Pseudo-gap and vertex correction of electron-phonon interaction

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The standard strong-coupling theory has no bound on \( T_c \). Recently, the Eliashberg functions \( \alpha^2 F(\omega) \) extracted from the measurements of infrared optical conductivity [1] and ARPES spectrum [2] for copper-oxides superconductors predicted very strong electron-phonon interaction and very high \( T_c \) over the experimental values [1]. The \( T_c \) in mean-field approximation of Eliashberg theory is higher than experimental \( T_c \). The \( T_c \) in evolving from weak-coupling region to strong-coupling region. The doping-dependent \( T_c \) of cuprate superconductors and most importantly the pseudo-gap can be explained as the effects of vertex correction.

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The strong-coupling Eliashberg theory plus vertex correction is used to calculate the maps of transition temperature (\( T_c \)) in parameter-space characterizing superconductivity. Based on these \( T_c \) maps, complex crossover behaviors are found when electron-phonon interaction increases from weak-coupling region to strong-coupling region. The doping-dependent \( T_c \) of cuprate superconductors and most importantly the pseudo-gap can be explained as the effects of vertex correction.

The standard strong-coupling theory has no bound on \( T_c \). Recently, the Eliashberg functions \( \alpha^2 F(\omega) \) extracted from the measurements of infrared optical conductivity [1] and ARPES spectrum [2] for copper-oxides superconductors predicted very strong electron-phonon interaction and very high \( T_c \) over the experimental values [1]. The \( T_c \) in mean-field approximation of Eliashberg theory is higher than experimental \( T_c \). The \( T_c \) in evolving from weak-coupling region to strong-coupling region. The doping-dependent \( T_c \) of cuprate superconductors and most importantly the pseudo-gap can be explained as the effects of vertex correction.

The pseudogap and phase diagram with same topology as the phase diagram of doping-dependent \( T_c \) for cuprate superconductor are explained as the effects of vertex correction. The interplay of vertex correction and Coulomb interaction can suppress theoretical \( T_c \) to access experimental values [1].

The calculations of vertex corrections are greatly simplified under isotropic approximation because the electron-phonon interactions are included in the vertex corrections only by the functions of electron-phonon interaction \( \lambda_n \) defined as \( \lambda_n = 2 \int_0^{\infty} d\omega\alpha^2 F(\omega)\omega/\omega^2 + \omega_n^2 \). When temperature is very close to \( T_c \) the energy-gap equation [3, 4] is simplified to \( \sum_{n'=\pm\infty} K_{nn'}(\Delta_n'/|\omega_n'|) = 0 \). The kernel matrix is expressed as

\[
K_{nn'} = [\lambda_{n-n'}B_{nn'} - \mu^* + C_{nn'}]|a_n' - \delta_{nn'}H_{n'}, \quad (1)
\]

where the parameters \( A_{nn'} = 1 - V_{nn'}^A, B_{nn'} = 1 - V_{nn'}^B, s_n = \omega_n/|\omega_n| \) and \( a_n = (2/\pi)\arctan(E_B/Z_n|\omega_n'|) \). The three parameters of vertex correction \( V_{nn'}^A, V_{nn'}^B \) and \( C_{nn'} \) can be found in Ref. The Coulomb pseudopotential is defined as \( \mu^* = \mu_0/(1 + \mu_0\ln(E_B/\omega_0)) \), where \( \mu_0 = N(0)U \). The Coulomb interaction between electrons and \( \omega_0 \) characteristic energy of typical phonon related to superconductivity. If the vertex corrections are ignored, three parameters \( V_{nn'}^A, V_{nn'}^B \) and \( C_{nn'} \) are all equal to zero and the kernel Eq. of energy-gap reduction enters to the normal form without vertex correction after some symmetrizations and simplifications. It’s convenient that the \( K_{nn'} \) matrix is symmetrized as in Ref. [14]. The Eliashberg functions \( \alpha^2 F(\omega) \) have the same approximation as in Ref. [12]. Other details in our calculations can be found in Ref. [3, 11].

The parameter \( \Omega_c/E_B \) measures and controls the magnitude of vertex correction in perturbing calculation.

