Slave-Boson Three-Band Model with O-O Hopping for High-T_c Superconductors

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Slave boson mean-field approximation is carried out analytically for weakly doped CuO2 conduction planes, characterized by Cu-O charge transfer energy Δpd, Cu-O hopping t0, O-O hopping t' and repulsion U_d between holes on Cu site taken as infinite. At zero doping d, finite negative t'.t' < t0/2, expands the range of stability of the covalent, conducting state on the expense of the insulating state which, however, remains stable at larger Δpd. For sufficiently large Δpd the renormalized charge transfer energy saturates at 4|t'| instead of decreasing to zero, as at t' = 0 case.

In contrast to t', finite d suppresses the insulating state nearly symmetrically with respect to the sign of d. The regime with charge transfer energy renormalized close to 4|t'| fits remarkably well the ARPES spectra of Bi2212 and LSCO, and, in the latter case, explains the observed strong doping dependence of the Cu-O hopping.

ARPES measurements of the electron spectra in the high-T_c superconductors [1,2] have shown that the characteristic band energy scales fall into the range between 0.1 and 1 eV. On the other hand, the high-energy spectroscopies indicate considerably larger characteristic energies, of the order of several eV [2]. This implies that the renormalization of the electron spectrum in low energy range measured by ARPES is strong. Recent results on La2−xSrxCuO4 (LSCO) [1] have shown in addition that the shape of the Fermi surface varies strongly with doping, indicating again strong renormalization of band parameters. Further argument in favor of the strong renormalization comes from the approximate electron-hole symmetry of the phase diagram of the high-T_c superconductors [2]. If the couplings were weak, band renormalization small, the approximate electron-hole symmetry would occur with respect to the (optimal) necessary to bring the Fermi level to the logarithmic van Hove singularity. This would be accompanied by the activation of the Umklapp scattering, i.e. tendency towards Mott localization. Thus far such tendency has not been observed and the approximate symmetry occurs with respect to δ = 0 rather than with respect to δ_c. This rules out weak coupling and raises the question whether intermediate [6] to strong [7] coupling can account for such behavior.

It is usually assumed that the largest coupling is the local hole-hole interaction U_d on the Cu-site of the conducting CuO2 planes. The interaction problem is often treated within the Emery model [3] which describes the three-site structure of the CuO2 plane by copper and oxygen site energies ϵ_d and ϵ_p respectively, the Cu-O hopping t0 and the O-O hopping t_0', the single-particle parameters in addition to U_d. The strong renormalization of the band structure characterized by ϵ_d, ϵ_p, t0 and t_0' is thus expected only when the number of holes on the Cu-site is close to unity, because only then large U_d is effective. In the opposite case, when the holes tend to reside on oxygen sites, the renormalization should decrease. Bearing this in mind, the limit of large U_d is discussed here, taking U_d larger than Δpd = ϵ_p − ϵ_d, t0, t_0'. The limit of infinite U_d is, as usual, treated within mean-field slave boson approximation [3,10], neglecting the AF and SC effects. The latter occur on the energy scales of the 0.01 eV, an order of magnitude below the band energy scales of interest here.

Previously, similar slave boson calculations were carried out analytically for the t0, t_0' 1d (CuO) analog of the 2d (CuO2) case [4], and, for the latter, numerically for some particular choices of the bare parameters [4,11]. The 2d three-band structure is considerably richer than its 1d two-band counterpart, therefore, similar holds for the corresponding mean-field slave boson theory. In particular, the 2d case is sensitive to the sign of t_0'. Two bands may anticross, as in the 1d case, but in 2d case, band-touching is also possible [3,12]. Above all, in contrast to 1d model, the parameter t_0' removes in 2d case Fermi energy of the half-filled band from the van Hove singularity, i.e. introduces a finite doping δ_c required to bring it back [12]. The question whether the electron-hole symmetry occurs for δ = 0 or δ_c should therefore be discussed at finite t_0'.

