Coexistence of Band Jahn Teller Distortion and superconductivity in correlated systems

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The co-existence of band Jahn-Teller (BJT) effect with superconductivity (SC) is studied for correlated systems, with orbitally degenerate bands using a simple model. The Hubbard model for a doubly degenerate orbital with the on-site intraorbital Coulomb repulsion treated in the slave boson formalism and the interorbital Coulomb repulsion treated in the Hartree-Fock mean field approximation, describes the correlated system. The model further incorporates the BJT interaction and a pairing term to account for the lattice distortion and superconductivity respectively. It is found that structural distortion tends to suppress superconductivity and when SC sets in at low temperatures, the growth of the lattice distortion is arrested. The phase diagram comprising of the SC and structural transition temperatures $T_c$ and $T_d$ versus the dopant concentration $\delta$ reveals that the highest obtainable $T_c$ for an optimum doping is limited by structural transition. The dependence of the occupation probabilities of the different bands as well as the density of states (DOS) in the distorted-superconducting phase, on electron correlation has been discussed.

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The dependence of $T_c$ on structural properties is rather less understood and had been a crucial question since the discovery of the high temperature superconductivity (HTSC) in the cuprates. On the other hand, the dominant effect of electron correlation on the normal and SC properties of the cuprates had been realized soon after the discovery [[1]]. The structural transitions associated with the crystallographic symmetry has been observed in many intermetallic compounds [[2]] as well as in the high $T_c$ cuprates [[3]] and fullerenes [[4]]. A common feature to all these systems is the existence of the Fermi level (FL) in an orbitally degenerate band. The essence of the Band Jahn-Teller (BJT) distortion is the following. If the Fermi level of a system lies in an orbitally degenerate band then there can be a net gain in electronic energy if the degeneracy is removed by the lowering of the lattice symmetry due to production spontaneous strain which results in a structural transition. The production of strain will cost elastic energy, therefore, the strain will be stabilized if the gain in the electronic energy overcomes the cost in elastic energy. The system will like to optimize the distortion so as to maximize the gain in energy, which will happen when the lower band is maximally occupied and the upper split band is minimally occupied. The system would however remain metallic in case of a small but finite distortion, as the two splitted bands can overlap. On the other hand, a split band with a gap and a resultant insulating phase would arise because of large distortion. On deviating from the half-filled situation by doping holes into the system will result in lowering of the band filling, thereby reducing the gain in energy, hence the magnitude of strain is expected to reduce. Thus the difference in the occupation probability of the two bands will couple to the lattice strain which defines the Jahn-Teller Hamiltonian. However, the redistribution of the density of state associated with Jahn-Teller distortion is expected to affect the occurance of superconductivity in the system. A drastic reduction in the density of states at the FL due to BJT distortion would suppress superconducting transition. On the other hand, if the superconducting pairing is phonon mediated one can expect an enhancement in the transition temperature because the distortion of the lattice will soften the frequency of some phonons resulting in an enhancement of the coupling constant. In this paper therefore, we present a model study of the coexistence of BJT distortion and superconductivity in narrow band systems.

The electron correlation is known to play a significant role in shaping the physical properties of the normal and SC states of the correlated systems. It is believed that the single band Hubbard model contains all the necessary physical ingredients to describe electron correlation in narrow band systems. One of the recently contrived methods to solve the Hubbard model for any filling and any value of correlation ($U$) is the slave - boson technique, as formulated by Kotliar and Ruckenstein (KR) [[5]] which introduces four auxiliary boson fields corresponding to the occupancy of a site, namely empty ($e_i$), doubly occupied ($d_i$), singly occupied ($p_{i\sigma}$) with spin $\pm \sigma$ respectively. In terms of the slave boson field operators the single band Hubbard model takes the form

$$H = \sum_{ij,\sigma} t_{ij} z_i^j c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i d_i^\dagger d_i - \mu \sum_i c_{i\sigma}^\dagger c_{i\sigma} + \sum_i \lambda_i (1 - c_i^\dagger e_i$$


\[-d_i^j d_i - \sum_{\sigma} p_{i\sigma}^\dagger p_{i\sigma} \]  
\[+ \sum_{\sigma} \lambda_{i\sigma} (c_{i\sigma} c_{i\sigma} - d_i^j d_i - p_{i\sigma}^\dagger p_{i\sigma}) \]  