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From electron point of view, the vertex correction or nonadiabatic effect can be controlled by the effective band-width \( E_B \), on the other hand, from ion point of view, it can be controlled by the cutoff \( \omega_0 \) of phonon energy or \( \Omega_P \) in Einstein model. In this work, the vertex correction is controlled by the effective band-width \( E_B \) within the range from 0.5 eV to 5 eV. The situation \( E_B = \infty \) is equivalent to no vertex correction. The smaller \( E_B \) means possible the stronger vertex correction.

The Fig.1(a,b,c) illustrate the evolution of \( T_c \) map on \( \lambda-\Omega_P \) plane with decreasing strengths of vertex corrections (decreasing effective band-width \( E_B \)) with (a) \( E_B = \infty \), (b) \( E_B=1.7 \) eV and (c) \( E_B=1 \) eV. The Coulomb pseudo-potential \( \mu^* = 0.1 \).

The Fig.2(a) is the \( T_c \) change along two arrows shown in Fig.1(c) with fixed phonon energies \( \Omega_P=80 \) meV and 95 meV respectively. (b) The \( T_c \) change along two arrows shown in Fig.3(c) with fixed Coulomb pseudo-potentials \( \mu^* = 0.10 \) and 0.25 respectively.

The Fig.3(a) shows the changes of \( T_c \) with \( \mu^* \) along two arrows A and B shown in Fig.1(c). If \( \Omega_P=80 \) meV, the \( T_c \) monotonously increases with \( \mu^* \). However for \( \Omega_P=90 \) meV, the \( T_c \) first increases with \( \lambda \), reaches the maximum at \( \lambda \sim 1.5-1.7 \) and then quickly decreases with increasing \( \lambda \). Further increasing \( \lambda > 2 \), \( T_c \) will be very low due to strong vertex correc-

FIG. 1: The evolution of \( T_c \) map on the \( \lambda-\Omega_P \) plane with increasing strengths of vertex corrections (decreasing effective band-width \( E_B \)) with (a) \( E_B = \infty \), (b) \( E_B=1.7 \) eV and (c) \( E_B=1 \) eV. The Coulomb pseudo-potential \( \mu^* = 0.1 \).

FIG. 2: (a) The \( T_c \) change along two arrows shown in Fig.1(c) with fixed phonon energies \( \Omega_P=80 \) meV and 95 meV respectively. (b) The \( T_c \) change along two arrows shown in Fig.3(c) with fixed Coulomb pseudo-potentials \( \mu^* = 0.10 \) and 0.25 respectively.

FIG. 3: The evolutions of \( T_c \) map on the \( \mu^* - \lambda \) plane (\( \Omega_P=69 \) meV) with decreasing effective band-width (a) \( E_B = \infty \), (b) \( E_B=1.7 \) eV and (c) \( E_B=1.0 \) eV.
tions. The non-monotonous $\lambda$-dependent $T_c$ in Fig(2a) had been found in the non-adiabatic theory of superconductivity [6]. Some crossover behaviors from weak coupling to strong coupling region had been predicted in Holstein-Hubbard model solved numerically by quantum Monte Carlo method [7] and in polaron theory [8]. It’s very reasonable that the non-monotonous $\lambda$-dependence $T_c$ is equivalent to the crossovers found in QMC calculation [6] and polaron theory [8]. So only the leading vertex correction can describe qualitatively well the electron-phonon interaction in strong coupling region.

The $T_c$ map on $E_B-\lambda$ plane with $\mu^*=0.25$ and $\Omega_P=72$ meV. (b) The open circle line is the evolution of $T_c$ from P1 to P2 in (a) but $\mu^*$ linearly decreases from 0.3 to 0.1. The solid line $T_c$ is the standard results in strong coupling theory without vertex correction. (c) The $\delta-\lambda$ relation is adopted in Ref.[1]

