MODIFIED BCS GAP EQUATION FOR JAHN-TELLER DISTORTED HIGH TEMPERATURE SUPERCONDUCTORS

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In this communication we report the interplay of the normal electron-phonon (EP) interaction, dynamic Jahn-Teller (DJT) distortion and superconductivity in high temperature superconductors in presence of a static lattice strain. This model consists of a degenerate two orbital band separated by Jahn-Teller (JT) energy modified by the DJT interaction in the conduction band. The superconductivity is assumed to be s-wave type present in the same band. The interaction Hamiltonian is solved by Green's function method and a modified BCS gap equation is obtained with a modified conduction band energy $\tilde{\varepsilon}_{\alpha k}$ and modified BCS order parameter $\tilde{\Delta}_{\alpha}$ with $\alpha = 1, 2$ designating the two orbitals. This interplay displays some new interesting results which are different from the effect of the static lattice strain on superconducting (SC) order parameter. The interplay is studied by varying the normal EP coupling, the DJT coupling, the SC coupling, the phonon vibration frequency, the phonon wave vector and other model parameters of the system.

Keywords: High-Tc Superconductivity; Dynamic Jahn-Teller Effect; Electron-Phonon Interaction.

1. Introduction

The high-Tc copper oxide superconductors exhibit a pseudogap (PG) state as observed in the anomalous transport, thermodynamic, and optical properties below a temperature, larger than the superconducting transition temperature $T_c$. One of the challenging issues of the SC mechanism is the origin of the PG. The PG phase is detected in the underdoped region, which has been interpreted in terms of

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preformed pairs, a circulating current phase, and many more. In many cuprate superconductors in the underdoped region, the static stripe phases play an important role, which may be incommensurate unidirectional spin and charge-density waves. Also it has been reported that bismuth-based cuprates conventionally exhibit the "out-of-plane disorder," which strongly affects superconducting transition temperature $T_c$ This suggests that the out-of-plane disorder is a potentially important factor concerning the superconducting properties of high-$T_c$ superconductors and hence it proves the importance of Jahn-Teller effect.

The dependence of the SC transition temperature on the structural properties is little understood for the high temperature SC compounds. In this system, the Fermi level (FL) lies within the degenerate band of the two orbitals. The molecular distortion is produced when the electronic degeneracy is removed by some symmetry breaking interactions. This type of distortion is called Jahn-Teller distortion. There is a change in the electronic density of states (DOS) around the FL associated with such a transition. Therefore, it is expected that the band Jahn-Teller (BJT) distortion would strongly influence the superconductivity in such a system.

There is a large number of experimental evidences indicating the strong influence of the structural distortion on the SC transition temperature. The neutron scattering measurements of the temperature dependence of the spontaneous strain have been reported by Paul et al. for $La_{2-x}Ba_xCuO_4$ ($T_c \approx 38K$). The system exhibits a structural transition at 180K. The magnitude of the strain rises on lowering the temperature and shows an anomalous suppression below 75K. This anomaly is expected to be associated with the appearance of the superconductivity in the system. The evidence for such interplay between lattice distortion and superconductivity in $La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_6.5$ and even in electron doped cuprate system $Nd_{2-x}Ce_xCuO_4$ has been reported by Lang et al. from thermal expansion measurements. Moreover, the suppression of the lattice distortion in the SC state has also been observed for 2212 and 2223 Bi-superconductors as shown by extended X-ray absorption measurements. Further, the structural transition from tetragonal to orthorhombic phase in $La_{2-x}Sr_xCuO_4$ takes place at temperatures higher than the SC transition temperature $T_c$ is also reported for $La_{2-x}M_xCuO_4$ ($M = Ca, Sr$). These measurements clearly demonstrate that there exists a strong interplay between superconductivity and structural distortion.

The introduction of an electron-phonon mechanism that can achieve high-$T_c$ superconductivity is challenging in the theoretical point of view. For the theoretical study of the high-$T_c$ superconductivity the onsite and/or intersite bipolarons, JT bipolarons and different mechanisms of carrier dynamics such as Bose-Einstein condensation and tunneling-percolation have been proposed. The JT polaron pairing effect was originally proposed as a possible explanation for the superconductivity in $La_{2-x}Ba_xCuO_4$ by Bednorz and Müller. Since then this effect has been discussed by a number of authors in different contexts and many features have
been observed experimentally supporting the general concept of JT effect\cite{26,27}. A dynamic Jahn-Teller effect arises, when there is a degeneracy in both of electronic levels and of molecular vibrations and when two independent distortions have the same JT energy lowering. The DJT effects have been proposed to play a role in a number of materials of current interest including cuprates\cite{24,28,29} and manganites\cite{30} etc.

Ghosh et al. have reported a simple model study of the interplay between the superconductivity and the static JT distortion\cite{31}. In another report the same authors have reported the coexistence of the static JT effect with the superconductivity for the correlated orbitally degenerated bands of the cuprate systems taking into account one band Hubbard model\cite{32}. In the present report, we consider the interplay between static lattice strain and superconductivity in presence of a normal electron-phonon interaction and dynamic JT interaction. The rest of the work in the paper is organized as follows. The theoretical model for the DJT is described in section 2. In the dynamic limit calculation, the electron Green’s functions are calculated and solved in such a way that it gives rise to the modified BCS gap equation. The lattice strain relation is calculated in section 3, the results and discussion are presented in section 4 and finally the conclusion is given in section 5.

