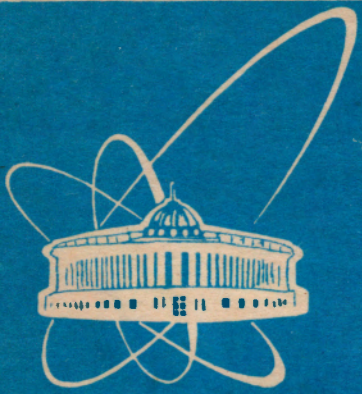

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TWO-BAND SINGLET-HOLE MODEL FOR THE COPPER OXIDE PLANE

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1 INTRODUCTION

An important contribution to the understanding of the low-energy electronic spectrum of copper-oxides has been done by Zhang and Rice [1] who pointed out the remarkable role of singlet formation for doped oxygen holes due to strong Coulomb correlations. Starting from the original *p-d* model proposed by Emery [2] and Varma et. al. [3] they have derived an effective one-band *t-J* model for the copper oxide plane. The appearance of singlet quasiparticle states inside the *p-d* gap was proved by different methods based on exact diagonalization [4], cluster calculations [5, 6], projection technique [7] and other calculations. It should be noted that the commonly used local density approximation [8] cannot describe such a singlet band formation due to the insufficient treatment of electronic correlations which questions the results of these calculations.

Recently [9, 10], the original Zhang-Rice procedure has been considerably improved in terms of the so-called cell-perturbation method (see also [11, 12]). It results in simple analytical formulas to reduce the *p-d* model to an effective singlet-triplet model. Applying the equation of motion method for Green's functions (GF) it has been found, however, that the coupling between singlet and triplet band is very small [10]. So we are left with a one-band *t-J* like model. One can also use this formalism as a basis to investigate the pairing which may be induced by either the electron-phonon or the exchange interaction [13].

The reduction to a *t-J* model has some disadvantages, however, which may be listed as follows: First of all, it neglects completely the charge fluctuations between the singlet and the one-hole *d*-like states. As will be seen in the following, such a hybridization modifies the spectrum in a considerable way and cannot be neglected. Secondly, the *t-J* model does not reproduce in a

correct way the spectral weight transfer which occurs with doping [14, 15]. More important difficulties may arise if one would like to calculate the pairing induced by the exchange interaction: The J-term in the Hamiltonian describes this effect only in a static and instanteneous way. That is quite similar to the BCS Hamiltonian for the electron-phonon mechanism. It does not deal with the dynamical effects of the exchange interaction as has been done for instance in [16] in analogy to the Eliashberg theory of the electron-phonon case. To solve *all* these problems we present in the following the reduction to an effective Hubbard model for one-hole d-like states and two-hole singlet states and avoid the further second order perturbation theory to obtain the J-term in the Hamiltonian. That keeps the possibility to describe the dynamical effects of the exchange interaction in terms of Green's functions.

The main purpose of the present work consists in the presentation of a new Hamiltonian in large analogy to the Hubbard model. In contradistinction to the usual case one ends up with an asymmetric model with different hopping integrals for the singlet and the one-hole bands. That may give a good starting point to study the differences between electron and hole doping. The use of such a Hamiltonian has also some practical reasons since several techniques are easier to apply for a Hubbard model than for a t-J model. That is especially true for the Green's functions decoupling scheme which is used here.

Then we apply the projection technique for the two-time matrix GF in terms of Hubbard operators. One ends up with a self-consistent system of equations for the one-particle GF. Their solution gives a two-band spectrum for d-like holes and Zhang-Rice-singlets. We consider in the present work only the paramagnetic state which may have, however, strong short-range antiferromagnetic correlations (spin-liquid state). The system of equations depends on these spin correlation functions as parameters. The second task of our

calculation consists in an analysis of the strong influence of short range antiferromagnetic spin fluctuations on the dispersion relation of the one-particle GF. It will be shown that its character changes dramatically by decreasing the spin-spin correlations.

The paper is organized as follows: after presenting the reduction procedure from the p-d model to an effective two-band Hubbard model in Sect. 2, we define the one-particle GF in Sect. 3. In Sect. 4 we derive the self-consistent system of equations and we present the results of a numerical calculation in Sect. 5. Finally we summarize the results.

2 TWO-BAND MODEL HAMILTONIAN

We consider the original p-d model [1, 2] in the limit of strong correlations at the copper sites, $U_d \to \infty$. By taking into account only the most important terms it can be written in a simple form:

$$H = \epsilon_d \sum_{i,\sigma} \tilde{d}^+_{i\sigma} \tilde{d}_{i\sigma} + \epsilon_p \sum_{m,\sigma} p^+_{m\sigma} p_{m\sigma} + t \sum_{i,m,\sigma} S_{im} \left(\tilde{d}^+_{i\sigma} p_{m\sigma} + h.c. \right), \qquad (1)$$

where $\tilde{d}^+_{i\sigma} = d^+_{i\sigma}(1 - n_{i\bar{\sigma}})$ denotes the creation of a hole on a copper site i provided there is no other hole with spin $\bar{\sigma} = -\sigma$, $p^+_{m\sigma}$ creates a hole on an oxygen site m and $S_{im} = \pm 1$ depending on the position of the site m in the unit cell i in agreement with [1]. The hopping p-d integral t and the difference between the hole energy levels for oxygen and copper, $\Delta = \epsilon_p - \epsilon_d$, are the only two parameters in the model (1).

