# Exchange enhancement of the electron-phonon coupling in metals

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It is well known that ferromagnetic tendency is destructive to superconductivity through the spin-fluctuation coupling effect. Experimentally, however, the relation between superconductivity and magnetism is not that simple. Recently, we pointed out that by softening phonons the exchange interaction between electrons enhances the electron-phonon coupling constant $\lambda_p$, and, accordingly, superconductivity. If the effect of the exchange enhancement of $\lambda_p$ overrides the destructive effect of the spin-fluctuation coupling, resultantly, superconductivity can be helped by magnetism. In order to substantiate the above idea, in the present paper we carry out a quantitative estimation of $\lambda_p$ for a model in which deviations from the jellium model are conveniently included by a parameter $\xi$. The size of the exchange enhancement of $\lambda_p$ is found to depend very sensitively on $\xi$. Thus, assuming different values for $\xi$, we can explain why in Pd the exchange enhancement of $\lambda_p$ is small, resulting in the absence of superconductivity, whereas it is large in $V_3Si$, producing high superconducting transition temperature.

## I. INTRODUCTION

The effects of the electron-phonon interaction on the electronic properties of metals can be conveniently described by the electron-phonon coupling constant $\lambda_p$. The BCS superconducting transition temperature $T_s$ is given as $k_B T_s \simeq \hbar\omega_D e^{-1/\lambda_p}$, where $\omega_D$ is the Debye frequency, and the electronic-specific-heat mass $m^*$ is given as $m^* = (1+\lambda_p)m$, where $m$ is the band mass of an electron. In spite of many efforts,[1] however, still we do not fully understand how $\lambda_p$ is determined from various factors in a metal.

Recently[2] we pointed out the possible importance of taking into account the exchange interaction between electrons in estimating $\lambda_p$. We noted that $\lambda_p$ can be significantly enhanced by the exchange effects. As for the effect of the exchange interaction on superconductivity, only the destructive aspect (spin-fluctuation coupling)[3] was known previously. According to our new viewpoint, however, if the constructive effect of the exchange enhancement of $\lambda_p$ dominates the destructive one, resultantly superconductivity can be even enhanced.

In the present paper we carry out a quantitative model calculation of $\lambda_p$ to substantiate the above argument. Within our model we demonstrate that under certain conditions the constructive effect of the exchange interaction can become more important than the destructive one.

Note actually it has long been perceived that in a certain way magnetism seems to help superconductivity. For instance, the uranium compounds are either ferromagnetic or superconducting and this close link between superconductivity and ferromagnetism was considered even to indicate the electron-phonon interaction may not be the dominant cause for superconductivity in these materials.[4] Both superconductivity and magnetic phase are observed most widely among the transition metals.[5] Generally the $A15$ compounds with high superconducting transition temperatures such as $Nb_3Sn$ and $V_3Si$ have large and strongly temperature dependent magnetic susceptibilities.[6] Our new viewpoint seems to be useful in qualitatively understanding these observations.

In Sec. II we present an explicit derivation of the expression for the electron-phonon coupling constant $\lambda_p$ including the effect of the exchange interaction between electrons. Based on the result of Sec. II, in Sec. III we carry out a model calculation of $\lambda_p$ and discuss some experimental data in the light of our results in Sec. IV.

## II. EFFECT OF THE EXCHANGE INTERACTION ON THE ELECTRON-PHONON COUPLING CONSTANT

In this paper we use the following form of Hamiltonian for a metallic electron-phonon system.[7]

$$\mathcal{H} = \sum_{\vec{k},\sigma} \epsilon_{\vec{k}} a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma} + \sum_{\vec{q},\lambda} \Omega_{\vec{q}\lambda} b^\dagger_{\vec{q}\lambda} b_{\vec{q}\lambda} + \frac{1}{2} \sum'_{\substack{\vec{k},\vec{k}',\vec{q} \\ \sigma,\sigma'}} V(\vec{q}) a^\dagger_{\vec{k}+\vec{q}\,\sigma} a^\dagger_{\vec{k}'-\vec{q}\,\sigma'} a_{\vec{k}'\sigma'} a_{\vec{k}\sigma} + \sum_{\substack{\vec{k},\vec{q} \\ \sigma,\lambda}} \alpha_\lambda(\vec{q}) a^\dagger_{\vec{k}-\vec{q}\,\sigma} a_{\vec{k}\sigma} (b^\dagger_{\vec{q}\lambda} + b_{-\vec{q}\,\lambda}) . \quad (1)$$

The first and second terms, respectively, represent the energies of free electrons and phonons, where $a^\dagger_{\vec{k}\sigma}$ is the creation operator of an electron with energy $\epsilon_{\vec{k}}$ and spin $\sigma$, and $b^\dagger_{\vec{q}\lambda}$ is the creation operator of a phonon with wave number $\vec{q}$ and polarization $\lambda$. The third term is the Coulomb repulsion between electrons, where the prime on the summation indicates to exclude $q = 0$ from the sum.