2. Theoretical Methods

The present model study attempts to investigate the effect of DJT distortion on the superconducting gap in high-\(T_c\) superconductors (HTSs). If the Fermi level lies on a degenerate conduction band and the degeneracy is removed by lowering of the lattice symmetry, a spontaneous lattice strain is produced in the band resulting in the structural transition. This strain in the band is stabilized, if the gain in electronic energy overcomes the cost in elastic energy. Depending on the magnitude of the lattice distortion, the system can behave as a metal or insulator. The difference in the occupation probability of the two bands will couple to the lattice strain which gives rise to JT distortion. The Hamiltonian for such a system is reported earlier\cite{33,34,35} and the same Hamiltonian is written here.

\[
H_c = \sum_{k\sigma} \epsilon_k \left( c_{1k\sigma}^\dagger c_{1k\sigma} + c_{2k\sigma}^\dagger c_{2k\sigma} \right),
\]

\[
H_{c-L} = G \sum_{k\sigma} \left( c_{1k\sigma}^\dagger c_{1k\sigma} - c_{2k\sigma}^\dagger c_{2k\sigma} \right).
\]

The Hamiltonian \(H_c\) represents the hopping of the electrons between the two nearest neighbors for the two degenerate orbitals designated as 1 and 2. The dispersion of the degenerate band in a two dimensional CuO\(_2\) plane is written as \(\epsilon_k = -2t_0(\cos k_x + \cos k_y)\). Here \(c_{\alpha k\sigma}^\dagger(c_{\alpha k\sigma})\), for \(\alpha = 1\) and 2, are creation (annihilation) operators of the conduction electrons of copper ions for two orbitals with momentum \(k\) and spin \(\sigma\). The Hamiltonian \(H_{c-L}\) represents the static JT interaction where \(G\) is the strength of the electron-lattice interaction and \(e\) is the strength of the isotropic
static lattice strain. The lattice strain splits the single degenerate band into two bands with energies $\epsilon_{1,2k} = \epsilon_k \pm Ge$. The elastic energy of the system is $\frac{1}{2}Ce^2$ with $C$ representing the elastic constant. The minimization of the free energy of the electron including the elastic energy helps to find the expression for lattice strain. It is shown earlier that the static lattice strain suppresses the SC gap parameter in the interplay region of the two order parameters.

In order to investigate the phonon response in the HTSs, we consider the phonon interaction to the density of the conduction electrons of both the orbitals as well as the phonon coupling to the difference in electron densities of the JT distorted orbitals of the conduction band. The electron-phonon interaction Hamiltonian is written as

$$H_{e-p} = \sum_{\alpha,k,\sigma} f_1(q) \left( c_{\alpha k+q\sigma}^\dagger c_{\alpha k\sigma} \right) A_q - \sum_{\alpha,k,\sigma} (-1)^\alpha f_2(q)e \left( c_{\alpha k+q\sigma}^\dagger c_{\alpha k\sigma} \right) A_q$$

$$= \sum_{\alpha,k,\sigma} s_\alpha(q) \left( c_{\alpha k+q\sigma}^\dagger c_{\alpha k\sigma} \right) A_q.$$  \hspace{1cm} (3)

The strength of the EP coupling $s_\alpha(q)$ is defined as $s_\alpha = f_1(q) - (-1)^\alpha f_2(q)e$ in which $f_1(q)$ is the normal EP coupling and $f_2(q)$ is the dynamic Jahn-Teller EP coupling. The $q^{th}$-Fourier component of the phonon displacement operator is $A_q = b_q + b_q^\dagger$ with $b_q^\dagger$ ($b_q$) defining the phonon creation (annihilation) operator for wave vector $q$. Further the free phonon Hamiltonian $H_p$ is given in harmonic approximation as

$$H_p = \sum_q \omega_q b_q^\dagger b_q,$$  \hspace{1cm} (4)

with $\omega_q$ being the free phonon frequency.

Our main objective in the present report is to study the effect of dynamic JT distortion on the superconductivity in HTSs. The $d$-wave models have gained substantial support recently over $s$-wave pairing as the mechanism by which high temperature superconductivity might be explained. The establishment of $d$-wave symmetry in cuprates does not necessarily specify a high-$T_c$ mechanism. It does not impose well defined constraints on possible models for this mechanism. While the spin fluctuation pairing mechanism leads naturally to an ordered parameter with $d$-wave symmetry, the conventional BCS electron phonon pairing interaction give rise to $s$-wave superconductivity. As a first step, it is assumed that $s$-wave like BCS pairing interaction mediated by some boson exchange exist within the same orbitals of a sub lattice and the same strength of the interaction is taken for the orbitals. The BCS type pairing Hamiltonian is considered here for the two orbitals.

$$H_I = -\Delta \sum_{\alpha,k} \left( c_{\alpha k\uparrow}^\dagger c_{\alpha,-k\downarrow} + c_{\alpha,-k\uparrow} c_{\alpha k\downarrow} \right).$$  \hspace{1cm} (5)

In order to simulate an attractive interaction to produce Cooper pairs, the energy
dependence of the interaction potential is taken as
\[ U(\epsilon) = U_0 \left[ 1 - \left(\frac{\epsilon - \epsilon_F}{\omega_D^4}\right)^{\frac{1}{4}} \right], \tag{6} \]
where \( U_0 \) is the effective attractive Coulomb interaction, \( \omega_D \) is cut-off energy and \( \epsilon_F \) represents the Fermi energy. In order to produce band splitting due to JT distortion, we consider an energy dependent density of state \( N(\epsilon) \) around the center of the conduction band in the system. Such a logarithmic model density of state\( ^{35} \) is given by
\[ N(\epsilon) = N(0) \sqrt{1 - |\epsilon_D| \ln \frac{|D|}{\epsilon^2}}, \tag{7} \]
where \( 2D = W \) is the conduction band width. The total Hamiltonian describing the dynamic JT effect and SC interaction in high-\( T_c \) cuprate systems can be written as
\[ H = H_c + H_{e-L} + H_I + H_{e-p} + H_p. \tag{8} \]