To derive the singlet band it is reasonable to simplify this Hamiltonian (1) further, following mainly [9, 10]. Let us summarize the main steps: introducing the symmetric combination of oxygen operators $p^{(s)}_{i\sigma}$ in the unit cell i according

to [1] we can define the orthogonal Wannier states $c_{i\sigma}$ by the equation

$$p^{(s)}_{i\sigma} = \frac{1}{2}\sum_m S_{im} p_{m\sigma} = \sum_j \nu_{ij}\ c_{j\sigma}\ . \qquad (2)$$

The overlapping parameters

$$\nu_{jl} = \frac{1}{N}\sum_k \sqrt{1 - \frac{1}{2}(\cos k_x + \cos k_y)}\ \mathrm{e}^{ik(j-l)} \qquad (3)$$

decrease rapidly, but nonexponentially with the distance $(j-l)$: $\nu_0 = \nu_{jj} \simeq 0.96$, $\nu_1 = \nu_{j\ j\pm a_{x/y}} \simeq -0.14$, and $\nu_2 = \nu_{j\ j\pm a_x \pm a_y} \simeq -0.02$. (see [9]). Taking into account in the following inter-cell perturbation theory *all* the Wannier coefficients ν_{jl} we would obtain an artificial sharp cusp in the dispersion curve at the Γ-point ($k = (0,0)$) [10]. That is a known artefact of the Wannier representation for nonisolated bands [17]. Therefore, we consider in the present calculation the Wannier coefficients ν_0, ν_1 and ν_2, only. Using the orthogonal Wannier states $c_{i\sigma}$ in (2) we can write the Hamiltonian in the form:

$$\begin{aligned} H &= \sum_{i\sigma}\{\epsilon_d\ \tilde{d}^+_{i\sigma}\tilde{d}_{i\sigma} + \epsilon_p\ c^+_{i\sigma}c_{i\sigma} + V_0\ (\tilde{d}^+_{i\sigma}c_{i\sigma} + h.c.)\} \\ &+ \sum_{i\neq j\sigma} V_{ij}\ \{\tilde{d}^+_{i\sigma}c_{j\sigma} + h.c.\}\ , \end{aligned} \qquad (4)$$

where $V_{ij} = 2t\ \nu_{ij}$ and $V_0 = 2t\ \nu_0$. Since $|V_{ij}| \ll V_0$ one can consider the last inter-cell term in (4) as a small perturbation to the intra-cell part given by the first term in (4).

As was shown in [9, 10] the first intra-cell part can be diagonalized within one unit cell. That gives for the lowest one-hole d-type state

$$|D_\sigma\rangle = \cos\theta_1\ d^+_\sigma|0\rangle - \sin\theta_1\ c^+_\sigma|0\rangle\ , \qquad (5)$$

and the two-hole state with the lowest energy is the singlet state

$$|\psi\rangle = \cos\theta_2\ \frac{1}{\sqrt{2}}\ (d^+_\uparrow c^+_\downarrow - d^+_\downarrow c^+_\uparrow)\ |0\rangle - \sin\theta_2\ c^+_\uparrow c^+_\downarrow\ |0\rangle\ , \qquad (6)$$

where the vacuum state $|0\rangle$ has no holes and $\tan 2\theta_1 = 2V_0/\Delta$, $\tan 2\theta_2 = 2\sqrt{2}V_0/\Delta$. The corresponding one-hole E_D and two-hole energies E_ψ are given by:

$$E_D = \frac{1}{2}(\epsilon_d + \epsilon_p) - \frac{1}{2}\sqrt{\Delta^2 + 4V_0^2}\ , \qquad (7)$$

$$E_\psi = \frac{1}{2}(\epsilon_d + 3\epsilon_p) - \frac{1}{2}\sqrt{\Delta^2 + 8V_0^2}\ . \qquad (8)$$

Another one-hole p-type state has higher energy then the d-type state (5) and can be neglected in the subspace of one-hole states. The singlet states (6) are the lowest among the two-hole states and have to be filled first with doping. At small doping we can also neglect the triplet states with the energy $E_\tau = (\epsilon_d + \epsilon_p)$ since the mixing between singlet and triplet bands is rather small [10].

By introducing the Hubbard operators in the subspace of the one-hole states $|D_\sigma\rangle$ (5) and the singlet states $|\psi\rangle$ (6)

$$X^{\sigma\sigma}_i = |D_{i\sigma}\rangle\langle D_{i\sigma}|, \quad X^{\sigma 0}_i = |D_{i\sigma}\rangle\langle 0|\ , \qquad (9)$$

$$X^{22}_i = |\psi_i\rangle\langle\psi_i|\ , \quad X^{20}_i = |\psi_i\rangle\langle 0|\ , \quad X^{2\sigma}_i = |\psi_i\rangle\langle D_{i\sigma}|\ , \qquad (10)$$

we can write the intra-cell part of the effective Hamiltonian in the form

$$H_0 = E_D\sum_{i\sigma} X^{\sigma\sigma}_i + E_\psi\sum_i X^{22}_i\ . \qquad (11)$$

