Roles of phonon interaction on the pairing in high $T_c$ superconductors

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Abstract. The effects of phonon interactions for the superconducting pairing, in the background of a d-wave pairing mediated by Antiferromagnetic (AFM) spin fluctuations, are studied. We found that anisotropic phonon interaction, together with the AFM spin fluctuations interaction, can dramatically enhance the d-wave pairing itself and therefore $T_c$. This $(D_{AFM} + D_{ph})$ type pairing, however, exhibits strongly reduced isotope coefficient despite the large enhancement of $T_c$.

1. Introduction
Recent Angle Resolved Photoemission Spectroscopy (ARPES) experiments revived the interest of phonons in the high $T_c$ cuprates [1]. The systematic measurements and analysis [2] of the kink structures in the quasiparticle dispersion near the Fermi surface (FS) strongly suggested that (1) the origin of the kink is electron-phonon coupling and its coupling is very strong, (2) the typical energy of the phonon(s) is $\sim 40 - 50$ meV, and (3) the coupling matrix is quite anisotropic. Therefore, there is a good motivation to investigate possible roles and effects of phonons, in particular, for the superconducting (SC) pairing in the high $T_c$ cuprates (HTC).

In this paper, we assume that the d-wave pairing in HTC is mainly mediated by an AFM spin fluctuations [3]. Then we add a phonon interaction to study the effect(s) of phonons for the SC gap and $T_c$. We took a simplest approach for this and solved the coupled BCS gap equations of multiple gaps in the single band with two pairing interactions, i.e., AFM interaction and anisotropic phonon interaction. We found that the anisotropic phonon interaction can induce an additional d-wave component ($D_{ph}$) to the AFM interaction induced d-wave component ($D_{AFM}$). As a result, $T_c$ is dramatically enhanced with a help of the phonon interaction. The condition for the anisotropy of the phonon, for this effect, is also clarified. We then derived an analytic $T_c$ equation for this $(D_{AFM} + D_{ph})$ case and showed that phonon isotope effect can be strongly reduced due to the interplay between the AFM and phonon interactions despite the large increase of $T_c$ by phonon. This result can explain a long standing puzzle of the small phonon isotope effect in HTSC. In view of experiments[2], the best anisotropic phonon can be the $B_{1g}$ buckling phonon mode, which fulfills all necessary qualifications for our model.

2. Model
We start with the Hamiltonian of free electrons with two phenomenological interactions: AFM spin fluctuations $V_{AFM}$ and phonon $V_{ph}$.

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Hamiltonian in the mean field theory can be written as
\[ H = \sum_{k\sigma} \epsilon(k) c_{k\sigma}^\dagger c_{k\sigma} + \sum_{kk'\uparrow\downarrow} V_{AFM}(k, k') c_{k\uparrow}^\dagger c_{-k'\downarrow} + \sum_{kk'\uparrow\downarrow} V_{ph}(k, k') c_{k\uparrow}^\dagger c_{-k'\downarrow} \]  
(1)
where \( \epsilon(k) \) is the dispersion of the quasiparticles created by \( c_{k\sigma}^\dagger \) as standard notation. \( V_{AFM}(k, k') \) and \( V_{ph}(k, k') \) are the effective interactions originating from the AFM spin fluctuations and phonon(s), respectively. For simplicity, the real two dimensional FS is simplified as a circular FS and the interactions are also modelled accordingly as follows.
\[ V_{AFM}(\Delta \phi) = V_M \frac{\phi_0^2}{(\Delta \phi + \phi_{AFM})^2 + \phi_0^2} \]  
(2) 
and
\[ V_{ph}(\Delta \phi) = \begin{cases} -V_P & \text{for } |\Delta \phi| < \phi_{AN} \\ 0 & \text{for } |\Delta \phi| > \phi_{AN} \end{cases} \]  
where \( \Delta \phi = \phi - \phi' \) and \( \phi_{AFM} = \pi/2 \) represent the exchanged momentum \( k - k' \) and the AFM ordering vector \( Q \) in the circular FS, respectively. \( V_M \) and \( V_P \) are chosen to be positive, so that \( V_{AFM} \) is all repulsive and \( V_{ph} \) is all attractive in momentum space. Now the reduced BCS Hamiltonian in the mean field theory can be written as
\[ H = \sum_{\phi\xi} \epsilon(\xi) c_{\phi\xi\sigma}^\dagger c_{\phi\xi\sigma} + \sum_{\phi\xi} \Delta_{AFM}(\phi) c_{\phi\xi\downarrow} c_{-\phi\xi\uparrow} + \sum_{\phi\xi} \Delta_{ph}(\phi) c_{\phi\xi\downarrow} c_{-\phi\xi\uparrow} \]  
(4)
where \( \Delta_{AFM}(\phi) \) is the SC gap function induced by \( V_{AFM} \) and \( \Delta_{ph}(\phi) \) is the one induced by \( V_{ph} \). The two gap functions \( \Delta_{AFM}(\phi) \) and \( \Delta_{ph}(\phi) \) may or may not have the same symmetry. After diagonalizing the above Hamiltonian we obtain two self-consistent equations as
\[ \Delta_{AFM}(\phi) = \sum_{\phi'\xi} V_{AFM}(\phi - \phi') c_{\phi'\xi\downarrow} c_{-\phi'\xi\uparrow} >, \]  
(5) 
\[ \Delta_{ph}(\phi) = \sum_{\phi'\xi} V_{ph}(\phi - \phi') c_{\phi'\xi\downarrow} c_{-\phi'\xi\uparrow} >. \]  
(6)