The slave boson procedure [6] amounts to searching the ground state band energy E_0 at a given number of holes 1+δ, subjected to the restriction that the number of holes n_d on the Cu-site is smaller than 1, as required by large U_d. In the mean-field approximation E_0 is the energy of the free holes with the renormalized band parameters Δ, t, t', chosen to fulfill the requirement ⟨n_d⟩ < 1, which becomes [6]

⟨n_d⟩ + t^2/t_0' = 1, \quad ⟨n_d⟩ = −\frac{\partial E_0}{\partial Δ}. \quad (1)

The minimization of E_0 with respect to the remaining parameter t, gives the second slave boson equation

...
\[
\langle n_B \rangle = 2 \frac{t(\Delta_{pd} - \Delta)}{t_0^2}, \quad \langle n_B \rangle = \frac{\partial E_0}{\partial \delta},
\]

denoting renormalized bond charge on the Cu-O bond.

The solution of the coupled integro-differential equations (1) and (2) gives \( \Delta \) and \( t \) as functions of \( \Delta_{pd} \), \( t_0 \), \( t' \) and \( \delta \) (remembering that \( t_0' = t' \)). The present slave boson calculation is carried out for arbitrary \( \Delta_{pd} \) and \( t_0 \), assuming \( 2|t'| < t_0 \) and \( |\delta| << 1 \). The assumption \( 2|t'| < t_0 \) is in the spirit of the Emery model [3], but the opposite limit will nevertheless be briefly commented upon. On the other hand, the results obtained here for \( |\delta| << 1 \) do not cover all the physically achieved doping, but rather indicate the tendencies associated with finite \( \delta \).

It is possible to transform [3] the integro-differential equations (1) and (2) to the coupled algebraic equations for all interesting regimes of parameters by calculating \( E_0(\Delta, t, t', \delta) \) analytically and then \( \langle n_d \rangle \) and \( \langle n_B \rangle \) from Eqs. (1) and (2). Leaving the details of the calculation for the extended publication [13], the final results will be discussed here.

These results are best understood starting from the \( t' = 0 \) situation. \( \varepsilon_p \), which does not renormalize, is chosen for the energy origin, \( \varepsilon_p = 0 \). Only one band, \( \varepsilon_0^0(k) \), out of three is occupied for \( \delta \leq 1 \),

\[
\varepsilon_0^0(k) = -\frac{1}{2}(\Delta_0 + \sqrt{\Delta_0^2 + 16t^2f_1}),
\]

\[
f_1 = \sin^2 \frac{k_x}{2} + \sin^2 \frac{k_y}{2},
\]

setting \( \Delta(t' = 0) = \Delta_0 \). Using \( \varepsilon_0^0(k) \) to calculate \( E_0 \), leads to the solution of the \( t' = 0 \) slave boson equations (1) and (2) for arbitrary \( \Delta_{pd} \) and \( t_0 \) (taken without loss of generality). The behavior of \( t \) for \( \delta = 0 \) is fairly simple: \( t/t_0 = 0 \), starting from large \( \Delta_{pd} \) to \( \Delta_{pd}^{cr} = 4.7t_0 \), where the angular point in \( t/t_0 \) occurs. For \( \Delta_{pd} \) close below \( \Delta_{pd}^{cr}, t \) is given by a Landau-like expression \( t\sqrt{\Delta_{pd}^{cr} - \Delta_0} \), which describes Brinkman-Rice (BR) phase transition from the insulating state \( t = 0 \) to the conducting phase. The overall behavior can be obtained by expanding Eq. (3) in terms of \( t^2/\Delta_0^2 \) including the terms of the order of \( t^3 \) close below \( \Delta_{pd}^{cr} \).