By projecting the original p- and d-operators in the inter-cell part of the Hamiltonian (4) onto the subspace of one- and two-hole states (5), (6)

$$c^+_\sigma = 2\sigma A_c X^{2\bar{\sigma}} - \sin\theta_1 X^{\sigma 0} \qquad \tilde{d}^+_\sigma = 2\sigma A_d X^{2\bar{\sigma}} + \cos\theta_1 X^{\sigma 0} \qquad (12)$$

where $2\sigma = \pm 1$ we can write the inter-cell term in (4) in the form

$$H_{int} = \sum_{i\neq j\sigma}\{t^\psi_{ij}X^{2\sigma}_i X^{\sigma 2}_j + t^D_{ij}X^{\sigma 0}_i X^{0\sigma}_j + 2\sigma t^{\psi D}_{ij}(X^{2\bar{\sigma}}_j X^{0\sigma}_j + X^{\sigma 0}_i X^{\bar{\sigma}2}_j)\}\ . \qquad (13)$$

The effective hopping parameters are given by [10]:

$$\begin{aligned} t_{ij}^{\psi} &= V_{ij} K_{\psi\psi} \qquad & K_{\psi\psi} &= 2A_d A_c \\ t_{ij}^{D} &= V_{ij} K_{DD} \qquad & K_{DD} &= -2\sin\theta_1 \cos\theta_1 \\ t_{ij}^{\psi D} &= V_{ij} K_{\psi D} \qquad & K_{\psi D} &= A_c \cos\theta_1 - A_d \sin\theta_1 \end{aligned} \tag{14}$$

with the coefficients

$$\begin{aligned} A_d &= -\frac{1}{\sqrt{2}} \sin\theta_1 \cos\theta_2 , \\ A_c &= \sin\theta_1 \sin\theta_2 + \frac{1}{\sqrt{2}} \cos\theta_1 \cos\theta_2 . \end{aligned} \tag{15}$$

Therefore, the total Hamiltonian of the two–band model for d-like holes and singlets takes the form:

$$H = H_0 + H_{int} - \mu N , \tag{16}$$

where we have introduced the chemical potential μ and the number operator

$$N = \sum_i N_i = \sum_i (2X_i^{22} + \sum_\sigma X_i^{\sigma\sigma}) . \tag{17}$$

It is easy to prove that the number operator (17) acting in the subspace of one- and two-hole states (5) and (6) satisfies the necessary condition $[N, H_0 + H_{int}] = 0$. This condition is not satisfied for the number operator for the original p- and d-holes in (1) written in terms of the Hubbard operators given by (12) since the higher energy one– and two–hole states were ignored in the model Hamiltonian (16).

To prove the importance of the hybridization term in (13) between D-holes and singlets we estimate the hopping parameters (14) for the case of strong intra–cell coupling: $2t = \Delta = \epsilon_p - \epsilon_d$. Direct calculation in (14) gives us

$$K_{\psi\psi} \simeq -0.477, \quad K_{DD} \simeq -0.887, \quad K_{\psi D} \simeq 0.834 . \tag{18}$$

This estimation shows that the ψ-D hybridization is rather strong being much larger than the singlet–triplet coupling $K_{\psi\tau}$ considered in [10]: $K_{\psi D} >> | K_{\psi\tau} | \simeq 0.08$. In the limit of small p-d hybridization, $t/\Delta \to 0$, while all the coefficients $K_{\psi\psi}$, K_{DD} and $K_{\psi\tau}$ tend to zero, $K_{\psi D}$ has a finite value, $K_{\psi D} \to 1/\sqrt{2}$. Therefore, in this limit the effective hopping parameter $t_{ij}^{\psi D}$ vanishes linearly with $V_{ij} \propto t$ while all the others, $t_{ij}^{\psi}, t_{ij}^{D}$, are proportional to (t^2/Δ). As a result, the inter–band ψ-D hybridization gives a rather strong renormalization of the singlet band dispersion being of the same order of (t^2/Δ) as the original one t_{ij}^{ψ}.

The two–band Hubbard–like model (16) in comparison with the original p-d model (1) takes into account the formation of a new singlet band for doped p–holes due to strong Coulomb correlations on copper sites. The appearance of the singlet band due to many–body correlations was proved by different methods (see [4]-[7]) while it cannot be obtained in the framework of standard band–structure calculations based on the local–density approximation [8]. On the other hand, the one–band t-J model for singlets [1] considers the one–hole d–like band only in a static way by an effective exchange J-term and it neglects charge–carrier fluctuations that prevents a proper study of charge transport in the CuO_2 planes. In general, the two–band (p-d) model (16) can be considered as the standard Hubbard model with one–hole and two–hole (lower and upper) subbands but with highly asymmetric hopping parameters (14) and the single–site correlation energy $U \simeq \Delta = \epsilon_p - \epsilon_d$. Therefore we can apply to this model well–developed methods in the theory of the standard Hubbard model.

3 GREEN'S FUNCTIONS

To consider the hole spectrum for the two–band model (16) we employ the equation of motion method for the two–time Green function (GF). By using the projection technique we obtain the Dyson equation which will be solved in a generalized mean–field approximation neglecting finite lifetime effects.

