# Phonon contribution to the Stoner enhancement factor: Ferromagnetism and possible superconductivity of $ZrZn_2$

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(Received 11 April 1979)

The contribution of phonons to the Hubbard-type exchange interaction parameter is shown to be much smaller than the electron-phonon mass-enhancement parameter $\lambda$ as a consquence of Migdal's theorem. Application to $ZrZn_2$ and the connection with $p$-state pairing are briefly discussed.

## I. INTRODUCTION

Enz and Matthias[1] (hereafter denoted by EM) have recently proposed that the electron-phonon interaction plays an essential role in the magnetism of $ZrZn_2$. They attempted to show that a dominant one-dimensional soft phonon contributes a positive (repulsive) term to the short-range Hubbard interaction parameter $I$. They found this term to be of the form $N(0)I_{\text{el-ph}} \simeq \lambda > 0$ where $N(0)$ is the density of states and $\lambda$ is the usual electron-phonon mass-enhancement parameter.[2]

We have considered this problem more generally and find that $N(0)I_{\text{el-ph}} \sim \lambda(\omega_D/E_F) \sim \lambda(m/M)^{1/2}$ where $\omega_D$ is the Debye energy and $m$ and $M$ are the electron and ion masses, respectively. This result is basically a manifestation of Migdal's theorem[2,3] and does *not* depend on the assumption of a soft phonon mode, although it is also valid in this special case. The particular contribution to $I_{\text{el-ph}}$ considered by EM can in fact be calculated *exactly* and, in addition to being order $(\omega_D/E_F)$, it is *negative*. There are however additional diagrams, not considered by EM, that contribute at this order. These diagrams, which are usually neglected (by invoking Migdal's theorem!), cannot be accurately evaluated at present and thus the sign of the complete $N(0)I_{\text{el-ph}}$ is still uncertain.

In Sec. II we describe the general formalism and in Sec. III we give the exact calculation of the contribution considered by EM. Section IV consists of a brief discussion of the general case and in Sec. V we make some general remarks on $ZrZn_2$ and the connection with $p$-state pairing.

## II. GENERAL FORMULATION

We consider the effect of phonons on the Stoner factor $S$ of a paramagnetic Fermi system at zero temperature. By definition,

$$S \equiv \lim_{\vec{q}\to 0}\lim_{q_0\to 0}\frac{\chi(q)}{\chi_0(q)} \equiv \frac{1}{1-N(0)I} \quad , \tag{1}$$

where $\chi(q)$ is the dynamic susceptibility, $\chi_0(q)$ is the susceptibility of the noninteracting system, and we employ the four-vector notation $q \equiv (\vec{q}, q_0)$. Here the appropriate limit is $q_0/v_F|\vec{q}| \to 0$ and $\chi_0(0) = N(0)$. The susceptibility is shown in Fig. 1 in terms of the single-particle propagator $G$, the vertex function $\Gamma$, and the irreducible particle-hole interaction $\tilde{I}$, which is represented as a Hubbard-type Coulomb interaction $I_c$ plus terms involving phonons. For $G \to G_0$ and $\tilde{I} \to I = \text{const}$, the usual RPA susceptibility is obtained. The Coulomb contribution $I_c$ is presumably well approximated by a constant. The extent to which the contributions to $\tilde{I}$ containing electron-phonon interactions can be considered constant is however not so clear. We avoid this difficulty by restricting our discussion to the Stoner factor. Thus it should be kept in mind that our $I_{\text{el-ph}}$ is really $I_{\text{el-ph}}(\vec{q}=0, q_0=0)$ and extrapolations away from $q=0$ should be viewed with suspicion.

