbands.

In order to study the temperature dependence of ΔC, we have evaluated F_1 and F_2 as a function of temperature for some values of U,J and filling of the band using simple form of DOS $\rho(\varepsilon)=\frac{3}{2}(1-\varepsilon^2)$. The results are given in Figs. 1–3. Figure 1 corresponds to the half-filled fully saturated state whereas Figs. 2 and 3 present the results for weak ferromagnetic cases. The trends of the numerical results can be summarized as follows.

(1) The decrease in the value of ΔC between $T=0$ and $T=T_c$ and also the rate of decrease depend on the value of J. The sign of A in F_2 plays an important role in this change of ΔC. For $A>0$, this variation is larger than that for $A<0$ for a given value of $U+J$. With decreasing J the tendency towards the tetragonal transformation increases. The cubic-to-tetragonal transition occurs when $(U-5J+4G^2/C_0)\rho_0 > 1$.[11] The system can gain energy either by lifting degeneracy or going into the magnetic state. So there is a competition between the large moment state and the incipient band Jahn-Teller effect reflected in softening of shear modulus. Therefore, the maximum softening from $T=0$ to $T=T_c$ occurs for systems with large moment. Near $T \approx T_c$, the change in shear modulus varies as m^2. Consequently, iron with large magnetic moment at $T=0$ shows appreciable softening of C'. For weak moment system the decrease from $T=0$ to $T=T_c$ in the shear modulus is, therefore, smaller (Fig. 3).

(2) The contribution to ΔC from electron-lattice coupling at $T=0$ is small for the saturated moment case and is not sensitive to the value of A whereas for the weak ferromagnetic case it is large and depends more strongly on J.

(3) The rate of variation of ΔC with temperature is larger for $T<T_c$ than that for $T>T_c$. The magnitude of the slope decreases with the increase of J.

(4) For high temperatures ($T>T_c$) the shear modulus increases from its value at $T=T_c$. But to get correct temperature dependence of C', the thermal variation of C_0 has to be included. Normally in metals, the elastic constant C_0 decreases with temperature. At low T such variation is small so that the thermal variation of C' is solely

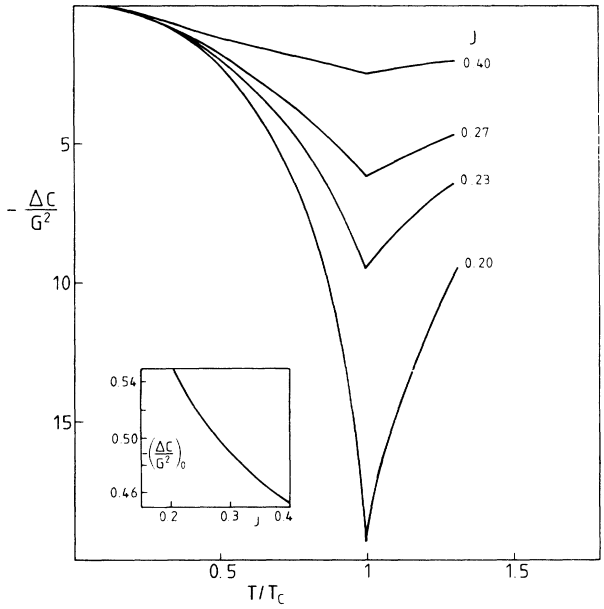

FIG. 1. Variation of the decrease of shear modulus from its value at $T=0$ K with temperature T/T_c for different values of J corresponding to the half-filled band case with $U+J=2.0$. The saturation moment is 1.99. Inset gives the reduction at $T=0$ K for different values of J.