To study the two–band problem we have to introduce the matrix Green's function

$$\hat{G}_{ij\sigma}(t-t') = \langle\langle \hat{X}_{i\sigma}(t); \hat{X}^{+}_{j\sigma}(t') \rangle\rangle \,, \tag{19}$$

where we have used Zubarev's notations [18] for the anticommutator GF for the two–component operators

$$\hat{X}_{i\sigma} = \begin{pmatrix} X_i^{\sigma 2} \\ X_i^{0\bar{\sigma}} \end{pmatrix} \qquad \hat{X}^{+}_{j\sigma} = \begin{pmatrix} X_j^{2\sigma} & X_j^{\bar{\sigma}0} \end{pmatrix} . \tag{20}$$

By differentiating the GF (19) over time t we get for the Fourier component the following equation

$$\omega \hat{G}_{ij\sigma}(\omega) = \delta_{ij}\hat{\chi} + \langle\langle \hat{Z}_{i\sigma} \mid \hat{X}^{+}_{j\sigma} \rangle\rangle_{\omega} \tag{21}$$

where $\hat{Z}_{i\sigma} = [\hat{X}_{i\sigma}, H]$ and

$$\hat{\chi} = \begin{pmatrix} \chi_\psi & 0 \\ 0 & \chi_D \end{pmatrix} \tag{22}$$

with the matrix elements

$$\chi_\psi = \langle \chi^{\psi}_{i\sigma} \rangle = \langle X_i^{22} + X_i^{\sigma\sigma} \rangle \qquad \chi_D = \langle \chi^{D}_{i\sigma} \rangle = \langle X_i^{\sigma\sigma} + X_i^{00} \rangle \,. \tag{23}$$

Here and in what follows we consider a spin–singlet state for which the correlation functions (23) do not depend on the spin σ. For the two–band model (16) we have

$$X_i^{00} + \sum_{\sigma} X_i^{\sigma\sigma} + X_i^{22} = 1 \tag{24}$$

that implies $\chi_D = 1 - \chi_\psi$.

Now, we project the many–particle GF in (21) on the one–hole one by introducing the irreducible (irr) part of the $\hat{Z}_{i\sigma}$ operator

$$\langle\langle \hat{Z}_{i\sigma} \mid \hat{X}^{+}_{j\sigma} \rangle\rangle = \sum_k \hat{E}_{ik\sigma} \langle\langle \hat{X}_{k\sigma} \mid \hat{X}^{+}_{j\sigma} \rangle\rangle + \langle\langle \hat{Z}^{(irr)}_{i\sigma} \mid \hat{X}^{+}_{j\sigma} \rangle\rangle \,. \tag{25}$$

The projection is defined by the condition

$$\langle \{ \hat{Z}^{(irr)}_{i\sigma}, \hat{X}^{+}_{j\sigma} \} \rangle = 0 \tag{26}$$

that results in the equation for the frequency matrix

$$\hat{E}_{ij\sigma} = \langle \{ [\hat{X}_{i\sigma}, H], \hat{X}^{+}_{j\sigma} \} \rangle \, \hat{\chi}^{-1} \,. \tag{27}$$

Here $\{A, B\}$ and $[A, B]$ are the anticommutator and the commutator for the A, B operators, respectively. After performing the necessary commutations of the Hubbard operators with the Hamiltonian (16) we obtain the following representation for the matrix (27):

$$\hat{E}_{ij\sigma} = \delta_{ij} \begin{pmatrix} E_\psi - E_D - \mu + \Delta^{\psi\psi}_\sigma & \Delta^{\psi D}_\sigma \\ \Delta^{D\psi}_\sigma & E_D - \mu + \Delta^{DD}_\sigma \end{pmatrix} + (1-\delta_{ij}) V_{ij} \begin{pmatrix} K^{\psi\psi}_{ij\sigma} & K^{\psi D}_{ij\sigma} \\ K^{D\psi}_{ij\sigma} & K^{DD}_{ij\sigma} \end{pmatrix} . \tag{28}$$

The components of the matrix are determined by the energy-shifts

$$\begin{aligned}
\Delta^{\psi\psi}_\sigma \chi_\psi &= \sum_{k\neq i} V_{ik} (K_{\psi\psi} \langle X_i^{2\bar{\sigma}} X_k^{\bar{\sigma}2} \rangle + K_{DD} \langle X_i^{0\sigma} X_k^{\sigma 0} \rangle) \\
\Delta^{DD}_\sigma \chi_D &= -\sum_{k\neq i} V_{ik} (K_{\psi\psi} \langle X_i^{\bar{\sigma}2} X_k^{2\bar{\sigma}} \rangle + K_{DD} \langle X_i^{\sigma 0} X_k^{0\sigma} \rangle) \\
\Delta^{\psi D}_\sigma \chi_D &= -\sum_{k\neq i} V_{ik} (K_{DD} \langle X_i^{\bar{\sigma}2} X_k^{\sigma 0} \rangle + K_{\psi\psi} \langle X_i^{\sigma 0} X_k^{\bar{\sigma}2} \rangle) - \\
&\quad -2\sigma \sum_{k\neq i} V_{ik} K_{\psi D} \langle X_i^{\bar{\sigma}2} X_k^{2\bar{\sigma}} + X_i^{\sigma 0} X_k^{0\sigma} \rangle \,,
\end{aligned} \tag{29}$$

and by the renormalized hopping parameters

$$K^{\psi\psi}_{ij\sigma} \chi_\psi = K_{\psi\psi} \langle X^{\psi}_{i\sigma} X^{\psi}_{j\sigma} + X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} \rangle - K_{DD} \langle X_i^{02} X_j^{20} \rangle$$

$$K_{ij\sigma}^{DD}\ \chi_D = -K_{\psi\psi}\langle X_i^{02}X_j^{20}\rangle + K_{DD}\langle \chi_{i\sigma}^D\chi_{j\sigma}^D + X_i^{\sigma\bar{\sigma}}X_j^{\bar{\sigma}\sigma}\rangle$$
$$K_{ij\sigma}^{\psi D}\ \chi_D = -2\sigma K_{\psi D}\langle \chi_{i\sigma}^{\psi}\chi_{j\sigma}^D - X_i^{\sigma\bar{\sigma}}X_j^{\bar{\sigma}\sigma} + X_i^{02}X_j^{20}\rangle\ . \qquad (30)$$