(1)

where \( z_{i\sigma} = (1 - d_i^j d_i - p_{i\sigma}^\dagger p_{i\sigma})^{-1/2} (c_{i\sigma} c_{i\sigma} - d_i^j d_i - p_{i\sigma}^\dagger p_{i\sigma})^{-1/2} \) and the boson field operators are not independent of each other but are constrained by the requirements of completeness and local charge conservation at a site, hence the fourth and fifth terms are added in the Hamiltonian with the help of Lagrange multipliers \((\lambda_i, \lambda'_i)\). The values of the boson field operators and Lagrange multipliers are determined by minimizing the free energy in the saddle point approximation. This approximation diagonalizes the \( U \) term whereas renormalizes the hopping term as \( \tilde{q}_{ij} \) with \( \tilde{q} = z^j z \); \( \tilde{q} \) usually being a complicated function of the reduced correlation \( u (= \frac{U}{\epsilon}) \), and the dopant concentration \( (\beta) \).

In this approach solutions are obtained for the paramagnetic state for all values of \( u \) and band fillings that reproduces the correct Brinkmann-Rice result for metal-insulator transition at a critical value of correlation \((U_e)\) at half-filling. Approximately, in the weak correlation limit \( \tilde{q} = 1 - u^2 \) and in case of strong correlation and small values of \( \beta, \tilde{q} = \frac{2q}{\sqrt{1-q^2}} \) (for details please see ref. [2]).

We generalize the above formalism to a model system in which the electrons are in a two-fold degenerate \( e_g \) band and interact with the lattice as well as between themselves, the later via a BCS kind of pairing interaction mediated by some boson exchange. The Hamiltonian for such a system can be written as,

\[ H = \sum_{k,\sigma=1,2} \left[ \{ \hat{q} \epsilon_k - \mu + 2U' < n_{\beta} > \} n_{k\sigma} - (-1)^\alpha Ge n_{k\sigma} \right] + \frac{1}{2} cc^\dagger + \sum_{k,\alpha=1,2} \left( \Delta c_{k,\alpha,\uparrow}^\dagger c_{-k,\alpha,\downarrow}^\dagger + h.c. \right) \]

\[ + \text{bosonic terms} \]  

(2)

The first term corresponds to band-energy of the correlated electrons in a two-fold orbitally degenerate \( e_g \) band; where \( U' \) is the strength of the inter-orbital Coulomb correlation treated within the mean field Hartree-Fock approximation, and the band renormalization factor \( \tilde{q} \) depends on the on-site intra-band coulomb interaction \( U \). The second term within the square bracket corresponds to the symmetry breaking electron - lattice interaction that lifts the degeneracy of the bands by differently populating them and thereby producing the lattice strain \((\epsilon)\). The cost in lattice energy due to such strain is given by the second term whereas the third term represents the usual BCS Cooper pairing between the quasiparticles of the correlated systems in which only intra-band pairing is considered for simplicity assuming the strength of pairing interactions to be of equal magnitudes \([3]\). The bosonic terms in the Hamiltonian being C-numbers do not contribute to the dynamics of the system. In the normal undistorted phase, it is possible to show that the strain is exactly proportional to the population difference between the shifted sub-bands. The self-consistent equations for the strain \((\epsilon)\) and the SC-order parameter\((\Delta)\) are given below,

\[ e = - \sum_{k,\sigma,\alpha} (-1)^\alpha n_{k\sigma} = -\frac{G}{\epsilon} \sum_{k,\sigma,\alpha} (-1)^\alpha \frac{\epsilon_{\alpha}(k)}{E_{\alpha}(k)} \tanh \frac{\beta E_{\alpha}(k)}{2} \]