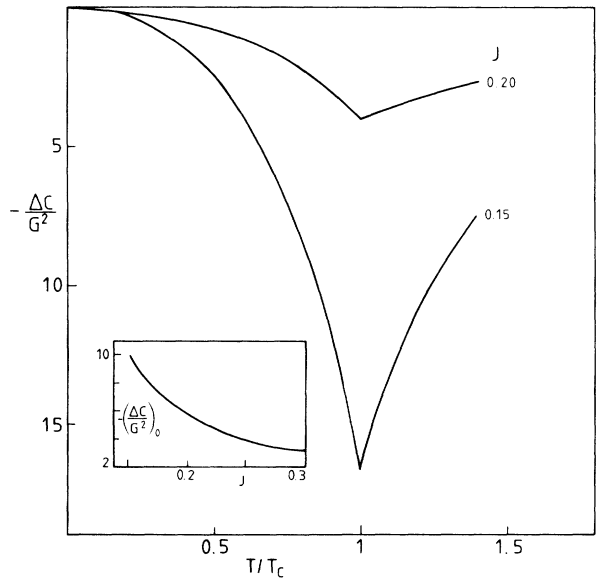

FIG. 2. Same as Fig. 1 with $U+J=1.5$ for the half-filled case. The saturation moment is 1.55. Inset gives contribution at $T=0$ K due to electron-lattice coupling for different J values. Note it is much larger than the preceding case.

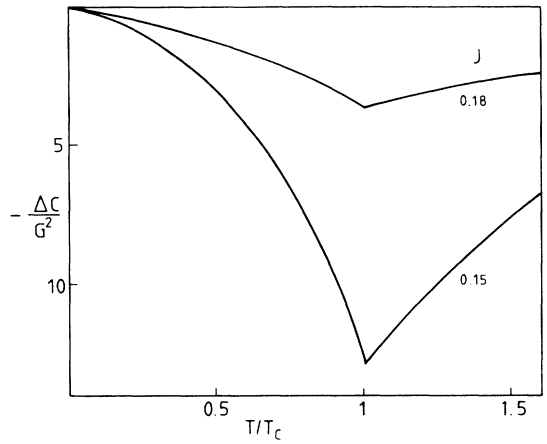

FIG. 3. Same as Fig. 2 with $U+J=1.5$, band filling $n=2.8$ and moment is 0.71.

due to electron-lattice coupling. At high T, the thermal decrease of C_0 becomes important so as to cause slower variation of C'. For $T \gg T_c$, the elastic constant is nearly C_0 and hence decreases again.

III. ANTIFERROMAGNETIC CASE

Since the antiferromagnetic case is the particular case of spin-density wave (SDW) with wave vector $Q=\pi/a$, a being the lattice constant, we can define an order parameter[11]

$$b_{\alpha\sigma}=\sum_{\mathbf{k},\mathbf{Q}}(C^{\dagger}_{\mathbf{k}+\mathbf{Q},\alpha\sigma}C_{\mathbf{k},\alpha\sigma}) \ . \tag{16}$$

In order to get maximum amplitude of this order parameter we take

$$b_{\alpha\sigma}=-b_{\alpha-\sigma}=b_{\alpha} \tag{17}$$

and

$$n_{\alpha\sigma}=n_{\alpha-\sigma} \ .$$

This gives the moment per site in each band as

$$S_{\alpha z}=\tfrac{1}{2}(b_{\alpha\uparrow}-b_{\alpha\downarrow})e^{i\mathbf{Q}\cdot\mathbf{R}i}=b_{\alpha}e^{i\mathbf{Q}\cdot\mathbf{R}i} \ . \tag{18}$$

The total moment

$$S_z=\sum_{\alpha}S_{\alpha z}=be^{i\mathbf{Q}\cdot\mathbf{R}i} \ , \tag{19}$$

where $b=b_1+b_2$. As the strain lifts the orbital degeneracy the orbital parameter b_α would not be the same for the two orbitals and we therefore introduce

$$\delta b=b_1-b_2 \ . \tag{20}$$

Solving the Hartree-Fock Hamiltonian for the antiferromagnetic (AF) case we get the following Hamiltonian in the diagonal form (assuming complete nesting condition for the bare band energies),

$$H^{\mathrm{AF}}=\sum_{\mathbf{k}\alpha\gamma}E_{\mathbf{k}\alpha\gamma}\hat{n}_{\mathbf{k}\alpha\gamma}+\frac{B}{2}b^2+\frac{D}{2}(\delta b)^2-\frac{A}{8}(\delta n)^2 \ , \tag{21}$$

where

$$E_{\mathbf{k}\alpha\gamma}=\alpha X+\gamma[\varepsilon_{\mathbf{k}}^2+\delta\alpha^2)]^{1/2} \ . \tag{22}$$

Here $\alpha=+1$ for orbital 1 and -1 for orbital 2, $\gamma=\pm$ for higher and lower Slater spin subbands, respectively, $\delta_\alpha=(B/2)b-\alpha(D/2)\delta b$ and $X=Ge+(A/4)\delta n$. We have neglected a constant term in $E_{\mathbf{k}\alpha\gamma}$.