For $E_{ij\sigma}^{D\psi}$ we have the equation

$$E_{ij\sigma}^{D\psi}\ \chi_\psi = (E_{ij\sigma}^{\psi D})^+\chi_D\ . \qquad (31)$$

Now we introduce the zero-order GF in the generalized mean-field approximation by neglecting finite lifetime effects due to $\hat{Z}_{i\sigma}^{irr}$:

$$\hat{G}_{ij\sigma}^0(\omega) = \{\omega\hat{\tau}_0\delta_{ij} - \hat{E}_{ij\sigma}\}^{-1}\hat{\chi} \qquad (32)$$

where $\hat{\tau}_0$ is the unity matrix. By writing the equation of motion for the irreducible part of the GF in (25) with respect to the second time t' and performing the same procedure as in (25) for the right-hand side operator $\hat{X}_{j\sigma}^+(t')$ we get

$$\langle\langle \hat{Z}_{i\sigma}^{(irr)} \mid \hat{X}_{j\sigma}^+\rangle\rangle_\omega = \sum_k \langle\langle \hat{Z}_{i\sigma}^{(irr)} \mid \hat{Z}_{k\sigma}^{(irr)^+}\rangle\rangle\ \hat{\chi}^{-1}\ \hat{G}_{kj\sigma}^0(\omega)\ . \qquad (33)$$

By using (21), (25) and (33) we can obtain the Dyson equation for the GF (19) in the form

$$\hat{G}_{ij\sigma}(\omega) = \hat{G}_{ij\sigma}^0(\omega) + \sum_{kl}\hat{G}_{ik\sigma}^0(\omega)M_{kl\sigma}(\omega)\hat{G}_{lj\sigma}(\omega) \qquad (34)$$

where the self-energy operator $\hat{M}_{kl\sigma}(\omega)$ is defined by the equation

$$\hat{T}_{ij\sigma}(\omega) = \hat{M}_{ij\sigma}(\omega) + \sum_{kl}\hat{M}_{ik\sigma}(\omega)\hat{G}_{kl\sigma}^0(\omega)\hat{T}_{lj\sigma}(\omega)\ . \qquad (35)$$

The scattering matrix is given by the equation

$$\hat{T}_{ij\sigma}(\omega) = \hat{\chi}^{-1}\langle\langle \hat{Z}_{i\sigma}^{(irr)} \mid \hat{Z}_{j\sigma}^{(irr)^+}\rangle\rangle_\omega\ \hat{\chi}^{-1}\ . \qquad (36)$$

Eqs.(32), (34)-(36) give an exact representation for the one-hole GF (19). To calculate it, however, one has to apply some approximation for the many-particle GF in the scattering matrix (36) which describes finite lifetime effects.

4 SELF-CONSISTENT SYSTEM OF EQUATIONS

In the present section we consider an approximate solution for the zero-order GF (32). For that we introduce the **q**-representation for the GF (32) and the matrix elements in Eq. (28):

$$G_\sigma^{\alpha\beta}(\mathbf{q},\omega) = \sum_j G_{oj\sigma}^{\alpha\beta}(\omega)e^{-i\mathbf{qj}}$$
$$K_\sigma^{\alpha\beta}(\mathbf{q}) = \sum_j K_{0j\sigma}^{\alpha\beta}e^{-i\mathbf{qj}}$$
$$\gamma(\mathbf{q}) = 2\sum_{j\neq 0}\nu_{oj}e^{-i\mathbf{qj}} = \gamma_1(\mathbf{q}) + \gamma_2(\mathbf{q}) \qquad (37)$$

where γ_1 and γ_2 correspond to the nearest (n.n) and next nearest neighbours (n.n.n.), overlapping parameters $\nu_{ij}(3)$. Then we can solve Eq. (32) in the form

$$\hat{G}_\sigma^0(\mathbf{q}\omega) = \{\omega\tau_0 - \hat{E}_\sigma(\mathbf{q})\}^{-1}\hat{\chi}\ , \qquad (38)$$

where the **q**-representation for the matrix (28) can be written as

$$\hat{E}_\sigma(\mathbf{q}) = \begin{pmatrix} \omega_\psi(\mathbf{q}) & W_\sigma^{\psi D}(\mathbf{q}) \\ W_\sigma^{D\psi}(\mathbf{q}) & \omega_D(\mathbf{q}) \end{pmatrix}\ . \qquad (39)$$

Here, the energy spectra for unhybridized singlets and D-holes are defined by the functions

$$\omega_\psi(\mathbf{q}) = E_\psi - E_D - \mu + \Delta_\sigma^{\psi\psi} + V_\sigma^{\psi\psi}(\mathbf{q})$$
$$\omega_D(\mathbf{q}) = E_D - \mu + \Delta_\sigma^{DD} + V_\sigma^{DD}(\mathbf{q}) \qquad (40)$$

while the hybridization interaction is given by

$$W_\sigma^{\psi D} = \Delta_\sigma^{\psi D} + V_\sigma^{\psi D}(\mathbf{q})\ . \qquad (41)$$

The effective interaction in (40)-(41) according to (28), (37) has the form

$$V_\sigma^{\alpha\beta}(\mathbf{q}) = \frac{t}{N}\sum_k \gamma(\mathbf{k})K_\sigma^{\alpha\beta}(\mathbf{k}\text{-}\mathbf{q})\ . \qquad (42)$$