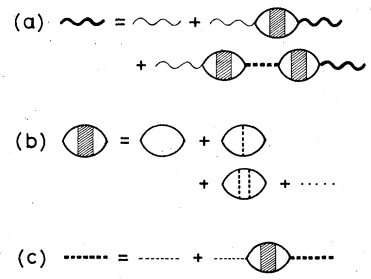

FIG. 1. Phonon renormalization by the electron-phonon interaction, (a). Thick and thin wavy lines represent, respectively, phonons with and without the effects of the electron-phonon interaction. A thick dotted line is for the screened Coulomb interaction, (c), whereas thin dotted lines are for the bare Coulomb interaction. The effects of the exchange interaction are included by shading the electron-hole bubble, (c).

Note for plane-wave electronic states, which we assume, $V(q)=4\pi e^2/q^2$, with unit volume normalization. The last term in Eq. (1) represents the electron-phonon interaction.

Let us first review how the phonon frequency is affected by the exchange interaction between electrons. As described in detail elsewhere[8] if we include the effects of the electron-phonon and electron-electron interactions as shown in Fig. 1, we obtain the following phonon Green's function:

$$D_\lambda(\vec{q}, i\nu_l) = -2\Omega_{\vec{q}\lambda}\Big/\nu_l^2+\Omega_{\vec{q}\lambda}^2\left(1-\frac{2}{\Omega_{\vec{q}\lambda}}\,|\,\alpha_\lambda(\vec{q})\,|^2 \times\frac{2\tilde{F}(\vec{q}, i\nu_l)}{1+2V(\vec{q})\tilde{F}(\vec{q}, i\nu_l)}\right) \quad (2)$$

in the standard notations,[9,13] where we put

$$\tilde{F}(\vec{q}, i\nu_l)=F(\vec{q}, i\nu_l)/[1-\tilde{V}(\vec{q})F(\vec{q}, i\nu_l)]$$

with $\nu_l=2l\pi/\beta$ and

$$F(\vec{q}, i\nu_l)=-\beta^{-1}\sum_{\vec{p},n} G(\vec{p}+\vec{q}, i\omega_{n+l})G(\vec{p}, i\omega_n) =-\sum_{\vec{p}}\frac{f(\epsilon_{\vec{p}+\vec{q}})-f(\epsilon_{\vec{p}})}{\epsilon_{\vec{p}+\vec{q}}-\epsilon_{\vec{p}}-i\nu_l},$$

where $G(\vec{p}, i\omega_n)=(i\omega_n-\epsilon_{\vec{p}})^{-1}$, with $\omega_n=(2n+1)\pi/\beta$ is the electron Green's function, $f(\epsilon_{\vec{p}})$ is the Fermi distribution function, and $\tilde{V}(q)$ is the effective exchange interaction between electrons. Note that $\tilde{F}(\vec{q}, i\nu_l)$ represents the shaded (exchange enhanced) electron-hole bubbles in Fig. 1 whereas $F(q, i\nu_l)$ stands for the unshaded ones. Without the exchange effects Eq. (2) reduces to the familiar result with $\tilde{F}(q, i\nu_l)$ replaced by $F(q, i\nu_l)$. The renormalized phonon frequency is obtained from the pole of the above phonon Green's function analytically continued to the real frequency axis from the upper half $\omega$ plane.[9] Thus in the adiabatic approximation we obtain[2,8]

$$\omega_{\vec{q}\lambda}^2=[\Omega_{\vec{q}\lambda}^2-2\Omega_{\vec{q}\lambda}\,|\,\alpha_\lambda(\vec{q})\,|^2/V(\vec{q})] +\frac{2\Omega_{\vec{q}\lambda}\,|\alpha_\lambda(\vec{q})\,|^2/V(\vec{q})}{1+V(\vec{q})\chi_m(\vec{q})}, \quad (3)$$

where we noted that in the mean-field approximation the exchange-enhanced paramagnetic spin susceptibility of the electrons $\chi_m(\vec{q})$ is given as (with $\mu_B^2=1$)

$$\chi_m(\vec{q})=2F(\vec{q}, 0)/[1-\tilde{V}(\vec{q})F(\vec{q}, 0)]. \quad (4)$$

The meaning of the effective exchange interaction $\tilde{V}(q)$ may have become clearer from Eq. (4).