3. Results of \((D_{AFM} + D_{ph})\) case
We consider here the possibility that \( V_{ph} \) also supports a d-wave gap, therefore it is assumed that \( \Delta_{AFM}(\phi) = \Delta_{d1} \cos(2\phi) \) and \( \Delta_{ph}(\phi) = \Delta_{d2} \cos(2\phi) \). The coupled gap equations are
\[ \Delta_{d1}(\phi) = -\sum_{\phi'} V_{AFM}(\phi - \phi') \Delta_{d1}(\phi') \chi(\phi', \omega_{AFM}), \]  
(7) 
\[ \Delta_{d2}(\phi) = -\sum_{\phi'} V_{ph}(\phi - \phi') \Delta_{d2}(\phi') \chi(\phi', \omega_{ph}), \]  
(8) 
\[ \chi(\phi', \omega_{AFM,ph}) = N(0) \int_0^{\omega_{AFM,ph}} d\xi \frac{\tanh(\frac{E(\xi)}{2T})}{E(\xi)}. \]  
(9)
where $V$ change the anisotropy angle of $\phi$. Calculated magnitudes of $D$ angles $\phi_{\text{AN}}$ cases $N_{d}$ component ($\Delta_{d}$) for different phonon anisotropy angles $\phi_{\text{AN}} = \pi/8, \pi/4, \pi/2, \pi$. For all cases $N(0)V_{M} = 2.0$, $N(0)V_{p} = 0.5$ and $\omega_{ph}/\omega_{AFM} = 0.5$.

Also the effective dimensionless coupling constants $\lambda_{AFM,ph}$ are defined below as a projected average with a SC gap function.

$$\lambda_{AFM,ph} = N(0) \frac{\sum_{\phi,\phi'} V_{AFM,ph}(\phi - \phi') \eta(\phi) \eta(\phi')}{\sum_{\phi} \eta^{2}(\phi)} \quad \text{(10)}$$

where $\eta(\phi) = \cos(2\phi)$ for d-wave gap and $\eta(\phi) = 1$ for s-wave gap.

In Fig.1, we plot $\Delta_{d1}$ and $\Delta_{d2}$ separately; between the same symbols the smaller value is the phonon induced d-wave gap $\Delta_{d1}$ and the larger one is the AFM induced d-wave gap $\Delta_{d1}$. We change the anisotropy angle of $V_{ph}(\Delta_{d})$ with the fixed interaction strengths of $N(0)V_{M} = 2.0$ ($\lambda_{AFM,D} = 0.332$) and $N(0)V_{p} = 0.5$. For the phonon anisotropy angle $\phi_{\text{AN}} = \pi/2$ and $\pi$, the phonon interaction has absolutely no effect on the d-wave pairing; this is simply because the d-wave projected averaged interaction Eq.(10) becomes zero for these two commensurate angles with our model potential Eq.(3). With a stronger anisotropy ($\phi_{\text{AN}} = \pi/4$; $\lambda_{ph,D} = 0.12$), the phonon scattering sees only a limited part of the d-wave gap, therefore the d-wave gap is seen effectively as a s-wave gap for the anisotropic phonon. In our model potential, $\phi_{\text{AN}} = \pi/4$ is the optimal anisotropy. Fig.1 demonstrates that the phonon interaction, with a proper anisotropy, can dramatically enhance the total gap ($\Delta_{d,tot} = \Delta_{d1} + \Delta_{d2}$) and $T_{c}$ with a relatively weak phonon interaction. Other authors [4] also obtained a similar result using different approaches.