The corresponding behavior of \( \Delta_0(\Delta_{pd}) \) is more important for further discussion. \( \Delta_0 \) has a single, maximum (angular at \( \delta = 0 \)) at \( \Delta_{pd} = \Delta_{pd}^{cr} \), where it reaches the value \( \Delta_0 = \Delta_{pd}^{cr}/2 \). For \( \Delta_{pd} \) well below \( \Delta_{pd}^{cr} \) the regime \( t > |\Delta_0| \) is reached. \( \langle n_d \rangle \) decreases, according to Eq. (4) and so do both renormalisation of \( t_0 \) to \( t \) and of \( \Delta_{pd} \) to \( \Delta_0 \). Before approaching asymptotically \( \Delta_{pd}/t_0 \), \( \Delta_0 \) crosses zero [4] at \( \Delta_{pd}/t_0 \approx 1.5 \): standard covalent situation \( \Delta_{pd} \approx t_0 \) renormalizes to the extreme \( \Delta_0 \approx 0 \) covalent limit. For \( \Delta > \Delta_{pd}^{cr}, |\Delta(\Delta_{pd})| \) decreases fast towards the asymptotic regime valid for large \( \Delta_{pd} \), when \( \Delta = 4.7t_0^2/\Delta_{pd} \) tends to zero (similarly to the site energy of the t-J model [4]).

Turning next to finite \( t' \), in the limit where \( 2|t'| < t_0 \), it is to be noted that under such condition (more precisely for \( 4|t'| < \Delta_{pd}^{cr}/2 = 2.4t_0 \)), \( 4|t'| \) intersects \( \Delta_0(\Delta_{pd}) \) at \( \Delta_{pd}^{cr} > \Delta_{pd}^{cr} \). When \( |t'| \ll t_0, \Delta_{pd}^{cr} = 4.7t_0^2/|t'| \). For \( \Delta_{pd} < \Delta_{pd}^{cr}, 4|t'| \) is smaller than \( \Delta_0 \) and/or \( t \) obtained from \( t'=0 \) solution, and a perturbative treatment of \( t' \) is possible. For \( \Delta_{pd} > \Delta_{pd}^{cr}, 4|t'| > \Delta_0 \) and full treatment of \( t' \) is required.

The perturbative corrections due to \( t' \) in the regime \( t > \Delta_0 \) at \( \Delta_{pd} \) well below \( 4.7t_0 \), are not of particular interest because only of the quantitative nature. The attention will be therefore focused here on the small \( t \) regime at \( \Delta_{pd} \) close below or above \( 4.7t_0 \). For this purpose a perturbative calculation can be carried out in terms of small \( t \), using (with \( \varepsilon_p = 0 \))

\[
\varepsilon_1^0(k) = -\Delta - 4\varepsilon_0^2(\Delta_{pd}^{cr} - \Delta_0) + O(t^4),
\]

\[
f_1 = \sin^2 \frac{k_x}{2} + \sin^2 \frac{k_y}{2}.
\]

This expansion, valid at \( \delta \approx 0 \) for \( 0 < t < \Delta - 4|t'| \) and arbitrary sign of \( t' \), reduces at \( t'=0 \) to the spectrum used in obtaining the BR transition, i.e. it is appropriate for following the evolution with \( t' \) of the small \( t \) slave boson solution.

In the first step Eq. (4) is used in the range \( 4.7t_0 < \Delta_{pd} < \Delta_{pd}^{cr} \), where it can be expanded further in terms of \( |t'/\Delta| < 1 \). The following results are obtained retaining the terms linear in \( t' \) and quadratic and quartic in \( t' \).

The corresponding analytical calculation of the position of the Fermi level \( \varepsilon_F \) has been carried out earlier [2], by systematical linearization with respect to \( t' \). The shift of the \( \varepsilon_F \) from the van Hove singularity at \( \Delta_0(\varepsilon_F = \varepsilon_p) = 2t_0^2|F| \) turned out to be

\[
x_F \ln \frac{1}{x_F} = \frac{8\pi^2(\delta_c - \delta)}{1 + 8\pi^2\delta_c},
\]

where \( \delta_c = -32t'/\pi^2\Delta_0 \) stands for the critical doping required to bring the Fermi level back to the van Hove singularity. Experimentally, this doping is positive i.e. \( \text{sign} t' = -\text{sign} \Delta \). The linearization procedure can be generalized to the calculation of \( E_0(\Delta, t, t', \delta) \) and then, straightforwardly, to the solution of the slave boson equations (1) and (2). Here, for brevity, small terms in \( E_0 \), linear in \( x_F \), discussed in Ref. [13], will be omitted in the description of this solution.

