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Role of Magnetism in the Volumic and the Elastic Anomalies in Ferromagnetic Materials

Sang Koo You and Chul Koo Kim
Department of Physics and Institute for Mathematical Sciences, Yonsei University, Seoul 120-749, Korea

Kyun Nahm
Department of Physics, Yonsei University, Wonju 220-710, Korea

The physical origins of anomalous volume effect (Invar effect) and elastic effect (Elinvar effect) are critically examined. We found that, unlike the volume effect, the shear elastic properties are not much influenced by the ferromagnetic transition. This finding shows that the two anomalies originate from different physical origins, thus contradicting the conventional wisdom. We discuss the consequences of this finding in the light of recent experiments.

I. INTRODUCTION

Since Guillaume first discovered that certain materials had zero or negative thermal expansion coefficients around the room temperature about one hundred years ago [1], enormous amounts of research efforts have been spent to elucidate the physical origin of this volumic anomaly which is generally called the invar effect. One of prominent features of the invar materials is that they also possess the elastic anomaly, which is called the elinvar effect [2]. In the elinvar materials, certain elastic constants decrease when temperature is lowered, whereas, in normal metals, all the elastic constants increase monotoneously with decreasing temperature. Since the two anomalous effects, the invar and the elinvar effects, occur simultaneously in the invar materials, it has been generally believed that they have the same physical origin [2].

However, recently, it has been observed that the elinvar type elastic anomalies could occur also in non-invar materials [3]. It was found by the authors that the elastic anomaly of nonmagnetic A-15 compounds could be explained using a theoretical scheme based on redistribution of electrons between strain-split d-bands [4]. The same theoretical scheme was later found applicable to the elastic anomalies of ferromagnetic [5], antiferromagnetic [6], and superconducting materials [7]. Although this theoretical scheme is based on the existence of narrow degenerate d-bands which is also true for the invar materials, it does not directly depend on the invar property. It raises doubt on the conventional wisdom that the two effects originate from the same physical mechanism. In this context, one of the interesting problems is the role of magnetism in the volumic and elastic anomalies. In all existing invar theories, the magnetism is known to play a dominant role [2,8]. Therefore, it is necessary to investigate whether the magnetism plays an important role in the elastic anomaly.

II. ROLE OF MAGNETISM IN THE ELASTIC ANOMALY

Majority of existing theories for the invar effect are based on the magnetic moment and the volume relationship as represented by the moment-volume instability theory by Wassermann [2]. Another important theoretical approach is the electron-phonon theory by Kim [8], in which the coupling between the longitudinal phonon and the itinerant electrons provides the necessary mechanism for the volumic anomaly. In both types of theories, magnetism plays a crucial role.

Below, we examine whether the mechanism leading to the invar effect has any physical bearing on the elastic anomaly. First, the moment-volume instability theory is examined. In this theory, there are two different volume states; namely the high and the low magnetic moment states. With temperature change, it is assumed that there occurs the transition between the two moment states, thus changing the volume of the materials. Here, we note that this theory is purely volumic and, thus, it is not possible to have any effect on the shear elastic constants. Thus, this theory does not have any direct relation to the elinvar effect.

Secondly, we examine the electron-phonon theory. In the electron-phonon theory, the electron-phonon interaction is shown to renormalize the longitudinal acoustic phonon frequency [8]. Since the phonon frequency is renormalized through the interaction with the electrons which go through the magnetic transition, the magnetism affects the phonon frequency and, consequently, the thermal expansion coefficient. So that the electron-phonon interaction plays a role in the elastic anomaly, the electron should couple to the transverse phonon instead of the longitudinal one. However, it is well known that the electron does not couple to the transverse phonon in the normal process. Therefore, it is necessary to consider the Umklapp process for the following electron-phonon Hamiltonian

$$H_{el-ph} = \sum_{kq\lambda} \sum_{\sigma,K_m} G_{q\lambda k}^{K_m} (b_{q\lambda} + b_{-q\lambda}^{\dagger}) a_{k+q+K_m,\sigma}^{\dagger} a_{k,\sigma} \tag{1}$$

where

$$G_{q\lambda k}^{K_m} = -\sqrt{\frac{N}{m}} \sqrt{\frac{1}{2\Omega_{q\lambda}}} V_{q+K_m} i(\vec{q} + \vec{K}_m) \cdot \hat{e}_{q\lambda} \times \int u(\vec{q} + \vec{K}_m + \vec{k}, r)^* u(\vec{k}, r) d\tau \tag{2}$$