One might be tempted at this point to conclude that the $g^2D$ contribution to $\tilde{I}$ in Fig. 1 would, in analogy to the situation in superconductivity, yield $N(0)I_{\text{el-ph}}$ of order $\lambda$. As will be seen in detail shortly, this is not correct. The point is that the phonon-induced electron-electron interaction $g^2D$ does not stand alone but must be considered as part of a larger diagram: a *particle-particle* $t$ matrix which diverges at the superconducting transition or, in the present case, a *particle-hole* $t$ matrix which diverges at the ferromagnetic transition. The analogy between the two cases cannot however be pushed too far. In the present case the quantity of interest is actually the susceptibility due to the interaction with an external magnetic field. Hence, to obtain $\chi$ from the particle-

 

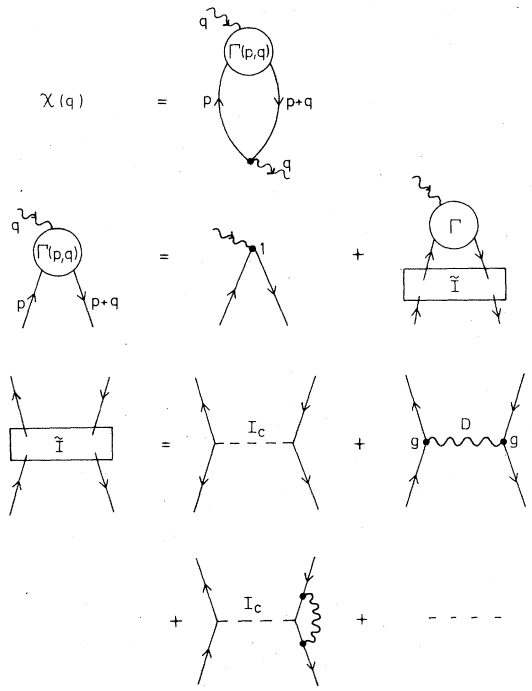


FIG. 1. Diagrammatic representation of the dynamic susceptibility $\chi$ in terms of the vertex function $\Gamma$ and the irreducible particle-hole interacton $\tilde{I}$. $I_c$ is the Hubbard-type contact interaction due to the Coulomb interaction, $D$ is the phonon propagator, and $g$ is the electron-phonon coupling constant. External lines have been included for clarity. The *external* wiggly line represents the interaction with an external magnetic field.

hole $t$ matrix the external lines of the $t$ matrix must be closed (i.e., integrated over). Thus the vertex function $\Gamma$ appears naturally as shown in Fig. 1 and the small factor $(\omega_D/E_F)$ arises as a result of Migdal's theorem. The situation is quite different for the particle-particle $t$ matrix that occurs in superconductivity theory. The external lines of the particle-particle $t$ matrix are not joined together to form a vertex ( this is, in fact, diagrammatically not possible). Consequently, Migdal's theorem does not apply and the contribution is formally of order $\lambda$.

## III. CALCULATION OF $N(0)I_{\text{el-ph}}$

The simplest method of obtaining an effective, constant, $I_{\text{el-ph}}$ is that employed by EM which we now discuss within our general formalism: One retains in $\Gamma(p,q)$ only the lowest-order correction to the bare vertex and takes for $\tilde{I}$ only the $g^2D$ term. This leads to $\Gamma^{(1)}(p,q)$ as shown in Fig. 2. It turns out that retention of only the first vertex correction in $\Gamma(p,q)$ is justified ( for the phonon diagrams), while neglecting the third contribution to $\tilde{I}$ shown in Fig. 1 is not. $\Gamma^{(1)}(p,q)$ is now evaluated for $|\vec{p}|=k_F$, $p_0=0$, $|\vec{q}|=0$, and $q_0/v_F|\vec{q}|=0$. Defining $\Gamma^{(1)}$ as this limit of $\Gamma^{(1)}(p,q)$ and recalling that $\chi_0(0)=N(0)$, we can identify the effective $I_{\text{el-ph}}$ by writing $\Gamma^{(1)}=N(0)I_{\text{el-ph}} \equiv \bar{I}_{\text{el-ph}}$. Of course it is not really correct to set $|\vec{p}|=k_F$ and $p_0=0$ since these variables must be integrated over to obtain $\chi$, i.e., one should actually evaluate diagram (a) of Fig. 3 and identify $I_{\text{el-ph}}$ with the constant multiplying $N^2(0)$ when $q\to 0$. For the moment though, the important thing to note is that $\Gamma^{(1)}(p,q)$ is *identical* with the "iteration step" in the particle-hole $t$ matrix considered by EM. EM have not evaluated $\Gamma^{(1)}$ correctly, however. From the point of view of the present formalism, and the fact that $q_0/v_F|\vec{q}| \ll 1$ is the essential criterion for the validity of Migdal's theorem,[2] it should not be surprising that the exact calculation gives $\bar{I}_{\text{el-ph}} = O(\omega_D/E_F) \ll \lambda$. The calculation of $\Gamma^{(1)}$ proceeds as follows: For arbitrary $p$ and $q$ we have