The BR transition is shifted to the new position \( \Delta_{pd}^{cr} = 4.7t_0 + 3.5\delta_c \), with \( \delta_c = 13.6t'/t_0 \), but it is not suppressed by \( t' \). This important result can be traced back to the outstanding feature of the expansion of Eq. (4) in terms of \( t'^2/\Delta \), generating the term \( t'^2/\Delta^2 \). The above term vanishes with \( t \), making the theory all along convergent.
with respect to \( t'/\Delta \), as exemplified by Eq.(6), where \( x_F \) is finite and small independently on \( t \).

\( \Delta_{cr} \), the value of \( \Delta \) in the angular point, is equal to the \( \Delta_{pd}^{cr} / 2 \), i.e. for \( \delta_c > 0 \) it is slightly increased with respect to the \( t' = 0 \) value, and \( \Delta \) remains above \( \Delta_0 = \Delta(t' = 0) \) in the whole range of convergence of this approach, \( \Delta_{pd}^{cr} < \Delta_{pd} < \Delta'_{pd} \).

These results can be extended to finite \( \delta > 0 \). In contrast to \( t' \), i.e. to \( \delta_c \), finite \( \delta \) suppresses the BR transition, turning it into crossover, in spite of Eq.(6), which suggests analogous roles of \( \delta_c \) and \( \delta \). In the vicinity of \( \Delta_{pd}^{cr} \), the angular behavior of \( \Delta \) is essentially modified by finite \( \delta \). For example, the value of \( \Delta \) at \( \Delta_{pd} = \Delta_{pd}^{cr} = 4.7t_0 + 3.5\delta_c \)

\[
\frac{\Delta_{pd}^{cr}}{2} - \Delta = 0.8(1 + 0.2\delta_c)\delta^{1/3}
\]

and correspondingly

\[
t^2/t_0^2 = 0.63(1 - 0.2\delta_c)\delta^{2/3},
\]

up to the leading orders in \( \delta \) and \( \delta_c \).

Finally we turn to the range \( \Delta_{pd} > \Delta_{pd}^{cr} \), where the stability of the \( t = 0 \) solution is to be discussed using Eq.(6) non-expanded in terms of \( t' \), but dropping out \( O(t'^4) \) term. The main contribution to the cohesive energy \( E_0 \) is weakly dependent on \( \varepsilon_F \) (i.e. \( \delta_c \)) and strongly dependent on lower cut-off, which is \( \Delta = \Delta - 4|t'| \) according to Eq.(6), i.e. \( \delta_c \). (Note in this respect that the \( \varepsilon_F \) dependency of \( E_0 \) was not very important even in the vicinity of the BR transition, Eqs.(5) and (7).) Expanding then Eq.(6) around \( k = (\pi, \pi) \) point, one finds immediately that \( E_0 \) is logarithmic in \( t^2/t'\Delta \), which, through slave boson equations, leads for \( \Delta_{pd} > \Delta_{pd}^{cr} \) at \( \delta = 0 \) to

\[
\bar{\Delta} = \Delta - 4|t'| \simeq 2|t'|e^{-\frac{|t'|\Delta_{pd}}{4t_0^2}},
\]

where \( c \) is a numerical factor. Eq.(8) shows that the asymptotic behavior of \( \Delta \) which at \( t' = 0 \) vanishes as \( \Delta_0 \sim t_0^2/\Delta_{pd} \), undergoes an essential modification to the exponential behavior, with the saturation at \( \Delta = 4t' \). Although the derivation of the result (8) does not suggest that this result is independent of the dimension, the similar behavior was obtained [3] at \( \delta = 0 \) in 1d. Moreover, it is easy to see that finite \( \delta > 0 \) leads to \( t \sim \sqrt{\delta} \) as before. However, the convergence of this result is reduced to \( t < \Delta \), which is itself (exponentially) small according to Eq.(8). The regime \( t \approx \Delta \) is quickly reached with doping and it is clear that, from the slave boson point of view, the limit \( t \geq \Delta \) is physically achievable.