3. Calculation of Order Parameters
In order to calculate the SC gap and the lattice strain, we calculate the Green’s functions for the electrons in the two orbitals \( (\alpha = 1 \text{ and } 2) \) of the conduction band by using the Zubarev’s technique of Green’s functions\( ^{36} \). For the calculation we use the total interaction Hamiltonian given in equation (8). The coupled Green’s functions for the two orbitals can be defined as
\[ A_{\alpha}(k, \omega) = \langle c_{\alpha k \uparrow} c_{\alpha k \uparrow}^\dagger \rangle_\omega; \quad B_{\alpha}(k, \omega) = \langle c_{\alpha -k \downarrow}^\dagger c_{\alpha k \uparrow}^\dagger \rangle_\omega. \tag{9} \]
The calculation of Green’s functions \( A_{\alpha} \) and \( B_{\alpha} \) couples to the higher order Green’s functions \( \Gamma_{\alpha}^1 \) and \( \Gamma_{\alpha}^2 \) involving the electron and the phonon operators. They are written as
\[ \Gamma_{\alpha}^1(k, q, \omega) = \langle c_{\alpha k-q \uparrow} A_q; c_{\alpha k \uparrow}^\dagger \rangle_\omega; \quad \Gamma_{\alpha}^2(k, q, \omega) = \langle c_{\alpha k-q \downarrow} A_q; c_{\alpha k \uparrow}^\dagger \rangle_\omega. \tag{10} \]
The equations (9) and (10) involve higher order Green’s functions which are truncated by applying mean-field approximation in order to obtain the close form solutions. By this calculation we obtain the second order terms in electron-phonon coupling in the final results. In this mean-field approximation there appears a term \( N_q = 2\nu_q \), where the Bose-Einstein distribution function is \( \nu_q = \frac{1}{\exp(w/k_BT) - 1} \).
These coupled equations for \( \Gamma_{\alpha}^1 \) and \( \Gamma_{\alpha}^2 \) are solved in terms of the Green’s functions \( A_{\alpha} \) and \( B_{\alpha} \) and they are written below as
\[ \Gamma_{\alpha}^1(k, q, \omega) = s_{\alpha} N_q \left[ \frac{A_{\alpha}(k, \omega) - \Delta B_{\alpha}(k, \omega)}{\omega^2 + E_{\alpha k-q}^2 - 2\epsilon_{\alpha k-q}} \right] \tag{11} \]
and
\[ \Gamma_{\alpha}^2(k, q, \omega) = s_{\alpha} N_q \left[ \frac{B_{\alpha}(k, \omega) + \Delta A_{\alpha}(k, \omega)}{\omega^2 + E_{\alpha k-q}^2 - 2\epsilon_{\alpha k-q}} \right]. \tag{12} \]
On substitution of $\Gamma_1^\alpha$ and $\Gamma_2^\alpha$ in equation (9), finally we obtain the Green’s functions $A_\alpha$ and $B_\alpha$ as

$$A_\alpha(k, \omega) = \frac{1}{2\pi} \left[ \frac{\omega + \tilde{\epsilon}_{\alpha k}}{\omega^2 - \tilde{E}_{\alpha k}^2} \right]$$

(13) and

$$B_\alpha(k, \omega) = \frac{1}{2\pi} \left[ \frac{-\tilde{\Delta}_{\alpha}}{\omega^2 - \tilde{E}_{\alpha k}^2} \right].$$

(14)

The modified SC quasi-particle energy band for the two orbitals can be written as $\tilde{E}_{\alpha k}^2 = (\tilde{\epsilon}_{\alpha k} + \tilde{\Delta}_{\alpha}^2)$. Again the modified conduction band $\tilde{\epsilon}_{\alpha k}$ can be written in general form as

$$\tilde{\epsilon}_{\alpha k} = \epsilon_{\alpha k} + \sum_q 2(\omega - \epsilon_{\alpha k-q})N_q (\omega - \epsilon_{\alpha k-q})^2 + \Delta^2,$$

(15)

where $\epsilon_{\alpha k-q} = \epsilon_{k-q} - \mu - (-1)^\alpha Ge$ and the Bose-Einstein distribution function $N_q$ is defined as $N_q = (e^{\beta\omega_q} - 1)^{-1}$, with $\beta = 1/k_BT$ and $\omega_q$ being the renormalized phonon frequency at temperature $T$.

The modified SC gap for the orbitals 1 and 2 in presence of normal phonon interaction as well as the dynamic JT interaction appears as

$$\tilde{\Delta}_{\alpha k} = \Delta + \sum_q 2\Delta N_q (\omega - \epsilon_{\alpha k-q})^2 + \Delta^2.$$

(16)

From equations (15) and (16), it appears that the degenerate conduction band $\epsilon_k$ and the BCS gap parameter are renormalized by the static Jahn-Teller effect through the EP coupling constants and lattice strain $e$. In absence of EP coupling, the quasi particle band can be written as $E_{\alpha k} = \sqrt{E_{\alpha k}^2 + \Delta^2}$, where $\epsilon_{\alpha k} = \epsilon_k - \mu - (-1)^\alpha Ge$. This agrees with the calculation of Ghose et al. [31] for static lattice strain. Thus, the static Jahn-Teller effect only renormalizes the energy of the doubly degenerate conduction electron band, but not the superconducting gap parameter. Due to the interplay of both the order parameters i.e., superconducting gap and lattice strain, the lattice strain changes when the temperature decreases down to below transition temperature $T_c$ [31]. In the absence of lattice strain, the quasi particle of BCS model is reproduced i.e., $E_k = \sqrt{E_k^2 + \Delta^2}$.