By using the matrix representation (39) the zero–order GF takes the final form

$$\hat{G}^0_\sigma(\mathbf{q},\omega) = \left\{ \begin{array}{cc} [\omega-\omega_D(\mathbf{q})]\chi_\psi & W^{\psi D}_\sigma \chi_D \\ W^{D\psi}_\sigma \chi_\psi & [\omega-\omega_\psi(\mathbf{q})]\chi_D \end{array} \right\} \cdot ([\omega-\Omega_\psi(\mathbf{q})][\omega-\Omega_D(\mathbf{q})])^{-1} , \tag{43}$$

where the hybridized spectra for singlets (ψ) and D-holes are given by

$$\Omega_{\psi,D}(\mathbf{q}) = \frac{1}{2}[\omega_\psi(\mathbf{q})+\omega_D(\mathbf{q})] \pm \frac{1}{2}\{[\omega_\psi(\mathbf{q})-\omega_D(\mathbf{q})]^2 + 4W^{\psi D}_\sigma W^{D\psi}_\sigma\}^{1/2} \tag{44}$$

To obtain a closed system of equations we have to calculate self–consistently the correlation functions in (29). The energy shifts $\Delta^{\alpha\beta}_\sigma$ (29) can be readily calculated by using the spectral representation for the one–hole GF (43). For instance, one has

$$\sum_{j\neq i} V_{ij}\langle X^{\alpha\beta}_i X^{\gamma\delta}_j\rangle = \frac{t}{N}\sum_q \gamma(q)\langle X^{\alpha\beta}_q X^{\gamma\delta}_q\rangle =$$

$$= \frac{t}{N}\sum_q \gamma(q)\int_{-\infty}^{\infty}\frac{d\omega}{1+e^{-\beta\omega}}[-\frac{1}{\pi}\mathrm{Im}\langle\langle X^{\alpha\beta}_q \mid X^{\gamma\delta}_q\rangle\rangle_{\omega+i\delta}] . \tag{45}$$

But to calculate the two–particle correlation functions in $K^{\alpha\beta}_{ij\sigma}$ (29) we have to adopt some approximations. For instance, according to a procedure proposed by Roth [19] a two–particle correlation function, e.g.

$$\langle X^{02}_i X^{20}_k\rangle = \langle X^{0\sigma}_i X^{\sigma 2}_i X^{20}_k\rangle , \tag{46}$$

can be calculated from an equation of motion for the subsequent many–particle GF

$$\langle\langle X^{0\sigma}_i(t);\ X^{\sigma 2}_i X^{20}_k\rangle\rangle . \tag{47}$$

Such a technique was used for the original Hubbard model [20] giving the spectral function in good agreement with exact diagonalization results. It was found, however, that the Roth procedure underestimates slightly the value of the nearest neighbour spin-spin-correlation near to half filling. Therefore, we

consider in the following calculation the spin-correlation functions like parameters and deal with their doping dependence only phenomenologically.

In the present paper we decouple the product N_iN_j of the numbers operators N_i (17) on different lattice sites $i \neq j$ like in the Hubbard-I approximation but we keep spin correlations. By using the representation

$$\chi^\psi_{i\sigma} + X^{\sigma\bar{\sigma}}_i = \frac{1}{2}(\sum_\sigma X^{\sigma\sigma}_i + 2X^{22}_i) + \frac{1}{2}(X^{\sigma\sigma}_i - X^{\bar{\sigma}\bar{\sigma}}_i) + X^{\sigma\bar{\sigma}}_i = \frac{1}{2}N_i + 2\sigma S^z_i + S^\sigma_i \tag{48}$$

where $2\sigma = \pm 1$, $S^z_i = \pm 1/2$ and $S^\sigma_i = S^\pm_i$, we can write

$$\langle\chi^\psi_{i\sigma}\chi^\psi_{j\sigma}\rangle + \langle X^{\sigma\bar{\sigma}}_i X^{\bar{\sigma}\sigma}_j\rangle = \langle(\frac{1}{2}N_i + 2\sigma S^z_i)(\frac{1}{2}N_j + 2\sigma S^z_j) + S^\sigma_i S^{\bar{\sigma}}_j\rangle \simeq \chi_\psi\chi_\psi + \langle \mathbf{S_iS_j}\rangle \tag{49}$$

and analogous expressions for $\langle\chi^\psi_{i\sigma}\chi^D_{j\sigma}\rangle$, $\langle\chi^D_{i\sigma}\chi^D_{j\sigma}\rangle$. We neglect also correlations in the creation and annihilation of pairs

$$\langle X^{02}_i X^{20}_j\rangle \simeq \langle X^{02}_i\rangle\langle X^{20}_j\rangle = 0 . \tag{50}$$

For a spin–singlet state without long–range magnetic order the GF (43) and the one–hole spectrum (44) do not depend on the spin $\sigma = \pm 1/2$. But short–range magnetic fluctuations may give a considerable contribution for the spin correlation function $\langle \mathbf{S_iS_j}\rangle$ in (49). As it is well established, antiferromagnetic spin fluctuations are very strong in CuO_2 planes even in the metallic region at low temperatures and they should be taken into account in the renormalization of the hole spectrum.