The corresponding fits of the ARPES data for the Fermi surfaces of LSCO [3] (green dots) and the three band model fits (solid). (f) fitting parameters in units of \( t' \) with \( \Delta \) small

Equally good fits (c.f. Fig.3(b)) were however obtained earlier [2] assuming \( |\Delta| < 4|t'| \) rather than \( |\Delta| < 4|t'| \). Since it was shown here that the latter is the solution of the \( \Delta \approx 0 \) slave boson theory when \( 2|t'| < t_0 \), the former can only occur at \( \Delta \approx 0 \), if \( 2|t'| > t_0 \). While the behavior of \( \bar{\Delta} \) given by Eq.(8) can be visualized, assuming for the moment \( t = 0 \), as the avoided crossing of
the dispersionless (t=0) copper level and the pure oxygen band with the energy \(-4|t'|^2\) at \(k = (\pi, \pi)\) point, the limit \(|\Delta| < 4|t'|\) means that the Cu level has entered the oxygen band. The holes on Cu site are then necessarily transferred to the oxygen sites, i.e. \(\langle n_d \rangle < 1\). For \(n = 1 + \delta\), with \(\delta \approx 0\), Eq.\(^1\) then requires finite \(t\), i.e the solution \(t=0\) is unstable for \(2|t'| > t_0\). (For finite \(t\), copper band undergoes anticrossing (sign \(t' = -\text{sign} \Delta\), rather than touching (sign \(t' = \text{sign} \Delta\)) with the oxygen band. \([11,12]\)) With \(\langle n_d \rangle < 1\), the renormalization becomes small, analogously to the case of small and negative \(\Delta_\text{pd}\) at \(t'=0\). \(t \leq t_0\) and \(\Delta \leq \Delta_\text{pd}\) are not expected to depend much on doping \(\delta\). The appreciable experimental dependence of \(t\) on small \(\delta\) \([12]\) is therefore an indication in favor of the strongly renormalized \(2|t'| < t_0\) solution.

Let us finally point out that \(2|t'| < t_0\) solution, strongly dependent on doping, is approximately symmetric with respect to the electron (\(\delta < 0\)) or hole doping (\(\delta > 0\)). As the latter was discussed above, leading in particular to \(t/t_0 \sim \sqrt{\delta}\) for sufficiently large \(\Delta_\text{pd}\) > 4.7\(t_0\), the case \(\delta < 0\) will be briefly mentioned here. Since \(\langle n_d \rangle \leq n = 1 + \delta\), Eq.\(^1\) means that \(t \geq t_0\sqrt{-\delta}\), i.e., roughly speaking, \(t\) behaves as \(\sqrt{\delta}\), irrespectively of the sign of \(\delta\). \(t = 0\) line of the slave boson theory, obtained for the half-filled \(\delta = 0\) Cu-based band, is the singular line of the phase diagram, not only at \(t'=0\), but also for \(t' \neq 0\), as shown here. In the properties depending on the details of the band structure close to the Fermi surface, the simplest of which is perhaps the Hall constant, the symmetry is broken when a finite \(t'\) is taken into account. The corresponding asymmetry is the largest in the small \(t'/\Delta\) limit of Eq.\(^1\), when \(\delta > 0\) means doping towards and \(\delta < 0\) away from the vH singularity, whereas in the opposite limit of Eq.\(^1\), the Fermi level at \(\delta = 0\) is so far from the vH singularity, that the variation of the topology of the Fermi surface with doping becomes small. Overall, the asymmetry is much smaller than in the weak coupling limit.

In conclusion, the present work shows that the band structure of the high-\(T_c\) superconductors can be understood in terms of p-d bands in the CuO\(_2\) plane, renormalized by strong interaction on the Cu-site. According to the low energy ARPES data, the bare band parameters, measured by high energy spectroscopy, are renormalized by an order of magnitude. More profound understanding of the energy scales, of the order of 0.1 eV, i.e. the understanding of the approximate ground state on these energy scales, represents an appropriate prerequisite for consideration of the symmetry breaking, associated with AF and SC, on the energy scales of 0.01 eV.

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