The SC gap parameter is defined as

$$\Delta = -\sum_{\alpha k} \hat{U}_k \langle c_{\alpha k \uparrow} c_{\alpha,-k \downarrow} ^\dagger \rangle.$$

Finally the SC order parameter is found from the correlation functions calculated from the Green’s functions given in equation (14) and can be written as

$$1 = \int_{-\omega_D}^{\omega_D} U(\epsilon)N(\epsilon) d\epsilon_k \left[ \frac{1}{2E_{1k}} \tanh \left( \frac{1}{2} \beta \tilde{E}_{1k} \right) + \frac{1}{2E_{2k}} \tanh \left( \frac{1}{2} \beta \tilde{E}_{2k} \right) \right],$$

(17)
where $U(\epsilon)$ and $N(\epsilon)$ are defined in equations (8) and (7) respectively and the SC coupling constant is written as $g = N(0)u_0$. The equilibrium value of the static stress $e$ is found by minimizing the free energy which includes electronic as well as the lattice energies. The lattice strain is defined as

$$e = -\sum_{\alpha k \sigma} (-1)^\alpha \langle c_{\alpha k \sigma}^\dagger c_{\alpha k \sigma} \rangle .$$

(18)

The correlation functions of the electrons of the two orbitals are calculated from the Green’s functions $A_{\alpha}$ given in equation (13) and the equilibrium lattice strain can be written as

$$e = \left(-\frac{G}{c_0}\right) \int_{-W/2}^{W/2} N(\epsilon)d\epsilon_k \left[ \frac{\tilde{\epsilon}_{1k}}{2\tilde{E}_{1k}} \tanh \left(\frac{1}{2}\beta \tilde{E}_{1k}\right) - \frac{\tilde{\epsilon}_{2k}}{2\tilde{E}_{2k}} \tanh \left(\frac{1}{2}\beta \tilde{E}_{2k}\right) \right].$$

(19)

In order to study the mutual influence of the dynamic lattice distortion and superconductivity, one has to solve the above two coupled equations (17) and (19) self-consistently.

4. Results and Discussion

The electron Green’s functions $A_{\alpha}(k, \omega)$ and $B_{\alpha}(k, \omega)$ given in equations (13) and (14) are calculated from the total Hamiltonian consisting of SC and DJT interactions. The SC gap equation is written in the form of the modified BCS gap equation from electron correlation functions. The SC gap $\Delta$ and the lattice strain $e$ are calculated and given respectively in equations (17) and (19). These equations are solved self-consistently and their temperature dependence is shown in figures 1 to 12. All the physical parameters in the present calculation are scaled by the nearest neighbor hopping integral $2t_0 \approx 0.25\text{eV}$ for convenient self-consistent solutions. The dimensionless parameters are the SC coupling constant, $g = N(0)u_0$, the static JT coupling, $g_1 = G/2t_0$, the SC gap parameter, $z = \Delta/2t_0$, the static JT energy, $\tilde{c} = Gc/2t_0 = g_1 c$, and the phonon energy $c_q = v_F q$ corresponding to the electron velocity $v_F$ at the Fermi level. Further the other phonon parameters are the normal EP coupling $\lambda_1 = f_1/2t_0$, the DJT coupling, $\lambda_2 = f_2/2t_0$ for the JT distorted two orbitals, the phonon frequency, $\omega_1 = 0.0008$ at a given reduced temperature, $t = k_B T/2t_0$ and reduced external frequency, $c = \omega/2t_0 = 0.1$. The temperature dependent parameters $z(t)$ and $\tilde{c}(t)$ are solved self-consistently for a standard set of parameters i.e., $g = 0.031, g_1 = 0.152, \lambda_1 = 0.004$ and $\lambda_2 = 0.01$. The conduction band width, $W = 1\text{eV}$ and the cut-off frequency, $\omega_c = 250K$ for the SC pairing are taken for all further calculation.

Figure 1 shows the temperature variation of $z(t)$ and $\tilde{c}(t)$ for the static JT effect (red curves) and the DJT effect (green curves). The parameters are so adjusted that the JT distortion temperature ($t_c$) becomes greater than the SC transition temperature ($t_e$). The neutron scattering measurement of the temperature dependence of the spontaneous lattice strain for $La_{1.85}Ba_{0.15}CuO_4$ ($T_c \approx 38K$) exhibits a structural transition at $180K$ [16]. The magnitude of the strain rises on lowering.
the temperature and an anomalous suppression of strain below $T < 75K$. It may be associated with appearance of superconductivity. In static case, the SC order parameter $z$ shows mean-field behavior, while the JT energy gap $\tilde{\epsilon}$ shows depression within the interplay region; but $\tilde{\epsilon}$ shows mean-field behavior in the JT distorted phase for temperature $t > t_c$. Under DJT effects, the SC gap parameter is enhanced throughout the temperature range with the enhancement of the transition temperature $t_c$. This is contrary to the results obtained for the system under static limits as shown by mean-field calculations as well as the sophisticated Slave-boson calculations. It is found that the reduced SC gap size is $2\Delta_0/k_BT_c \simeq 3.64$ in the static JT limit, while the gap size is $2\Delta_0/k_BT_c \simeq 3.59$ in the DJT limit. The ratio is slightly less in the dynamic limit than its value in the static limit due to the enhancement of $t_c$ in the dynamic limit. The reduced gap sizes are comparable to the universal BCS value of 3.52. The evolutions of the two gap parameters are discussed below by varying the other parameters of the system as shown in the figures from 2 to 12.