The Fig(3a) is the normal $T_c$ map on $\mu^*-\lambda$ plane without vertex correction [8]. The figure shows that when $\mu^*>0.2$, $T_c$ is insensitive to the change of $\mu^*$. The breaking contour lines with $T_c=0$ K are because of the inaccurate calculations when $T_c<0.1$ K if only $N=200$ Matsubara energies are used. The contour lines with $T_c>0.1$ K are accurate enough. If the Coulomb pseudo-potential and vertex correction work together, the situation will change drastically and some new interesting results will appear. The large deformations are found in Fig(3c) if $E_B$ decreases to 1.0 eV. As expected, the large deformations and discontinuous changes of contour lines appear on the $T_c$ map when $\mu^*>0.20$. The contour lines with iso-values from $T_c=20$ K to 200 K are packed together within the rectangle region in Fig(3c) with $0.15<\mu^*<0.25$ and $\lambda>2$. The figure clearly shows that if the Coulomb pseudo-potential $\mu^*$ is larger enough, the $T_c$ will change with $\lambda$ non-monotonously. The changes of $T_c$ along two arrows with $\mu^*=0.1$ and 0.25 are plotted in Fig(2b). For $\mu^*=0.25$, $T_c$ first increases with $\lambda$ until reaches the maximum at $\lambda=2.2$ and then sharply decreases to smaller value at $\lambda=2.5$. The crossover behavior is enhanced by strong Coulomb interaction.

The $T_c$ map on $E_B-\lambda$ plane is presented in Fig(4a) with $\Omega_P=72$ meV. If $E_B$ increases but $\lambda$ keeps unchanged, the $T_c$ monotonously increases with $E_B$ until to the limit of non-vertex-correction. More interestingly, on this map, the $T_c$ is non-monotonous dependent on $E_B$ along straight line from P1 to P2 companying by
the decrease of $\lambda$ from 5.0 to 0.2. The non-monotonous dependence of $T_c$ on effective band-width $E_B$ is equivalent to the band-filling effect of $T_c$. Our results show that, if $\Omega_p > 80$ meV, the suppression of $T_c$ will be more prominently.

The values of $T_c$ obtained from standard strong-coupling theory are generally higher than those measured in experiments. The copper-oxides superconductors Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ and Bi$_2$Sr$_2$CuO$_{6+\delta}$ studied in Ref. [1, 2] have very strong electron-phonon interactions $\lambda > 2.36 - 2.85$ and overestimated $T_c$ in underdoped samples. With increasing doping $\delta$, the values of $T_c$ decrease to about 0.35 to 1.42 [1].

The effective band-widths $E_B$ of conducting electrons for these cuprates are distributed from 1 eV to 3 eV. The effective phonon energies are distributed from 50 meV to 80 meV. We re-calculate the $T_c$-doping phase diagram in underdoped region shown in Fig.4(b). The cooper-pairs degenerating with $T_c$ along straight line $P1-P2$ in Fig.4(a) under assumption that the Coulomb interaction is strong in underdoped region $\mu^* = 0.3$ at $P1$ and weak in overdoped region $\mu^* = 0.1$ at $P2$. For simplicity, $\mu^*$ linearly decreases from 0.3 at $P1$ to 0.1 at $P2$. As shown in Fig.4(b), if $\lambda < 4.0$, the values of $T_c$ are reduced from around 200 K to lower than 150 K and close to experimental values [1]. In strong-coupling region 4.0 $> \lambda > 3.0$, $T_c$ is very low. Our results are provided an explanation to pseudo-gap in underdoped region shown in Fig.4(b). The Cooper-pairs pre-form at $T^*_c$, the transition temperature of mean field theory (MFT) or the standard strong-coupling theory. However strong non-adiabatic effects induce the instability of Cooper-pairs and the real $T_c$ has lower value. The $T^*_c$ degenerating with $T_c$ in overdoped region is similar to the example (1) of Fig.9 in Ref. [15].

An interesting result is that at very strong coupling $\lambda > 4.0$, the effects of vertex corrections supercificially become weak. Even there are positive vertex correction that had been found in other work [2]. The electronic states in region $SP$ with $\lambda > 4.0$ are strong-coupling pairs [18]. The Fig.4(b) shows a crossover from BCS state to strong-coupling pairs state with increasing electron-phonon interaction $\lambda$. It’s obviously that Fig.4(b) has the same topology as the well-known $T_c$-doping phase diagram. It’s dependent on whether the parameter $\lambda$ electron-phonon interaction decreases with increasing doping or not. This point had been proved in recent experiments [1, 2]. The $\delta - \lambda$ curve in Fig.4(c) is based on data in Ref. [1]. It’s urged that there will be other experiments supporting this point.