$$\Gamma^{(1)}(p,q) = i\int \frac{d^4p'}{(2\pi)^4} G_0(p')G_0(p'+q) \times |g_{\vec{p}\,\vec{p}'}|^2 D_0(p-p') \quad . \tag{2}$$

Here we take

$$D_0(k) = \frac{2\omega_{\vec{k}}}{k_0^2 - \omega_{\vec{k}}^2 + i\delta} \tag{3}$$

and we assume

$$|g_{\vec{p}\,\vec{p}'}|^2 = |g_{\vec{p}-\vec{p}'}|^2 = g^2\omega_{\vec{p}-\vec{p}'} \quad , \tag{4}$$

where $g^2$ is a constant $\sim N(0)^{-1}$. In the limiting case $\Gamma^{(1)}(p,q)\to\Gamma^{(1)}$, we employ the method of Hertz *et al.*[4] and find

$$\Gamma^{(1)} = \bar{I}_{\text{el-ph}} = \frac{m}{(2\pi)^2 k_F}\int_0^{2k_F} |g_K|^2 k\,dk \int_0^\infty \frac{d\omega}{\pi}\,\mathrm{Im}D_0(k,\omega)\left[\frac{2(\omega+kv_F)}{(\omega+kv_F)^2-(k^2/2m)^2}\right] + \frac{m}{(2\pi)^2 k_F}\int_{2k_F}^\infty |g_k|^2 k\,dk \int_0^\infty \frac{d\omega}{\pi}\,\mathrm{Im}D_0(k,\omega)\left[\frac{2kv_F}{(kv_F)^2-(k^2/2m+\omega)^2}\right] \quad . \tag{5}$$

Equation (5) is exact for a spherically parabolic band structure. The first term in Eq. (5) was obtained in Ref. 4. In practice the second term is usually not important due to the large-phonon momenta involved. In our case this term does not contribute because we are calculating the static, uniform, susceptibility and therefore the intermediate state in Fig. 2 consists of a particle-hole pair of momentum $q$ with $q_0\to 0$ and $q\to 0$. This restricts

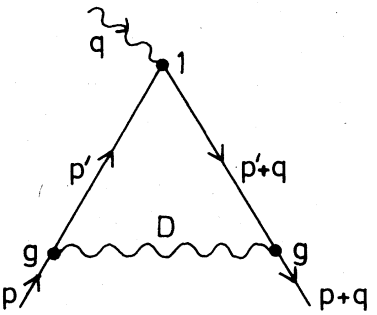


FIG. 2. Lowest-order phonon vertex correction $\Gamma^{(1)}(p,q)$.

the phonon momentum to $|\vec{k}| \leq 2k_F$. Corresponding to Eq. (3),

$$\mathrm{Im}D_0(k,\omega) = -\pi\delta(|\omega| - \omega_k)\mathrm{sgn}\omega \ . \tag{6}$$

The minus sign in Eq. (6) appears to have been omitted in Ref. 4. Using Eqs. (4) and (6), Eq. (5) becomes

$$\bar{I}_{\text{el-ph}} = -\bar{\lambda}\left(\frac{\omega_D}{E_F}\right)\int_0^1 dx \left(\frac{\omega_k}{\omega_D}\right)\frac{x(x+\omega_k/4E_F)}{(x+\omega_k/4E_F)^2 - x^4} \ , \tag{7}$$

where $x = k/2k_F$ and $\bar{\lambda} \equiv N(0)g^2 = O(1)$ is the same order magnitude as $\lambda$.