The fact that the exchange interaction between electrons softens phonons has been long known.[10] The exchange effect effectively reduces the Coulomb repulsion[11] and, accordingly enhances the screening of the ion-ion interaction in a metal to lower the phonon frequency. By relating the phonon frequency to the magnetic susceptibility as in Eq. (3) this situation may be shown most clearly. The larger is the spin susceptibility, the lower is the phonon frequency in the paramagnetic state of a metal.

Let us now proceed to discuss the effect of the exchange interaction on the self-energy of an electron due to the electron-phonon interaction as shown in Fig. 2(a). First note that if the exchange effect is included as in Figs. 2(b) and 2(c), the screened electron-phonon interaction, the shaded circle in Fig. 2(a), is given as

$$\bar{\alpha}_\lambda(\vec{q}, i\nu_l)=\alpha_\lambda(\vec{q})/\epsilon(\vec{q}, i\nu_l) \quad (5)$$

with the screening constant,

$$\epsilon(\vec{q}, i\nu_l)=[1+2V(\vec{q})\tilde{F}(\vec{q}, i\nu_l)] \times[1-\tilde{V}(\vec{q})F(\vec{q}, i\nu_l)]. \quad (6)$$

It is important to note that the exchange effects appear quite differently in screening the electron-

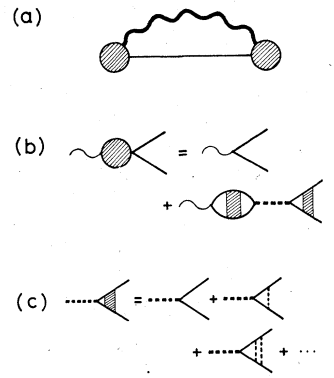

FIG. 2. Electron self-energy (a), and the screened electron-phonon interaction [(b), (c)].

phonon interaction, Eq. (6), and the ion-ion interaction, the denominator of the second term on the right-hand side of Eq. (3) or the first factor alone of the right-hand side of Eq. (6). The second factor of Eq. (6) comes from summing the diagrams of Fig. 2(c). The screening constant of the ion-ion interaction is enhanced by the exchange effects leading to the exchange softening of phonons. The screening constant of the electron-phonon interaction, on the contrary, is reduced by the exchange effects as is evident if we rewrite Eq. (6) as

$$\epsilon(\vec{q}, i\nu_l) = 1 + [2V(\vec{q}) - \tilde{V}(\vec{q})]F(\vec{q}, i\nu_l) .$$

Thus the electron-phonon interaction is enhanced by the exchange effects.

With the above preparation, the self-energy of an electron as represented in Fig. 2(a) is written down straightforwardly:

$$\Sigma(\vec{k}, i\omega_n) = -\beta^{-1} \sum_{\vec{k}', m} G(\vec{k}', i\omega_m) \times |\bar{\alpha}_\lambda(\vec{k} - \vec{k}', i\omega_n - i\omega_m)|^2 \times D_\lambda(\vec{k} - \vec{k}', i\omega_n - i\omega_n) . \quad (7)$$

Here if we put $\bar{\alpha}_\lambda(\vec{k} - \vec{k}', i\omega_n - i\omega_m) \simeq \bar{\alpha}_\lambda(\vec{k} - \vec{k}', 0) \equiv \bar{\alpha}_\lambda(\vec{k} - \vec{k}')$, and $D_\lambda(\vec{q}, i\nu_l) = -2\Omega_{\vec{q}\lambda}/(\nu_l^2 + \omega_{\vec{q}\lambda}^2)$ with $\omega_{\vec{q}\lambda}^2$ given by Eq. (3), Eq. (7) reduces to the familiar form. Then, following the procedure given in Sec. 21 of Ref. 9, for instance, we immediately obtain the real part of the self-energy of an electron near the Fermi surface

$$\mathrm{Re}\Sigma(k_F, \epsilon) \simeq -\lambda_p \epsilon$$

with the electron-phonon coupling constant

$$\lambda_p = N(\epsilon_F) \sum_\lambda \frac{1}{2k_F^2} \int_0^{k_1} \frac{q dq 2\Omega_{\vec{q}\lambda} |\bar{\alpha}_\lambda(\vec{q})|^2}{\omega_{\vec{q}\lambda}^2} . \quad (8)$$