By taking a limit $\Delta_{d1}, \Delta_{d2} \rightarrow 0$ for Eq.(7) and (8), we obtain the $T_{c}$ formula of the $(D_{AFM} + D_{ph})$ case as

Figure 1. Calculated magnitudes of $D_{AFM}$ component ($\Delta_{d1}/\omega_{AFM}$) and $D_{ph}$ component ($\Delta_{d2}/\omega_{AFM}$) for different phonon anisotropy angles $\phi_{\text{AN}} = \pi/8, \pi/4, \pi/2, \pi$. For all cases $N(0)V_{M} = 2.0$, $N(0)V_{p} = 0.5$ and $\omega_{ph}/\omega_{AFM} = 0.5$.

Figure 2. $T_{c}$ (symbols) calculated as a function of $\omega_{ph}/\omega_{AFM}$ for different strength of phonon interaction $N(0)V_{P} = 0.0, 0.2, 0.4$, and 0.6, normalized by $T_{c0}$ the transition temperature with $N(0)V_{P} = 0.0$. For all cases, $N(0)V_{M} = 2.0$ and $\phi_{\text{AN}} = \pi/4$. Lines are the results of the analytic formula of $T_{c}$ Eq.(15). The symbols and lines of the same colors have the same parameters set.

\begin{align*}
\lambda_{AFM,ph} &= N(0) \frac{\sum_{\phi,\phi'} V_{AFM,ph}(\phi - \phi') \eta(\phi) \eta(\phi')}{\sum_{\phi} \eta^{2}(\phi)} \quad \text{(10)}
\end{align*}
\[ T_c \simeq 1.13 \omega_{AFM}^{\lambda_{AFM}} \omega_{ph}^{\lambda_{ph}} e^{-1/\lambda_t}. \]  

where \( \lambda_t = (\lambda_{AFM} + \lambda_{ph}) \), \( \lambda_{AFM} = \lambda_{AFM}/\lambda_t \) and \( \lambda_{ph} = \lambda_{ph}/\lambda_t \), and \( \lambda_{AFM} \) and \( \lambda_{ph} \) are the dimensionless effective coupling constants obtained from Eq.(10) with d-wave gap average for both couplings. \( \omega_{AFM} \) and \( \omega_{ph} \) are the energy cutoffs of the AFM interaction and phonon interaction, respectively.

Fig.2 shows the \( T_c \)'s (symbols) calculated from Eq.(7) and Eq.(8) as well as the results of the analytic formula Eq.(11), showing a good agreement. Now we are in position to read the phonon isotope coefficient \( \alpha \) from Eq.(11), which is

\[ \alpha = \frac{1}{2} \lambda_{ph} = \frac{1}{2} \frac{\lambda_{ph}}{\lambda_{AFM} + \lambda_{ph}}. \]  

For example, with representative values of \( \lambda_{AFM} = 0.33 \), \( \lambda_{ph} = 0.1 \) and \( \omega_{ph}/\omega_{AFM} = 0.5 \), we obtain \( \alpha \approx 0.116 \), which is pretty small value compared to the standard BCS value of 0.5 while \( T_c \) is enhanced by about 100\% from \( T_{c0} \) the transition temperature without phonon interaction (see Fig.2; \( N(0)V_F = 0.6 \) is \( \lambda_{ph} = 0.142 \)).

4. Conclusion
In this paper we studied the effects of phonon interaction on the superconducting pairing, in particular, the role of anisotropy, in the background of d-wave gap already formed by the AFM interaction. Anisotropic phonon can boost the SC pairing together with the AFM interaction in the \( (D_{AFM} + D_{ph}) \) type solution. The \( T_c \) formula Eq.(11) explains how and why the phonon isotope effect is strongly reduced despite the large enhancement of \( T_c \) by phonon, the long-standing puzzle in HTSC [5].

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