The integral in Eq. (7) is always positive. In order that Migdal's theorem be valid, this integral must not yield a term proportional to $(E_F/\omega_D)$. For Debye spectrum, $\omega_k = ck$ with $c \simeq \omega_D/k_F$, Eq. (7) can be easily integrated with the result: $\bar{I}_{\text{el-ph}} \simeq -\bar{\lambda}(\omega_D/E_F) \times \ln(E_F/\omega_D)$. To verify that our result is also valid for soft phonons, we took $\omega_k = \omega_s + c|k - k_0|$ with $\omega_s \to 0$, which is similar to the dispersion considered by EM. The leading behavior of the integral in Eq. (7) arises from the logarithmic singularity at $x = 1$ $(k = 2k_F)$ for $\omega_D \to 0$. This leads again to a factor $\ln(E_F/\omega_D)$ (or simply a constant if all phonon momenta are less than $2k_F$). Thus we conclude that $\bar{I}_{\text{el-ph}} << \lambda$ also for soft modes which is reasonable since the condition $q_0/v_F|\vec{q}| << 1$ is certainly well satisfied in this case.

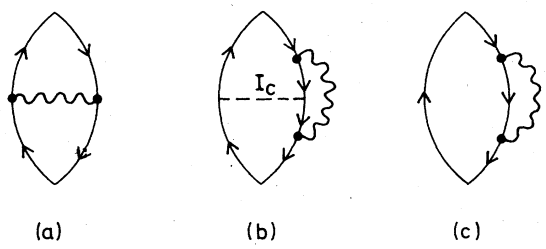


FIG. 3. Several contributions to $\chi_{\text{phon}}$.

## IV. GENERAL SUSCEPTIBILITY DIAGRAMS AT ORDER $(\omega_D/E_F)$

Since the effective $\bar{I}_{\text{el-ph}}$ calculated in Sec. III turned out to be $O(\omega_D/E_F)$, we cannot, *a priori*, neglect diagrams such as the third contribution to $\tilde{I}$ in Fig. 1. In order to discuss the general case it is convenient to express $\chi(q)$ as

$$\chi(q) = \frac{\chi_{\text{phon}}(q)}{1 - I_c\chi_{\text{phon}}(q)} \ , \tag{8}$$

where $\chi_{\text{phon}}$ is the bubble diagram $\chi_0$ completely renormalized by phonons. Several low-order contributions are shown in Fig. 3.

Determination of the sign of $\bar{I}_{\text{el-ph}}$ would require accurate evaluation of $\chi_{\text{phon}}$ to order $(\omega_D/E_F)$. This is a formidable task and, at present, we can only state the qualitative results of some rough calculations: Diagram 3(a) is the same order of magnitude as the effective $\bar{I}_{\text{el-ph}} = \Gamma^{(1)}$ calculated in Sec. III [i.e., $O(\omega_D/E_F)$] and is *probably* negative. Diagram 3(b) is also $O(\omega_D/E_F)$ but may be more important than Diagram 3(a) since we can replace the $I_c$ in this diagram with a full particle-hole $t$ matrix and thus obtain some enhancement effect. (A full Stoner factor does not appear here because the momentum argument of the $t$ matrix is integrated over.) Unfortunately, we can make no statement concerning the sign of Diagram 3(b). We have only shown that the particular limit, $\Gamma^{(1)}$, of $\Gamma^{(1)}(p,q)$ is negative. It appears however that $\Gamma^{(1)}(p,q)$ can be positive for certain ranges of $p$ and $q$. Now, since the arguments of the phonon vertex correction appearing in Diagram 3(b) are integrated over, a detailed analysis would be required to determine whether the positive or negative contributions dominate. All other contributions to $\chi_{\text{phon}}$ appear to be $O(\omega_D/E_F)^2$ or smaller. That self-energy corrections of the form of Diagram 3(c) do not contribute to $\chi$ at order $\lambda$ [i.e., $O(1)$] is well known.[5] We find that these corrections enter first at order $(\omega_D/E_F)^2$.