In the above the energy of an electron $\epsilon$ is measured from the Fermi level $\epsilon_F$, $N(\epsilon_F) = mk_F/2\pi^2$ is the density of states of electrons per spin at the Fermi surface for the parabolic energy band, and $k_1 = \min(2k_F, k_D)$, $k_D$ being the Debye wave number. For simplicity we assume $k_1 = 2k_F$ and use the notation

$$\int_0^{2k_F} q\, dq \cdots / 2k_F^2 = \langle\langle \cdots \rangle\rangle$$

which indicates taking an average over the momentum changes on the Fermi surface. Then Eq. (8) can be rewritten[12]

$$\lambda_p = N(\epsilon_F) \sum_\lambda \left\langle\!\!\left\langle \frac{2\Omega_{\vec{q}\lambda} |\bar{\alpha}_\lambda(\vec{q})|^2}{\omega_{\vec{q}\lambda}^2} \right\rangle\!\!\right\rangle . \quad (8')$$

Clearly $\lambda_p$ is exchange enhanced through (i) the exchange softening of phonon, and (ii) the exchange effect in the screening of the electron-phonon interaction.

## III. MODEL CALCULATION OF $\lambda_p$

In carrying out a quantitative estimation of the importance of the exchange effects on $\lambda_p$, retaining only the contribution from the longitudinal-acoustic phonon, we approximate Eq. (8') as

$$\lambda_p = N(\epsilon_F) \left\langle\!\!\left\langle \frac{\Omega_p^2 V(\vec{q})}{\epsilon(\vec{q}, 0)^2} \Big/ \left( \xi s_0^2 q^2 + \frac{\Omega_p^2}{1 + V(\vec{q})\chi_m(\vec{q})} \right) \right\rangle\!\!\right\rangle , \quad (9)$$

dropping the polarization subscript $\lambda$. In the above, the electron-phonon interaction is approximated by that of the jellium model, $2|\alpha(\vec{q})|^2 = \Omega_p V(\vec{q})$, $\Omega_p$ being the ionic plasma frequency,[7] and we put

$$\Omega_q^2 - 2\Omega_q |\alpha(\vec{q})|^2 / V(\vec{q}) = \xi s_0^2 q^2 , \quad (10)$$

where $s_0 = \Omega_p/[8\pi e^2 N(\epsilon_F)]^{1/2}$ is the Bohm-Staver sound velocity. Note that for the jellium model, where $\Omega_q = \Omega_p$, $\xi = 0$. Thus, through the parameter $\xi$ deviations from the jellium model are included in our model. If $\xi > 0$, phonon is harder than in the jellium model, whereas if $\xi < 0$ it is softer. Although our extension of the model beyond the jellium model is very primitive it turns out to be essential in our whole discussions.

Let us rewrite Eq. (9) more explicitly as

$$\lambda_p = N(\epsilon_F) \langle\!\langle V_{SC}(\vec{q}) / \{ [1 - \tilde{V}(\vec{q}) F(\vec{q}, 0)] + \tfrac{1}{2} \xi V_{SC}(\vec{q}) N(\epsilon_F) \} \rangle\!\rangle , \quad (11)$$

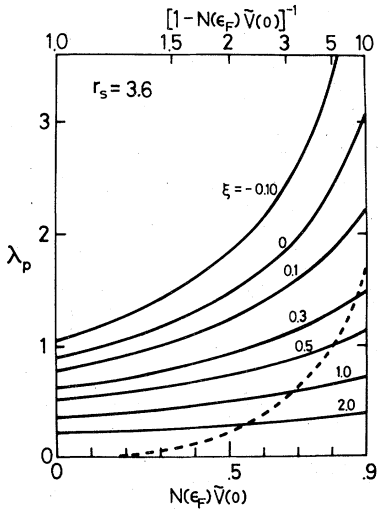


FIG. 3. Exchange enhancement of the electron-phonon coupling constant $\lambda_p$ for different values of $\xi$. The dotted line is for the spin-fluctuation coupling constant $\lambda_s$. $r_s = 3.6$ corresponds to the free-electron mass and $k_F = 10^8/\mathrm{cm}$.