Now, by using the corresponding $\gamma_1(\mathbf{q})$ and $\gamma_2(\mathbf{q})$ in (37), we can write the following equation for the effective interactions (42):

$$V^{\psi\psi}_\sigma(q) = tK_{\psi\psi}\chi_\psi \sum_i \gamma_i(\mathbf{q})(1+\chi^{(i)}_s/\chi^2_\psi) \tag{51}$$

$$V^{\psi D}_\sigma(\mathbf{q}) = -2\sigma tK_{\psi D}\chi_\psi \sum_i \gamma_i(\mathbf{q})(1-\chi^{(i)}_s/\chi_\psi\chi_D) \tag{52}$$

where $i = 1$ for n.n. and $i = 2$ for n.n.n. We have also $V_\sigma^{D\psi}(q) = V_\sigma^{\psi D}(\mathbf{q})(\chi_D/\chi_\psi)$ while $V_\sigma^{DD}(\mathbf{q})$ is given by (51) with the appropriate change of indexes, $\psi \to D$. Here we have introduced spin correlation functions for n.n.

$$\chi_s^{(1)} = \langle \mathbf{S}_i \mathbf{S}_{i\pm a_{x/y}} \rangle \tag{53}$$

and for n.n.n.

$$\chi_s^{(2)} = \langle \mathbf{S}_i \mathbf{S}_{i\pm a_x \pm a_y} \rangle \tag{54}$$

which are site–independent for a spin–singlet state. These correlation functions will be considered in the numerical calculations in the next section as phenomenological parameters.

Now we can perform self–consistent calculations for the one–hole spectra of D-holes and singlets and the corresponding density of states. To study the doping dependence of the spectra we have to find out also the position of the Fermi level μ from the equation for the average density of holes

$$\begin{aligned} n &= \frac{1}{N}\sum_i \langle N_i \rangle = \langle \sum_\sigma X_i^{\sigma\sigma} + 2X_i^{22} \rangle = \\ &= \frac{1}{N}\sum_q \int_{-\infty}^{\infty} \frac{d\omega}{e^{\beta\omega}+1} \{-\frac{2}{\pi}\mathrm{Im}[G_\sigma^{\psi\psi}(\mathbf{q},\omega+i\delta) + G_\sigma^{DD}(\mathbf{q},\omega+i\delta)]\} \end{aligned} \tag{55}$$

There is also a useful relation

$$\chi_\psi = 1 - \chi_D = n/2 \tag{56}$$

which follows from (24). In the next section we consider some numerical results of the self–consistent solution of the obtained system of equations.

5 NUMERICAL RESULTS

We will analyze three cases with hole numbers $n = 1, 1.2$ and 1.4, respectively. There are strong antiferromagnetic correlations in the undoped case $n = 1$.

We use in the present calculation the nearest and next nearest neighbour spin-spin correlations $\chi_s^{(i)}$ of the two dimensional Heisenberg model. Within the linear spin-wave approximation we obtain $\chi_s^{(1)} = -0.336$ and $\chi_s^{(2)} = 0.202$ [21]. That corresponds to an infinite spin-spin correlation length ξ. Neutron scattering experiments for $La_{2-x}Sr_xCuO_4$ [22] show a decreasing correlation length ξ with doping. Therefore, we expect reduced absolute values for $\chi_s^{(i)}$ in the doped case $n = 1.2$. For simplicity, let us assume a lorentzian shape for the static spin susceptibility χ_q

$$\langle \mathbf{S}_0 \mathbf{S}_j \rangle = \frac{1}{N}\sum_q \chi_q e^{i\mathbf{q}\mathbf{j}} \tag{57}$$

which is peaked around the antiferromagnetic wave vector (π, π):

$$\chi_q = \frac{C(\xi)}{1 + \xi^2[1 + \frac{1}{2}(\cos q_x + \cos q_y)]} \,. \tag{58}$$

The value of $C(\xi)$ is determined by the condition $\langle \mathbf{S}_i \mathbf{S}_i \rangle = 3/4$. Assuming for $n = 1.2$ a spin-spin correlation length ξ of the order of the lattice constant $\xi = 1$, we obtain from (57) and (58) $\chi_s^{(1)} = -0.10$ and $\chi_s^{(2)} = 0.03$. That values will be used for $n = 1.2$. For the overdoped case $n = 1.4$ we expect no antiferromagnetic spin-spin correlations and we set them equal to zero.

We calculated also the influence of the energy-shifts (29) on the spectrum. It turned out, however, that they are very small and their influence on the spectrum can be neglected. Therefore, we will present the results of our calculations without the inclusion of these energy shifts. Then, besides the spin-correlations, the parameters χ_ψ, χ_D and the position of the Fermi level depend on the doping. The Fermi level will be determined self-consistently from Eq. (55), while χ_ψ and χ_D are given from (56). So, with doping, the parameter χ_ψ which is proportional to the spectral strength of the singlet band increases and the corresponding parameter χ_D of the one-hole d-like band decreases.

In Fig. 1a-c we show the dispersion relation for both bands (44) for $n = 1, 1.2$ and 1.4 with the spin correlations discussed above. We chose the parameters $\Delta = 3eV$ and $t = 1.5eV$. For comparison we present also the result if we would neglect the hybridization between singlet and one-hole band. One may note that the hybridization between D-hole and singlet band is very crucial to obtain the correct dispersion relation for $n = 1$ and 1.2, but less important for $n = 1.4$. To study the influence of spin-correlations one should compare Fig. 1a with Fig. 1c. First of all, one observes a complete change of the dispersion due to the spin-correlations. Without them, in Fig. 1c, one has a simple nearest neighbour dispersion as for free holes. Qualitatively, the same behaviour may also be observed in all the slaved boson calculations or in the first analysis of the singlet-triplet model [10] neglecting the influence of the spin-system on the quasi-particle dispersion. The strong antiferromagnetic correlations suppress nearly completely the nearest neighbour dispersion. They allow only a motion on one sublattice, dominantly, which gives rise to a next nearest neighbour spectrum. Decreasing the spin-correlations from their value in the undoped system to zero one obtaines a continuous change of the shape of dispersion. Fig. 1b shows a intermediate stage where the dispersion of the singlet band is very flat between $(\pi, 0)$ and (π, π). A similar change of dispersion has been found recently in a variational study of the t-J model [23].