For the calculation of the shear elastic constant it is necessary to get an expression for δn in terms of e, b, and δb. From the definition of δn we obtain

$$\delta n=n_2-n_1=\sum_{\mathbf{k},\gamma}[f(E_{\mathbf{k}2\gamma})-f(E_{\mathbf{k}1\gamma})] \ . \tag{23}$$

Expanding the Fermi function about $f(E_{\mathbf{k}})$ and $f(-E_{\mathbf{k}})$ where $E_{\mathbf{k}}=[\varepsilon_{\mathbf{k}}^2+(Bb/2)^2]^{1/2}$ and keeping terms linear in e and δb we obtain finally

$$\delta n=-2XG_0+\frac{BD}{2}b\delta bG_1 \ , \tag{24}$$

where

$$G_0=\sum_{\mathbf{k}}\left[\frac{\partial f(E_k)}{\partial E_{\mathbf{k}}}+\frac{\partial f(-E_{\mathbf{k}})}{\partial E_{\mathbf{k}}}\right] , \tag{25}$$

$$G_1=\sum_{\mathbf{k}}\left[\frac{\partial f(E_{\mathbf{k}})}{\partial E_{\mathbf{k}}}+\frac{\partial f(-E_{\mathbf{k}})}{\partial E_{\mathbf{k}}}\right] .$$

In order to get expression δb in terms of e, we derive $b_{\alpha\sigma}$ by calculating $\langle C_{\mathbf{k}+\mathbf{Q},\alpha\sigma}C_{\mathbf{k},\alpha\sigma}\rangle$ through the Green's function formalism[11] and finally obtain

$$b\pm\delta b=-\sum_{\mathbf{k}}\frac{Bb\pm D\delta b}{(E_{\mathbf{k}1,2+}-E_{\mathbf{k}1,2-})}\times[f(E_{\mathbf{k}1,2+})-f(E_{\mathbf{k}1,2-})] \ . \tag{26}$$

Expansion of Fermi function in terms of X, b and δb gives δb in lowest orders of b and Ge as

$$\delta b=\frac{B}{2}XbG_1/G_2 \ , \tag{27}$$

where

$$\begin{aligned} G_2&=1+\frac{D}{2}G_3-\frac{B^2}{8}Db^2G_4 \ , \\ G_3&=\sum_{\mathbf{k}}\frac{1}{E_{\mathbf{k}}}[f(E_{\mathbf{k}})-f(E_{\mathbf{k}})] \ , \\ G_4&=\sum_{\mathbf{k}}\left[\frac{1}{E_{\mathbf{k}^3}}[f(E_{\mathbf{k}}-f(-E_{\mathbf{k}})]-\frac{1}{E_{\mathbf{k}^2}}[f'(E_{\mathbf{k}}-f'(-E_{\mathbf{k}})]\right] . \end{aligned} \tag{28}$$

Substituting this expression of δb in Eq. (24) we obtain

$$\delta n=-2Ge\frac{G_5}{G_6} \ , \tag{29}$$

where

$$G_5 = G_0 - \frac{B^2}{8} D \frac{G_1^2}{G_2} b^2 ,$$
$$G_6 = 1 + \frac{A}{2} G_5 . \tag{30}$$