![Figure 1](image)

**Fig. 1** The self-consistent plots of $z$ vs. $t$ and $\tilde{\epsilon}$ vs. $t$ for the SC coupling $g = 0.031$ and static JT coupling $g_1 = 0.152$ (red curves) and for the dynamic effect (green curves) for the same values of $g$ and $g_1$ with the fixed values of the phonon frequency $\omega_1 = 0.0008$, external frequency $c = 0.1$, normal EP coupling $\lambda_1 = 0.004$ and DJT coupling $\lambda_2 = 0.01$.

The effect of the static JT coupling $g_1$ on the SC parameter $z$ and the static JT energy gap $\tilde{\epsilon}$ is shown in figure 2. It is observed that the lattice strain energy ($\tilde{\epsilon}$) is reduced throughout the temperature range with decrease of static lattice coupling $g_1$. With the decrease of JT coupling to 0.145, the mean-field behavior disappears and the gap becomes nearly constant with temperature. On the other hand, the SC gap is enhanced throughout the temperature range with the decrease of the static JT coupling $g_1$ resulting in the enhancement of the SC transition temperature. The SC parameter shows mean-field behavior for all values of JT coupling ($g_1 = 0.145$ to 0.159). It is found that the reduced gap size $2\Delta_0/k_BT_c$ gradually decreases with
the decrease of the JT coupling $g_1$. This so happens because $t_c$ enhancement is more than the enhancement of the gap parameter $z$ due to the interplay of SC and lattice strain parameters. It appears that there exists a strong interplay between these two interactions. The band Jahn-Teller effect lifts the orbital degeneracy and lowers the electronic energy due to lattice distortion. Both structural transition $t_s$ and lattice strain $e(T = 0)$ are maximum, as the Fermi level lies at the singular point of the density of states. The suppression of SC transition temperature $t_c$ in presence of structural distortion is related to the removal of electronic states from the Fermi level due to the lifting of degeneracy. The larger the splitting of orbitals (with higher values of $t_s$ and $e$), the larger is the suppression of $t_c$.

Fig. 2 The self-consistent plots of $z$ vs. $t$ and $\tilde{e}$ vs. $t$ for fixed values of $g = 0.031$, $\lambda_1 = 0.004$, $\lambda_2 = 0.01$ and different values of static JT coupling $g_1 = 0.145$, 0.148, 0.152, 0.156 and 0.159.
The self-consistent plots of $z$ vs. $t$ and $\tilde{e}$ vs. $t$ for fixed values of $g = 0.031$, $g_1 = 0.152$, $\lambda_2 = 0.01$ and different values of normal EP coupling $\lambda_1 = 0.0$, 0.004, 0.010, 0.015 and 0.020. On increase of the normal EP coupling, the JT energy gap decreases throughout the temperature range with the suppression of JT distortion temperature. However, the JT gap remains nearly constant at low temperatures for any change in the normal EP coupling. It is observed that the SC gap parameter is enhanced accompanied by the enhancement of the SC transition temperature with the increase of the normal EP coupling, but the SC gap nearly remains constant with the increase of EP coupling at low temperatures. Under these circumstances, the reduced gap parameter $2\Delta_0/k_BT_c$ decreases with increase of the normal EP coupling. Hence it is concluded that the normal EP coupling $\lambda_1$ has profound effect on the SC transition temperature as well as the JT distortion temperature. It is further to note that the normal EP coupling can have $\lambda_1 = f_1/2t_0$ from 0 to 0.02, which is small compared to the value of the EP coupling $\lambda_1 = N(0)f_1^{2}/\omega_0$ lying between 0.10 to 0.15 for CDW superconductors [34]. The effect of the normal EP coupling $\lambda_1$ in the transition temperatures is shown in figure 4. The JT distortion temperature decreases with increase of the normal EP coupling $\lambda_1$. On the other hand, the SC transition temperature increases monotonically with increase of the normal EP coupling $\lambda_1$. Hence it is concluded that the decrease of JT transition temperature enhances the SC transition temperature for the optimum value of $\lambda_1 \approx 0.0175$. When the normal electron-phonon coupling ($\lambda_1$) increases, it strongly couples with at higher temperature ($t_c < t < t_d$), and it effectively reduces the static lattice energy $\tilde{e}$. In consequence there is the gain in electron energy. This results in enhancement of $t_c$. The existence of superconducting state at low temperature depends very sensitively on the strength of the EP coupling ($\lambda_1$) the effect of ionic size [19] of iso-electronic M (Sr, Ca, Ba) ions on the interplay of superconductivity and structural transition can be understood as the consequence of higher EP coupling.
The effect of the smaller values of the DJT coupling $\lambda_2(0 - 0.065)$ on the SC parameter and the JT energy gap is shown in figure 5. From figure 5 it is seen that the JT gap $\tilde{e}$ is suppressed throughout the temperature range with reduced distortion temperature $t_d$ with the increase of the DJT coupling $\lambda_2$. The DJT coupling has no effect on the magnitude of the JT gap at low temperatures. On the other hand, with increase of the DJT coupling, the SC gap parameter is enhanced accompanied by the enhancement of the SC transition temperature. Again it is seen that the DJT coupling has no effect on the SC gap at the very low temperatures. On further increasing the DJT coupling $\lambda_2 = 0.07$ to 0.20, the temperature dependent SC gap
$z(t)$ and the JT gap $\tilde{e}(t)$ show different behavior as shown in figure 6. For DJT coupling $\lambda_2 > 0.07$, the JT distortion temperature becomes smaller than the SC transition temperature. Under this condition, the increase of the DJT coupling $\lambda_2$, the JT gap parameter is suppressed throughout the temperature range accompanied by the large suppression of the JT transition temperature, but the DJT coupling has no effect on the JT gap $\tilde{e}$ at low temperatures. It is noted here that the SC gap magnitude and the SC transition temperatures are unaffected for the ranges of higher values of $\lambda_2$. However, the SC gap magnitude are enhanced within the temperature ranges $0 < t < t_c$. The reduced gap magnitude $2\Delta_0/k_B T_c \simeq 3.28$ remains constant for any change on the DJT coupling $\lambda_2$. The dependence of SC transition temperature $t_c$ and the distortion temperature $t_d$ on the DJT coupling $\lambda_2$ is shown clearly in figure 7. For lower values of DJT coupling $\lambda_2(0 - 0.063)$ the distortion temperature $t_d$ decreases rapidly with increase of $\lambda_2$, while the SC transition temperature increases slowly for all values of DJT coupling up to $\lambda_2 = 0.063$. On further increasing $\lambda_2$ to higher values ($\lambda_2 > 0.063$), the SC transition temperature remains unaffected while the distortion temperature $t_d$ decreases continuously on increasing DJT coupling $\lambda_2$ as shown in figures 5 and 6. On further increasing ($\lambda_2 > 0.063$), the modified static elastic energy becomes smaller than the electronic energy and the distortion temperature which is a measure of elastic energy, is suppressed as resulting in the situation $t_s < t_c$. Above the temperature $t_d$, all the electrons participate in the formation of Cooper Pairing and give rise to a constant $t_c$.