In order to analyze our results more deeply, we present individually the effects of non-adiabatic parameters $V_{nn'}^A$, $V_{nn'}^B$, and $C_{nn'}$ on $T_c$ in Fig.4(a). The $T_c$-$\lambda$ curve labeled with $V^B$ is calculated by allowing $V_{nn'}^B \neq 0$ and setting $V_{nn'}^A = 0$ and $C_{nn'} = 0$. Other curves are obtained with the same manner. We can find that the dome shape curve of $T_c$ in the region $\lambda < 4.0$ is generated by the effects of $V_{nn'}^B$. In the region $\lambda > 4.0$, the effects of $V_{nn'}^A$ and $C_{nn'}$ cancel the effects of $V_{nn'}^B$ so that the strong coupling pairs in mean field approximation are restored and even have higher $T_c$. This fact can be clarified from the Fig.4(b,c) in that the averages of the absolute values of diagonal and off-diagonal elements of parameter matrix $|A_{nn'}| = |1 - V_{nn'}^A|$, $|B_{nn'}| = |1 - V_{nn'}^B|$ and $|C_{nn'}|$ have larger changes mainly in the region $2.5 < \lambda < 4.0$. Moreover in the region $\lambda > 4.0$, the $|A_{nn'}|$ and $|B_{nn'}|$ are close to normal values 1.0 just as in weak coupling region. Additionally, the average values of diagonal elements of parameter matrix $|C_{nn'}|$ and $|B_{nn'}|$ steadily increase with $\lambda$ and lead to positive vertex-correction.

In summary the non-monotonous changes of $T_c$ with increasing $\lambda$ show the crossover behaviors near $\lambda = 2$ when $\lambda$ evolving from weak-coupling region to strong-coupling region. The crossovers can explain both the pseudo-gap phenomenon and the dome shape of doping dependent $T_c$ of cuprate superconductors. The $T_c$ maps in the previous paper [3] and the maps with vertex corrections in this paper provide very comprehensive understanding of superconductivity of superconductors. The author thanks Prof. E. Cappelluti for very helpful discussions.

[1] van Heumen E, Muhlethaler E, Kuzmenko A B, Eisaki H, Meevasana W, Greven M and van der Marel D 2009 Phys. Rev. B 79 184512.
[2] Ruiz H S and Badia-Majos A 2010 arXiv:1005.4770 [cond-mat].
[3] Kostur V N and Mitrović B 1994 Phys. Rev. B 50 12774.
[4] Grimaldi C, Pietronero L and Strässler S 1995 Phys. Rev. B 52 10530.
[5] Fan W 2009 Physica C 469 177.
[6] Paci P, Cappelluti E, Grimaldi C and Pietronero L 2001 Phys. Rev. B 65 012512.
[7] Freericks J K, Jarrell M and Scalapino D J 1993 Phys. Rev. B 48 6302.
[8] Nasu K 1990 Phys. Rev. B 42 6076.
[9] Fan W 2008 Chin. Phys. Lett. 25 2217.
[10] Fan W, Wang J L, Zou L J and Zeng Z, 2010 Chin. Phys. Lett. 27 087402.
[11] Ren Z A, Lu W, Yang J, Yi W, Shen X L, Li Z C, Che G C, Dong X L, Sun L L, Zhou F, Zhao Z X 2008 Chin. Phys. Lett. 25 2215.
[12] Scalapino D J, Schrieffer J R and Wilkins J W 1966 Phys. Rev. 148 263.
[13] McMillan W L 1968 Phys. Rev. 167 331.
[14] Allen P B and Dynes R C 1975 Phys. Rev. B 12 905.
[15] Norman M R, Pines D and Kallin C 2005 Advances in Physics 54 715.
[16] Xu Z A, Ong N P, Wang Y, Kakeshita T and Uchida S 2000 Nature 406 486.
[17] Wen H H, Wu G, Luo H Q, Yang H, Shan L, Ren C, Cheng P, Yan J and Fang L 2009 Phys. Rev. Lett. 103 067002.
[18] Chakraverty B K 1980 Nature 287 393.