with a screened Coulomb repulsion $V_{SC}(\vec{q}) = V(\vec{q})/\epsilon(\vec{q}, 0)$. If we put $\xi = 0$ and $\tilde{V}(\vec{q}) = 0$ in Eq. (11) it reduces to the familiar result[13] in the jellium model. In carrying out numerical calculation on Eq. (11) we assume a parabolic energy band for the electrons for which the Lindhard function takes the simple form,[7]

$$F(\vec{q}, 0) = N(\epsilon_F)\left\{\frac{1}{2} + [(1-x^2)/2x]\ln\left|(1+x)/(1-x)\right|\right\},$$

with $x = q/2k_F$. As for the effective exchange interaction we assume a Lorentzian, $\tilde{V}(\vec{q}) = \tilde{V}(0)/[1 + C(q/2k_F)^2]$, with $C = 1$.

In Figs. 3–5 we present our calculation of $\lambda_p$ varying the three parameters, the mean separation between electrons in the unit of the Bohr radius $r_s$, the strength of the exchange interaction $\tilde{V}(0)N(\epsilon_F)$, and $\xi$. In the simple jellium model[13] $r_s$ is the only parameter to determine $\lambda_p$. Our result shows that the two new parameters $\tilde{V}(0)N(\epsilon_F)$ and $\xi$ are as important as $r_s$. The effect of the exchange interaction on $\lambda_p$ depends very sensitively on $\xi$. It becomes especially important when $\xi$ is small or negative.

In Fig. 3 we included the calculation of the spin fluctuation coupling constant $\lambda_s$ which is given as[3]

$$\lambda_s = \tfrac{3}{2}N(\epsilon_F)\left\langle\!\!\left\langle \frac{[\tilde{V}(\vec{q})]^2 F(\vec{q}, 0)}{1 - \tilde{V}(\vec{q})F(\vec{q}, 0)} \right\rangle\!\!\right\rangle . \qquad (12)$$

From Eqs. (11) and (12), as well as from Fig. 3, it is evident that for negative $\xi$ the effect of the exchange enhancement of $\lambda_p$ can be larger than that of $\lambda_s$. That is, superconductivity can be enhanced by the exchange interaction between electrons if $\xi < 0$, or small.

Thus in our model whether the exchange effects can be important or not is determined by the values of the parameter $\xi$. The implication of this result can be understood from more general point of view. As can be seen from the denominator of Eq. (9), or, more generally, from Eq. (3), the phonon frequency or the ion-ion interaction consists of two components. The first component, $\Omega^2_{\vec{q}\lambda} - 2\Omega_{\vec{q}\lambda}\left|\alpha_\lambda(\vec{q})\right|^2/V(\vec{q})$ or $\xi s_0^2 q^2$, is not affected by the screening behavior of the conduction electrons. The effect of the conduction electron screening appears only in the remaining second component. Thus, if the first component is positive and large (compared with the second component) the role of the conduction electrons is not dominant in determining the phonon frequency. In such a system the exchange effects can not do much to enhance $\lambda_p$. If the first component is small or negative, on the other hand, the screening dependent second component becomes very important, and there $\lambda_p$ can be significantly enhanced by the exchange effects. In other words, a large exchange enhancement of $\lambda_p$ (or a large exchange softening of $\omega_{\vec{q}}$) is possible in a metal if the phonon spectrum of the metal is sensitively related to the conduction electron band structures. The result of present section, in which we used the simplification of Eq. (10), should be understood in this way.

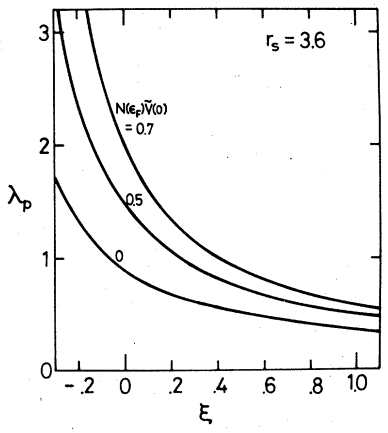


FIG. 4. $\xi$ dependence of $\lambda_p$ for different strengths of the exchange interaction.