It is not an easy task to evaluate the renormalization effect of the above Hamiltonian on the phonon frequency directly. Therefore we consider the phonon Green's function in the Zubarev notation [9]; $G_{AB}(\omega) = \langle\langle A; B \rangle\rangle$, which gives the equation of the motion

$$(\omega^2 - \Omega_{q\lambda}^2) \langle\langle \phi_{q\lambda}; \phi_{-q\lambda} \rangle\rangle = 2\Omega_{q\lambda} + 2\Omega_{q\lambda} \sum_{k\sigma K_m} G_{q\lambda k}^{K_m} \times \langle\langle \phi_{q\lambda}; a_{k+q+K_m,\sigma}^{\dagger} a_{k\sigma} \rangle\rangle \tag{3}$$

where $\Omega_{q\lambda}$ is the bare phonon frequency. Now approximating the higher order Green's function in the mean-field spirit, we obtain the renormalized phonon frequency

$$\omega_{q\lambda}^2 = \Omega_{q\lambda}^2 + 2\Omega_{q\lambda} \sum_{k\sigma K_m} \left| G_{q\lambda k}^{K_m} \right|^2 \times \frac{n_{k+q+K_m,\sigma} - n_{k\sigma}}{\omega_{q\lambda} + \epsilon_{k+q+K_m} - \epsilon_k} \times \frac{1 + \tilde{V}(q) \tilde{F}_{\sigma}(q, \omega_{q\lambda})}{1 + v(q)(\tilde{F}_{\sigma}(q, \omega_{q\lambda}) + \tilde{F}_{-\sigma}(q, \omega_{q\lambda}))} \tag{4}$$

where $\tilde{F}_{\sigma}(q, \omega)$ and $\tilde{V}(q)$ are defined as follows;

$$\tilde{F}_{\sigma}(q, \omega) = \frac{F_{\sigma}(q, \omega)}{1 - \tilde{V}(q) F_{\sigma}(q, \omega)} \tag{5}$$

$$\sum_{kK_m} v(\kappa) a_{k+q+K_m,\sigma}^{\dagger} a_{k\sigma} \simeq \tilde{V}(q) \sum_{kK_m} v(\kappa) a_{k+q+K_m,\sigma}^{\dagger} a_{k\sigma} \tag{6}$$

and $F_{\sigma}(q, \omega)$ is the well known *Lindhard function.*

If we neglect the Umklapp process by setting all $\vec{K}_m = 0$, then we readily recover the result of Kim [8]. However, when $\vec{K}_m \neq 0$, we have a more complicated situation. Since we are only interested in the static limit, we consider the limit $q \rightarrow 0$. Then the renormalized transverse phonon frequency is simplified to

$$\omega_{q\perp}^2 = \Omega_{q\perp}^2 + 2\Omega_{q\perp} \sum_{k_{ZB}\sigma K_m} \left| G_{q\perp k_{ZB}}^{K_m} \right|^2 \times \frac{n_{k_{ZB}+q+K_m,\sigma} - n_{k_{ZB}\sigma}}{\omega_{q\perp} + \epsilon_{k_{ZB}+q+K_m} - \epsilon_{k_{ZB}}} \times \frac{1 + \tilde{V}(q) \tilde{F}_{\sigma}(q, 0)}{1 + v(q)(\tilde{F}_{\sigma}(q, 0) + \tilde{F}_{\sigma}(q, 0))} \tag{7}$$

Evaluating the magnitude of order for $q \rightarrow 0$, we obtain $\omega_{q\perp}^2 \simeq \Omega_{q\perp}^2$. Therefore, we conclude that the transverse phonon frequency is not affected by the electron-phonon interaction to the first order. This also implies that the magnetic transition does not directly affect the elastic properties.

It has been shown that, in the elinvar theory of the electronic redistribution [3–7], the ferromagnetism is only weakly influence the elastic anomaly. Therefore, in conclusion, we believe that the magnetism does not play an important role to the elastic anomaly.

III. CONCLUSION

We have shown, in this paper, that the theories for the invar effect do not have direct bearing on the elastic anomaly. Thus, we conclude that the invar and the elinvar effects originate from different physical mechanisms although they may be closely related. Also it is shown that the magnetism does not play an important role to the elastic anomaly.

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