![Figure 6](image-url)  
*Fig. 6* The self-consistent plots of $z$ vs. $t$ and $\tilde{e}$ vs. $t$ for fixed values of $g = 0.031$, $g_1 = 0.152$, $\lambda_1 = 0.004$ and different values of DJT coupling $\lambda_2 = 0.07$, 0.09, 0.12, 0.14 and 0.20.
The effect of the reduced external frequency \( c \) on the SC gap parameter and the JT energy gap is shown in figure 8. With increase in frequency from \( c = 0.10 \) to 0.96, the magnitude of the JT gap is suppressed considerably accompanied by the suppression of the distortion temperature \( t_d \), but the gap magnitude at low temperatures remains unaffected with increase in frequency. On the other hand with increase of the frequency, the SC gap parameter is enhanced along with the SC transition temperature; but the magnitude of the SC gap remains unaffected at low temperatures. The change of the distortion temperature \( t_d \) and SC transition temperature \( t_c \) with the change of the external frequency is shown in figure 9. These two transition temperatures show different types of behavior for the lower external frequencies.
frequencies and higher external frequencies up to the frequency $c \approx 1$. For lower frequencies, the distortion temperature $t_d$ decreases; while the SC transition temperature slowly increases. On further increasing the frequency, the distortion temperature $t_d$ suddenly increases, then decreases rapidly and then remains constant for higher frequencies. On the other hand, on increasing the frequency to higher values, the SC transition temperature suddenly drops to a lower value, then slowly increases and then remains constant for higher frequencies. Figures 8 and 9 exhibit the influence of sound frequency ($c$) on the interplay of the SC and JT strain parameters. With the increase of the sound frequency, the coupling of the phonons to the band electrons becomes stronger i.e., the normal EP coupling ($\lambda_1$) and the DJT coupling ($\lambda_2$) become stronger. As discussed for $\lambda_1$ and $\lambda_2$, we will find that the increase of phonon frequency will reduce the static lattice energy resulting in the suppression of distortion temperature $t_s$ and enhancement of $t_c$. 

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**Fig. 9** The plots of $t_c$ and $t_d$ vs. $c$. 

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raw text: 

0 0.001 0.002 0.003 0.004 0.005 0.006 0.007

t 0.003 0.006 0.009 0.012 0.015

$\omega_1=0.00001$ $\omega_1=0.00005$ $\omega_1=0.00010$

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raw text: 

0 0.001 0.002 0.003 0.004 0.005 0.006 0.007

0 0.003 0.006 0.009 0.012 0.015
Fig. 10 The self-consistent plots of $z$ vs. $t$ and $\tilde{e}$ vs. $t$ for fixed values of $g = 0.031$, $g_1 = 0.152$, $\lambda_1 = 0.004$, $\lambda_2 = 0.01$ and different lower phonon vibrational frequencies $\omega_1 = 0.00001$, 0.00005, 0.00010 and 0.00020.