This expression of δn for the antiferromagnetic case is to be compared with that of the ferromagnetic case given by Eq. (7) where we get in the lowest order of m, $F_- \propto m^2$. The electronic contribution to C' in the antiferromagnetic case is then obtained as

$$\Delta C = \tfrac{2}{3} G^2 \frac{G_5}{G_6} . \tag{31}$$

In the paramagnetic limit we obtain the same expression as for the ferromagnetic case. Following the same procedure as earlier, we first solve the two self-consistent equations—one for b which is obtained from Eq. (26) in the limit of $e \to 0$ and $\delta b \to 0$ and the other for the chemical potential μ for each value of temperature. These are given below:

$$\frac{2}{U+J} = -\int_{-W}^{W} \frac{\rho(\varepsilon) d\varepsilon}{E} \times \left[\frac{1}{1+e^{\beta(E-\mu)}} - \frac{1}{1+e^{-\beta(E-\mu)}} \right] , \tag{32}$$

$$n = 2 \int_{-W}^{W} \rho(\varepsilon) d\varepsilon \left[\frac{1}{1+e^{\beta(E-\mu)}} + \frac{1}{1+e^{-\beta(E-\mu)}} \right] , \tag{33}$$

where $E = [\varepsilon^2 + (Bb/2)^2]^{1/2}$ and W is half of the bandwidth density of states. We have used the model density $\rho(\varepsilon) = \frac{3}{2}(1-\varepsilon^2)(2W=1)$ as in the ferromagnetic case. Using these values of b and μ, the integrals involved in G_5 and G_6 are numerically evaluated. The temperature variation of ΔC in units of G^2 are given in Fig. 4 for the half-filled band case. The value of b is 1.82 at $T=0$ and is, therefore, close to the saturated moment case. It is seen that though the results are qualitatively similar to those for the ferromagnetic case, there are some features worth mentioning for this case of antiferromagnets. First, J has more effect in reducing the value of C' between $T=0$ and $T=T_c$ and a small value of J is sufficient to reduce ΔC drastically. So in real antiferromagnetic systems with finite and nonnegligible J, ΔC, as the result of magnetic ordering, is expected to be small for the e_g electrons. Secondly, the electron-lattice contribution to ΔC is negligible around $T=0$ but it is large around $T=T_N$, particularly for small values of J. This is also very sensitive to the value of $A=U-5J$ even in the paramagnetic case. For more (or less) than half-filled cases and for weak antiferromagnets the results are similar to the ferromagnetic case. The elastic constant is reduced, although the variation between $T=0$ and $T=T_N$ is not large.

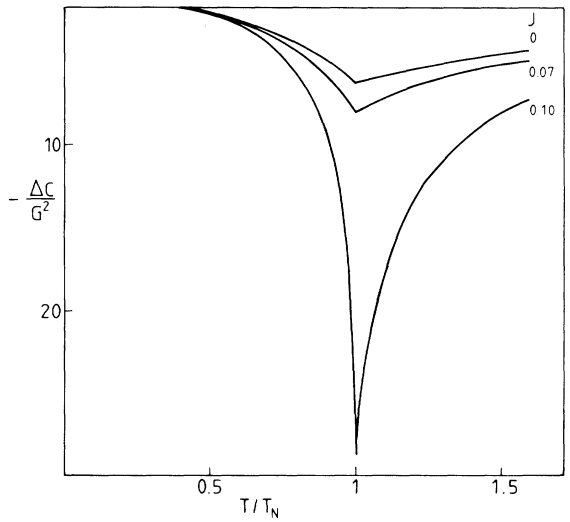

FIG. 4. Antiferromagnetic case with $U+J=1$, $n=2$, and the antiferromagnetic order parameter is 1.82 ($2W=1$ for all cases).