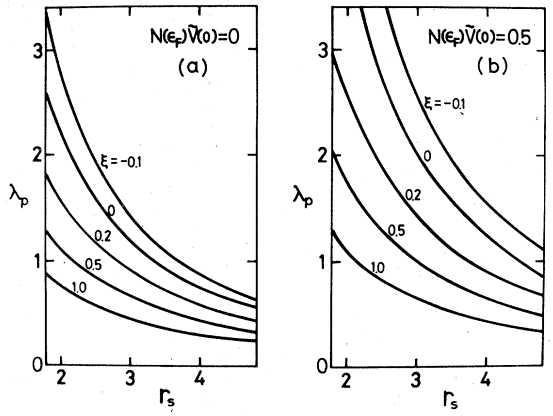


FIG. 5. $r_s$ dependence of $\lambda_p$ for different strengths of the exchange interaction, (a) $\tilde{V}(0)N(\epsilon_F) = 0$, and (b) $\tilde{V}(0)N(\epsilon_F) = 0.5$.

## IV. DISCUSSIONS

As an illustration let us see how the $A15$ compounds like $V_3Si$ can be understood from our point of view. According to the specific heat ($\gamma$) (Ref. 14) and magnetic susceptibility ($\chi$) data[15] on $V_3Si$, the effective electronic densities of states are given, respectively, as $N_\gamma(\epsilon_F) = 3.7$ states/(eV spin atom) and $N_\chi(\epsilon_F) = 6.1$ states/(eV spin atom). Note that these effective densities of states are related to the band density of states as $N_\gamma(\epsilon_F) = (1 + \lambda_p + \lambda_s)N(\epsilon_F)$ and $N_\chi(\epsilon_F) = N(\epsilon_F)/[1 - \tilde{V}(0)N(\epsilon_F)]$. A re-

cent band calculation,[16] on the other hand, gives $N(\epsilon_F) = 1.1$ states/(eV spin atom). If we compare $N_\chi(\epsilon_F)$ with the above $N(\epsilon_F)$ or $N_\gamma(\epsilon_F)$ it is almost evident that we have to consider the exchange enhancement effect.[17] Even if the orbital magnetic susceptibility is assumed to account for half the total susceptibility at low temperatures[15,17] we need the spin susceptibility enhancement factor of ~3, or $N(\epsilon_F)\tilde{V}(0) = 0.6$–$0.7$. Note the exchange-enhancement effect is required also to explain the temperature dependence, as well as the magnitude, of the susceptibility.[17] Now, with $\lambda_s = 0.5$, corresponding to $N(\epsilon_F)\tilde{V}(0) = 0.65$, we require $\lambda_p = 1.9$ to explain the above specific heat data. From the results of Figs. 3–5, however, it is not difficult to conceive this rather large value of $\lambda_p = 1.9$, if we assume small or negative $\xi$ in addition to the exchange interaction between electrons. As for the superconducting transition temperature, if we use the formula[3]

$$k_B T_s = \frac{\hbar\omega_D}{1.45} \exp\left(-\frac{(1+\lambda_p+\lambda_s)}{\lambda_p-\lambda_s-\mu^*}\right)$$

with $\hbar\omega_D/k_B = 330$ K,[18] and the above choice of $\lambda_p$ and $\lambda_s$, to reproduce the experimental value of $T_s = 17$ K, we require the Coulomb pseudopotential of $\mu^* = 0.08$. This appears to be rather reasonable. Note that the occurrence of structural instability in the $A15$ compounds can also be understood qualitatively from the present point of view[2,19] by assuming negative $\xi$.

As for Pd we believe $\xi > 1$. Thus, the temperature dependence of $\chi_m$ reflects on that of $\omega_{\vec{q}}$ much less than, for example, in $V_3Si$. Correspondingly, in Pd the exchange enhancement of $\lambda_p$ is not significant, resulting in the absence of superconductivity.

Recently an interesting analysis was carried out on the superconducting alloys $Mo_{1-x}Cr_x$.[20] Increase in $\lambda_p$ was observed as Cr concentration was increased to make the alloy more magnetic.

Obviously the model we used in Sec. III of the present paper is too unrealistic to discuss transition metals and the $A15$ compounds. The qualitative features of our result, however, should not be associated too closely with the model used. As illustrated above in analyzing some experimental data, our approach and result are to be understood as phenomenological. We calculated $\lambda_p$ as a function of $\tilde{V}(0)N(\epsilon_F)$, for instance, but we never dare to calculate the important quantity $\tilde{V}(0)N(\epsilon_F)$ within our model and approximation. We know that at present this quantity can not be calculated nonempirically. The same attitude should be taken on the meaning of the parameter $\xi$ as already emphasized at the end of Sec. III.

## ACKNOWLEDGMENT

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