Figure 10 shows the temperature dependence of the SC gap and the JT gap parameters for different values of the phonon vibrational frequency. With the increase of phonon vibrational frequency $\omega_1$, the JT gap increases throughout the temperature range and simultaneously the JT distortion temperature is also enhanced. This shows that the phonon vibrational frequency enlarges the JT gap. It is to note further that, in the interplay region of the lattice strain and the SC order, the SC parameter is suppressed at low temperatures. However, for the increase of the low vibrational frequencies the SC gap parameter is enhanced accompanied by the enhancement of its transition temperature. The effect of higher phonon vibrational frequency on the gap parameters is shown in figure 11. With the increase of the phonon vibrational frequency $\omega_1$, the JT gap is enhanced throughout the temperature range along with its transition temperature; but the JT gap magnitude, at very low temperature remains unaffected with $\omega_1$. On the other hand, the SC gap parameter is reduced throughout the temperature range with increase of the phonon frequency. Though the SC transition temperature is reduced with the phonon frequency, the magnitude of the SC gap remains unaffected at lower temperatures.
The dependence of the SC transition temperature and the JT distortion temperature on the phonon vibrational frequency $\omega_1$ is shown in figure 12. For lower frequencies up to $\omega_1 = 0.0013$, both the SC transition temperature $t_c$ as well as the JT distortion temperature $t_d$ increase with an increase of the phonon vibrational frequency. On further increasing phonon vibrational frequency $\omega_1$, the distortion temperature increases and remains constant for higher vibrational frequencies. Correspondingly the SC transition temperature decreases with the higher vibrational frequencies and then remains constant. Thus the $t_c$ and $t_d$ of the system are not affected for higher vibrational frequencies. The interplay between superconductivity and lattice distortion has been distinctively observed in $La_{2-x}M_xCuO_4$ [M = Sr, Ca, Ba\(^{19}\)]. The Ca-substituted compound has a higher value of the electron-lattice coupling constant than that of Sr-substituted system. The smaller is the ionic size, the larger will be the phonon vibration in the system. For lower phonon frequencies, both the lattice distortion temperature $t_s$ and SC transition temperature $t_c$ are enhanced\(^{19}\). For high frequency phonons the lattice distortion is enhanced resulting in the suppression $t_c$.

5. Conclusion

We report here a model study to treat the static and dynamic Jahn-Teller effects on high temperature copper oxide superconductors. The static JT effects are considered as the renormalization to the energy of the doubly degenerate conduction electron bands. Further, the dynamic JT effects renormalize both the conduction bands as well as the superconducting gap parameter under lattice strain through the electron-phonon coupling constant. The solutions are obtained by using the Zubarev double time Green’s function methods including the higher order mixing Green’s functions within mean-field approximations. We observe the changes in lattice strain, when the temperature decreases to below SC transition temperature $t_c$, as observed by
the calculation of Ghosh et al.\textsuperscript{31}. Further, we observe here some new results beyond mean-field approximation in a generalized model.

In the model calculation for the gap equation for the high-$T_c$ cuprates, we have considered the Jahn-Teller type lattice strain as a pseudogap interacting strongly with the superconducting pairing amplitudes. The static lattice strain suppresses the superconducting gap as reported by the neutron scattering studies and the theoretical calculation.\textsuperscript{31,32,33,34} Keeping in mind the important role played by the PG, we consider here the DJT effect on the superconducting gap in high-$T_c$ systems. In addition to the static band Jahn-Teller effect, we incorporate the normal phonon interaction to the electron densities of the degenerate conduction band and the DJT interaction to the difference in electron densities of the JT splitted two bands. The superconducting gap equation is calculated by the Zubarev’s technique of Green’s functions and the modified BCS gap equation is calculated from the modified conduction band energy $\tilde{\epsilon}_{\alpha k}$ and the modified SC gap parameter $\tilde{\Delta}_\alpha$. The lattice strain is calculated by minimizing the free energy. The SC gap and JT energy gap equations are solved self-consistently. It is observed that the SC gap and the SC transition temperature are enhanced by the DJT interaction as compared to the static case. The normal EP coupling suppresses the JT distortion temperature and enhances the SC transition temperature. Similarly, for smaller DJT coupling ($\lambda_2 < 0.075$), the JT distortion temperature is suppressed, while the SC transition temperature is enhanced. For higher values of the DJT coupling ($\lambda_2 > 0.075$), the JT distortion is suppressed, but the SC transition is not enhanced further. It is found that the external frequency suppresses the JT transition temperature but enhances the SC transition temperature for frequencies $\omega \leq 1$. It is further noticed that both the JT distortion temperature and the SC transition temperature are enhanced for the lower values of the phonon vibrational frequencies, while both the transition temperatures are not affected by the higher phonon vibrational frequencies. The electronic correlation effects and the $d$-wave symmetry are not discussed in the present model calculations. The present model study helps in understanding the interesting phenomenon of the interplay of dynamic structural transition with the superconductivity in cuprate systems. However, it will be interesting to study, how the antiferromagnetism spin fluctuations leading to $d$-wave pairing superconductivity will be influenced by the dynamic structural distortion. This will be the subject matter for a future study.