IV. DISCUSSION

The results presented in the preceding two sections point out the importance of the band Jahn-Teller interaction in determining the shear modulus C'. It depends on the magnetic state of the system. The amount of softening around T_c (or T_N) is more for systems with large saturation moment. On the other hand, the elastic constant is much reduced at $T=0$ for systems with weak saturation moment. The softening of the shear modulus can be understood from band Jahn-Teller mechanism. When the Fermi energy lies on a degenerate band the system wants to remove the degeneracy which involves the transfer of electrons from one orbital to another with consequent decrease in the band energy. This interorbital charge fluctuation causes a softening of shear modulus. For systems with large moments, such interorbital charge fluctuation is difficult due to large magnetic energy involved at $T=0$ but becomes important at $T \to T_c$ or T_N where ordering energy is less. This, therefore, causes a larger softening from $T=0$ to $T=T_c$ or T_N. Due to smaller magnetic energy involved for systems with weak saturated moments, interorbital charge transfer is easier and hence a larger reduction of C' at $T=0$ results. Apart from the electron-lattice interaction such reduction of C' depends on parameters U, U', and J. For a given value of U, the interorbital exchange J affects ΔC most through the parameter $A=U-5J$ which determines the amount of interorbital fluctuation. The present mean-field treatment gives the variation of C' with temperature in qualitative agreement with experimental results on bcc iron and γ-Mn (Ref. 12) doped with few percentage of Ni. But for a better comparison it is necessary to use a more realistic DOS and more appropriate values of U and J as well as spin-fluctuation effect around T_c or T_N. Since the purpose of this model calculation is to point out the role of the degeneracy of the band in which the Fermi energy lies, we refrain from pursuing further comparison with experimental results. Our results have similar qualitative features below the transition temperature as those given by Hasegawa *et al.* Our results show a rather large increase of C' for T larger than T_c; this may be due to the Hartree-Fock approximation used in our calculation and neglect of local moments. But the present self-consistent calculation

of the modifications of the effect of the electron-lattice interaction of C' due to magnetic moment formation treated within the Hartree-Fock approximation of the degenerate Hubbard Hamiltonian will serve as a starting point of further model calculations.

In conclusion, the present analysis of shear elastic constant based on the Hartree-Fock approximation indicates the importance of electron-lattice coupling in a degenerate band on the softening of shear modulus in the presence of magnetic interactions. The phenomenon is influenced strongly by interorbital exchange J. In order to get more quantitative results it is necessary to develop the present model further—particularly the effects of dynamics of spins through the generalized susceptibility approach. Also, large softening of C' at $T=T_c$ in iron indicates that phonons excited at T_c might modify the value of T_c. All these are under consideration now and will be reported in due course.

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[1]M. Weger and J. B. Goldberg, in *Solid State Physics,* edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1973), Vol. 28, p. 1; R. N. Bhatt Phys. Rev. B **16**, 1915 (1977); R. N. Bhatt and W. L. Mcmillan, *ibid.* **14**, 1007 (1976).

[2]W. Westerholt, F. Timmer, and H. Bach Phys. Rev. B **32**, 2985 (1985); S. K. Ghatak, D. K. Ray, and C. Tannous, *ibid.* **18**, 5379, (1978); P. J. Ford, W. A. Lambson, A. J. Miller, G. A. Saunders, H. Bach, and S. Methfessel, J. Phys. C. **13**, L697 (1980).

[3]R. J. Elliot, R. T. Harley, W. Hayes, and S. R. P. Smith, Proc. R. Soc. London, Ser. A **328**, 217 (1972); J. R. Sandercock, S. B. Palmer, R. J. Elliot, W. Hayes, S. R. P. Smith, and A. P. Young, J. Phys. C **5**, 3126 (1972).

[4]M. M. Von Choy *et al.*, in *Elastic, Piezoelectric, Pyroelectric, Piezooptic, Electrooptic Constants and Nonlinear Dielectric Susceptibilities of Crystals,* Vol. 11 of *Landolt-Börnstein: New Series,* edited by K.-H. Hellwege and A. M. Hellwege (Springer-Verlag, Berlin, 1979).

[5]S. K. Satija, R. P. Comes, and G. Shirane, Phys. Rev. B **32**, 3309 (1985).

[6]D. J. Kim, J. Phys. Soc. Jpn. **40**, 1244 (1976); **40**, 1250 (1976).

[7]H. Yamada, Solid State Commun. **37**, 841 (1981); S. Ami, N. A. Cade, and W. Young, J. Magn. Magn. Mater. **31-34**, 59 (1983).

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

[9]J. Labbe and J. Friedel, J. Phys. (Paris) **27**, 153 (1976); **27**, 303 (1966); J. P. Jardin and J. Labbe, J. Solid State Chem. **46**, 275 (1983).

[10]D. K. Ray and J. P. Jardin, Phys. Rev. B **33**, 5021 (1986).

[11]S. K. Ghatak and D. K. Ray, Phys. Rev. B **31**, 3064 (1985).

[12]G. A. Saunders (unpublished).