(3)

\[ \Delta = -V\tilde{q}^2 \sum_{k,\alpha} < c_{k\alpha,\uparrow} c_{-k\alpha,\downarrow} > = \sum_{k,\alpha} V\tilde{q}^2 \frac{\Delta}{2E_{\alpha}(k)} \tanh \frac{\beta E_{\alpha}(k)}{2} \]

(4)

where \( \epsilon_{\alpha}(k) = \tilde{q} \epsilon_k - \mu + 2U' < n_{\beta} > -(-1)^\alpha Ge \) is the band energy of the correlated normal state in the distorted phase and \( E_{\alpha}(k) = \sqrt{\epsilon_{\alpha}^2(k) + \Delta^2} \) is the SC quasiparticle energy in the band \( \alpha \).

In order to study the mutual influence of lattice distortion and superconductivity as a function of band filling one has to solve the above two coupled equations (3-4) self-consistently together with the equation for dopant concentration which can be obtained from the electron number conservation \((2 - \delta) = \frac{1}{N} \sum_{k\sigma} < n_{k\sigma} > \).

In order to solve these three equations the sum over \( \tilde{k} \) as usual is converted into an integral over energy variable \( \epsilon \), with an approximate peaked density of states \( N_0(\epsilon) \) at the centre of the unperturbed bands as given below,

\[ N_0(\epsilon) = N(0) \sqrt{1 - \frac{\epsilon}{B}} \ln \left| \frac{B^2}{\epsilon^2} \right| \]

(5)

where \( N(0) \) is the unperturbed density of states of the free electron system and \( 2B \) (which is chosen as 1 eV) is the band width.

Figure 1. shows the effect of electron correlation on the temperature dependence of the strain, i.e, \( e(T) \). In order to see this the curves for \( e(T) \) corresponding to the value of the coupling constants \( G = 1.2 \) and band occupation \( n = 0.9 \)
are plotted for different values of $u$ and $u'$. There is a suppression of strain around 40 K due to the appearance of superconductivity when $u$ and $u'$ are zero. As the intra-orbital intra-site Coulomb correlation is switched on with $u = 0.2$, while keeping $u' = 0$, the strain as well as $T_c$ has increased, and the SC transition temperature is lowered to around 22 K. Furthermore, when the inter-orbital intra-site Coulomb interaction strength is increased from zero to $u' = 0.001$, there is a further suppression of $T_c$ and an enhancement of $T_s$ as well as strain as can be seen from the dash - dotted curve. On further increasing $u'$ to 0.005 superconductivity almost vanishes (dotted curve) while $T_s$ and strain increases by a larger magnitude. Therefore, the present results predict that the suppression of strain will be lessened with increasing correlation in the superconducting state.

An unusual behavior in the temperature dependence of the SC order parameter $\Delta(T)$ and strain $e(T)$ is observed when the value of the SC transition temperature in the absence of strain ($T_c^0$) is comparable to the structural transition temperature $T_s$, which is depicted in Fig 2. The figure depicts the temperature dependence of $e$ and $\Delta$ for the same value of the coupling constant $G=1.2$eV as earlier but for a band filling $n = 0.7$. In this case the strain appears at the temperature of $T_s \approx 140K$, increases with decreasing temperature but drops precipitously to zero around 92 K, as soon as superconductivity appears. The SC order parameter rapidly increases within an extremely narrow range of temperature but it vanishes again with the recurrence of strain which attains a large value when the temperature is reduced slightly. Such alterations of SC and strain persist until the temperature is slightly less than 60 K below which the superconducting state stabilizes and the strain vanishes. This corresponds to a metastable situation that persists within a narrow range of temperature. While the SC state stabilizes at lower temperatures, the strain exists in the higher temperature range, with the two never co-existing in their respective regions of stability.

In figure 3, the occupation probability/per spin for different orbitals are plotted as a function of temperature. The occupation probability of the two orbitals are the same above the structural transition temperature $T_s$ but below $T_s$, the occupation probabilities being different creates a population difference between the orbitals and hence a net strain builds up. With lowering of temperature, the system undergoes SC transition and hence the electron density in each orbital is suppressed below $T_c$. Needless to say, this transition resembles to the orthorhombic to tetragonal transition in high-$T_c$ systems. However, as a result of reduction in the orbital population density below $T_c$, the growth of the spontaneous strain gets arrested.