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References

1. M.R. Norman, D.P. Pines, C. Kallin, \textit{Adv. Phys.} \textbf{54}, 715 (2005).
2. M.R. Norman, C. Pépin, \textit{Rep. Prog. Phys.} \textbf{66}, 1547 (2003).
3. J.L. Tallon, J.W. Loram, *Physica* **C349**, 53 (2001).
4. T. Ito, K. Takenaka, S. Uchida, *Phys. Rev. Lett.* **70**, 3995 (1993).
5. J.W. Loram, K.A. Mirza, J.M. Wade, J.R. Cooper, W.Y. Liang, *Physica* **C235-240**, 134 (1994).
6. T. Timusk, B. Statt, *Rep. Prog. Phys.* **62**, 61 (1991).
7. H.B. Yang, J.D. Rameau, P.D. Johnson, T. Valla, A. Tsvelik, G.D. Gu, *Nature (London)* **456**, 77 (2008).
8. B. Fauque, Y. Sidis, V. Hinkov, S. Pailhes, C.T. Lin, X. Chaud, P. Bourges, *Phys. Rev. Lett.* **96**, 197001 (2006).
9. M.E. Simon, C.M. Varma, *Phys. Rev. Lett.* **89**, 247003 (2002).
10. S. Chakravarty, R.B. Laughlin, D.K. Morr, C. Nayak, *Phys.Rev.* **B63**, 094503 (2001).
11. V. Hinkov, D. Haug, B. Fauque, P. Bourges, Y. Sidis, A. Ivanov, C. Bernhard, C.T. Lin, B. Keimer, *Science* **319**, 597 (2008).
12. V. Hinkov, P. Bourges, S. Pailhes, Y. Sidis, A. Ivanov, C.D. Frost, T.G. Perring, C.T. Lin, D.P. Chen, B. Keimer, *Nat. Phys.* **3**, 780 (2007).
13. V.J. Emery, S.A. Kivelson, J.M. Tranquada, *Proc. Natl. Acad. Sci. U.S.A* **96**, 8814 (1999).
14. H. Eisaki, N. Kaneko, D.L. Feng, A. Damascelli, P.K. Mang, K.M. Shen, Z.-X. Shen, M. Greven, *Phys. Rev. B69*, 064512 (2004).
15. K. Fujita, T. Noda, K.M. Kojima, H. Eisaki, S. Uchida, *Phys. Rev. Lett.* **95**, 097006 (2005).
16. D.Mck. Paul, G. Balakrishnan, N.R. Bernhoeft, W.I.F. David, W.T.A. Harrison, *Phys. Rev. Lett.* **58**, 1976 (1987).
17. M. Lang, R. Kürsch, A. Grañel, C. Geibel, F. Steglich, H. Rietschel, T. Wolf, Y. Hidaka, K. Kumagai, Y. Maeno, T. Fujita, *Phys. Rev. Lett.* **69**, 482 (1992).
18. J. Röhler, A. Larisch, in: *Electronic Properties of High-Tc Superconductors and Related Compounds*, Vol. **99**, Eds. H. Kuzmamy, M. Chring, J. Fink (Springer, Berlin) (1990) p.152.
19. B. Dabrowski, Z. Wang, J.D. Jogerson, R.L. Hitterman, J.L. Wagner, B.A. Hunter, D.G. Hinks, *Physica* **C217**, 455 (1993); B. Dabrowski, Z. Wang, K. Rogacki, J.D. Jorgensen, R.L. Hitterman, J.L. Wagner, B.A. Hunter, P.G. Radaelli, D.G. Hinks, *Phys.Rev. Lett.* **76**, 1348 (1996); J.B. Torrance, Y. Tokura, A.I. Nazzal, A. Bezinge, T.C. Huang, S.S.P. Parkin, *Phys. Rev. Lett.* **61**, 1127 (1988).
20. J. Miranda, T. Mertelj, V.V. Kabanov, D. Mihailovic, *J. Supercond. Nov. Magn.* **22**, 281 (2009).
21. D. Mihailovic, V.V. Kabanov, *Phys. Rev.* **B63**, 054505 (2001).
22. G. Bednorz, K.A. Müller, *Phys. B: Condens. Matter* **64**, 189 (1986).
23. M. Weger, R. Englman, *Physica* **A168**, 324 (1999).
24. R.S. Markiewicz, *Physica* **C200**, 65 (1992).
25. V.Z. Kresin, A. Bill, S.A. Wolf, Yu.N. Ochinnikov, *Phys. Rev.* **B56**, 107 (1997).
26. See for example : A. Bianconi, N.L. Saini, A. Lanzara, M. Missori, T. Rossetti, *Phys.Rev.Lett.* **76**, 3412 (1996); M. Acosta-Alejandro, et al., *J. Superconductivity* **15**, 355 (2002) and references therein.
27. E.S. Božin, S.J.L. Billinge, G.H. Kwei, H. Takagi, *Physica* **C341**, 1793 (2000); E.S. Božin, G.H. Kwei, H. Takagi, S.J.L. Billinge, *Phys. Rev. Lett.* **84**, 5856 (2000).
28. K.A. Müller, *J. Superconductivity* **12**, 3 (1999).
29. R.S. Markiewicz, *Physica* **C210-235**, 264 (1993).
30. A.J. Millis, F.B. Littlewood, B.I. Shraiman, *Phys. Rev. Lett.* **74**, 5144 (1995); A.J. Millis, B.I. Shraiman, R. Mueller, *Phys. Rev. Lett.* **77**, 175 (1996); A.J. Millis, *Phys. Rev.* **B53**, 8434 (1996).
31. H. Ghosh, S.N. Behera, S.K. Ghatak, D.K. Ray, *Physica* **C274**, 107 (1997).
32. H. Ghosh, M. Mitra, S.N. Behera, S.K. Ghatak, *Phys. Rev.* **B57**, 13414 (1998).
33. G.C. Rout, B. Pradhan, S.N. Behera, *phys. stat. solidi (c)**3**, 3617 (2006).
34. G.C. Rout, B. Pradhan, S.N. Behera, *Physica* **C444**, 23 (2006).
35. B. Pradhan, K.L. Mohanta, G.C. Rout, *Physica* **C475**, 14 (2012).
36. D.N. Zubarev, *Sov. Phys. Usp.* **3**(71), 320 (1960).
37. C.A. Balseiro, L.M. Falicov, *Phys. Rev. Lett.* **45**, 662 (1980).
38. G.C. Mohanty, S.N. Behera, *Pramana* **19**, 645 (1982).