## V. CONCLUSIONS AND DISCUSSION

In general, it seems safe to say that, for a nearly (or weakly) ferromagnetic system where $\bar{I}_c \equiv N(0)I_c \simeq 1$, $\bar{I}_{\text{el-ph}}$ is at most several percent of $\bar{I}_c$. The phonon corrections are thus only important in the rather anomalous case where $\bar{I}_c$ is *very* close to 1. Just this case was *assumed* by EM for $ZrZn_s$ in order to explain the concentration dependence of the Curie temperature in certain solid solutions as being due to phonon mode softening. Our results do not rule out this possibility since accurate evaluation of Diagrams 3(a) and 3(b) might well yield a positive $\bar{I}_{\text{el-ph}}$. However, before attemptimg to calculate these contributions, it would be wise to rule out other (perhaps more likely) explanations for the behavior of the Cu-

rie temperature, such as variation of $I_c$.

As pointed out by several authors,[1,6] the fact that the ferromagnetism of $ZrZn_2$ can be suppressed by a pressure of about 8 kbar raises the question of the possibility of $p$-state pairing in the nearly ferromagnetic region. First, we wish to point out that the absence of $s$-state superconductivity in $ZrZn_2$ can be accounted for by the strong spin fluctuations presumably present which should effectively suppress $s$-state pairing.[7]

Can one expect, therefore, that $p$-state pairing would be favored in the paramagnetic phase of $ZrZn_2$? In order to shed some light on this question we briefly discuss the conditions necessary for the appearance of $p$-state pairing. The strength of the $p$-state interaction is determined by the angular dependence of the electron-electron interaction $V(\vec{k},\vec{k}')$, that is, by the dependence of this function on the angle between $\hat{k}$ and $\hat{k}'$. $P$-state pairing is favored by a $V$ that is large and attractive for small-angle scattering and small, or repulsive, for large-angle scattering.[8] The electron-electron interaction due to spin-fluctuation exchange $V^{SF}$ does have a strong lobe in the forward direction, $\hat{k}\cdot\hat{k}'\sim 1$, and therefore it favors $p$-state superconductivity in exchange-enhanced transition metals as we have discussed elsewhere.[9] The phonons contribute to the pairing interaction in two ways: (i) directly, through the usual phonon-exchange mechanism and, (ii) indirectly, as suggested by EM and discussed here, by contributing to the exchange interaction $I$ and thus affecting $V^{SF}$ In $d$-band metals the $p$-state interaction due to phonon exchange $V_1^{ph}$ is weak for normal phonons and can be either repulsive or attractive. The reason for the weakness of the $p$-state interaction is that large-momentum (including umklapp) scattering is attractive and comparable in magnitude to the small-momentum scattering. For the case of Pd, $V_1^{ph}$ has been calculated by several authors[10,11] and found to almost vanish. We conclude then, that in order to yield a sufficiently strong and attractive $p$-state interaction, the ordinary large-momentum contribution to $V_1^{ph}$ would have to be compensated for by a repulsive large-momentum contribution from some other source.

## ACKNOWLEDGMENTS

One of the authors (D.F.) wishes to thank G. Grünewald, N. Schopohl, and K. Scharnberg for helpful conversations.

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[8]That such a behavior of $V$ favors the $p$-state interaction is readily seen for the case of a spherical Fermi surface. Here we can write $V(\vec{k},\vec{k}')=V(|\vec{k}|,|\vec{k}'|;\hat{k}\cdot\hat{k}')$, where $|\vec{k}|=|\vec{k}'|=k_F$. The angular momentum decomposition of $V$ yields the $p$-state ($l=1$) pairing coefficient, $V_1=\int \hat{k}\cdot\hat{k}'V(\hat{k}\cdot\hat{k}')d(\hat{k}\cdot\hat{k}')$. In simple metals, for example, $V_1^{ph}$ is comparable with $V_0^{ph}$ because the phonon-mediated interaction has a strong lobe in the forward direction $\hat{k}\cdot\hat{k}'\sim 1$, and is small for large-angle scattering, $\hat{k}\cdot\hat{k}'\sim 0$.

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