In figure 4, the detailed phase diagram comprising of $T_c \& T_s$ as a function of hole concentration is shown for different values of intra and inter orbital correlation strengths. The phase diagram (solid lines represent $T_c$ curves) demonstrates that the $T_c$ is largely suppressed in presence of structural distortion and the highest $T_c$ is obtainable for an optimum doping ($\delta_c$) where $T_s$ vanishes. It is to be noted that the suppression in $T_c$ is maximum at half-filling as the strain is the largest there. These results are in close agreement with experimental observations.

The structural transition in this model results from the competition between lowering of the electronic energy due to lifting of the orbital degeneracy (band Jahn-Teller effect) and the increase in elastic energy associated with the appearance of strain. The gain in energy in this process stabilizes the structural transition and this gain is largest when the Fermi level (FL) in the undistorted phase lies at the center of a peak in the DOS, because in that case a large number of electrons in higher energy states are transferred to lower energy states. This is realized in the present model at half filling of the degenerate band resulting in a splitting due to JT effect by an amount 2 Ge which leaves the lower band almost fully occupied whereas the upper band is nearly empty. Thereby, it creates maximum population difference between the two shifted sub-bands resulting in the largest strain. Consequently, the DOS at the FL gets reduced drastically so that the system is no longer favorable for superconductivity. However, as one moves away from half-filling of the bands (by doping holes) the FL moves away from the peak in the DOS resulting in a lesser gain in electronic energy which will tend to reduce the distortion as well as the structural transition temperature. As a result the DOS at the FL will increase thereby favoring superconductivity. Thus the SC-$T_c$ increases with increasing hole concentration.

On the other hand, the appearance of SC reduces the occupation probability of the bands exponentially due to the presence of the gap $2\Delta$ in the energy spectrum resulting in the reduction of the strain ($e$) below $T_c$. This explains the arresting of the growth of the strain at $T_c$ and its suppression below $T_c$. Such a picture becomes self-evident from Fig. 3. Our results presented in figures have close resemblance to experimental data of high temperature superconductors.

Finally, within the present formulation the electron correlation has the following effects. The band narrowing due to renormalizin factor $\bar{q}$ enhances the density of states which favors the Jahn - Teller splitting, while the pairing amplitude gets suppressed, due to the reduction of the strength of the interaction by a factor $\bar{q}^2$. Inclusion of inter orbital coulomb makes the J-T splitting asymmetric with respect to the centre of mass of the original band and hence enhances the lattice strain but suppresses SC further. Therefore, the present model study helps in understanding the interesting phenomenon of the interplay of structural transition with superconductivity in correlated systems like the cuprates. However, it remains to be seen how the antiferromagnetic spin fluctuations leading to d-wave pairing superconductivity is influenced by structural distortion. This is the subject matter for a future study.
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Figure Captions

Fig. 1 The thermal variation of the lattice strain ($\epsilon$) for $n = 0.9$ and $G = 1.2$ in presence of on-site coulomb correlation (intraband ($u$) as well as interband ($u'$ is denoted as $u_1$ in figures)).

Fig. 2 The temperature variation of the superconducting gap and the strain for $n = 0.7$, for $G = 1.2$. A metastable thermal regime from around 60 K - 90 K is worth noticing (the solid line indicates the $\Delta_{sc}(T)$ and the dotted one $\epsilon(T)$).

Fig. 3 The temperature variation of the occupation probabilities of the splitted bands for $n = 0.9$, $G = 1.2$ in presence of the onsite intraband ($u$) as well as ($u_1 \equiv u'$) coulomb correlations.

Fig. 4 The complete phase diagram in terms of the structural and superconducting transition temperatures ($T_s, T_c$) as a function of hole concentration ($\delta$) for $G = 1.16$. The curves with connected lines correspond to $T_c$ curves).