Besides the dispersion relation (44) we also calculate the density of states, i.e. the imaginary part of the Green's function $-\frac{2}{\pi}\mathrm{Im}(G^{\psi\psi} + G^{DD})$. That quantity is normalized such that it gives the number of holes if one integrates up to the Fermi level. The density of states is shown in Fig. 2a-c for the same parameters as the band structure Fig. 1a-c, respectively. To clarify the amount of hybridization between singlet and one-hole d-like band we present also the mixed Green's function $-\frac{2}{\pi}\mathrm{Im}G^{\psi D}$. The most remarkable detail consists in

the occurrence of van-Hove singularities near to the bottom of the singlet band in Figs. 2a and 2b. We find the Fermi level in the singlet band near to the maximum of the density of states for the doped case Fig. 2b. That may give a possible foundation for the van-Hove scenario of high-temperature superconductivity. The very high density of states in Fig. 2b in comparison with Figs. 2a and 2c is due to the flat dispersion region in Fig. 1b. The Fermi level of the overdoped system $n = 1.4$ is far away from the van-Hove singularity. Another interesting detail consists in the ratio between singlet and D-hole band. With doping, the integrated spectral weight of the D-hole band decreases, but the spectral weight of the singlet band increases in agreement with other studies of the spectral weight transfer [14, 10].

Let us discuss some details of the singlet band dispersion in the undoped case. In Fig. 1a we find minima of the singlet dispersion at $(\pi/2, \pi/2)$ and $(\pi, 0)$ which are nearly degenerate, but $(\pi, 0)$ is lower in energy. These two minima correspond also to the double-peak structure in the density of states. If we would neglect in the present calculation the next nearest neighbour hopping ν_2 we would obtain a complete degeneracy between $(\pi/2, \pi/2)$ and $(\pi, 0)$. The reason for that consists in our special decoupling procedure such that the spin correlation function

$$\chi_s^{(3)} = \langle \mathbf{S}_i \mathbf{S}_{i \pm 2a_{x/y}} \rangle \tag{59}$$

does not occur. Indeed, it was shown in [24] that the inequality $\chi_s^{(2)} < \chi_s^{(3)}$ gives rise to a minimum at $(\pi/2, \pi/2)$. So, it might be that an improvement of the present calculation shifts the minimum to $(\pi/2, \pi/2)$. That would also be in agreement with other studies of the one-hole motion in an antiferromagnetic state [25, 26]. It was shown by variational studies [27, 23] that the antiferromagnetic long range order is not a necessary condition to observe such a dispersion and that the main features are also preserved in a spin liquid state

ENERGY(eV)

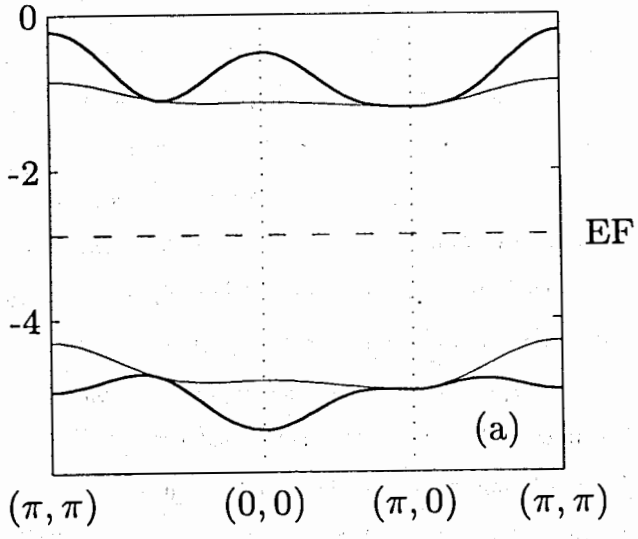

Fig. 1a.

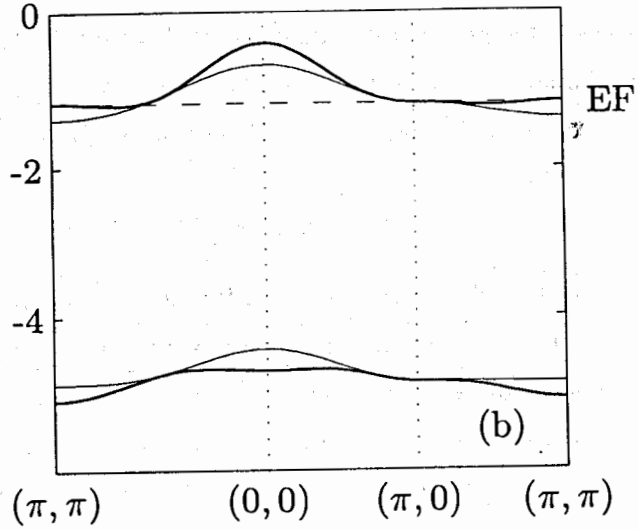

Fig. 1b.

ENERGY(eV)

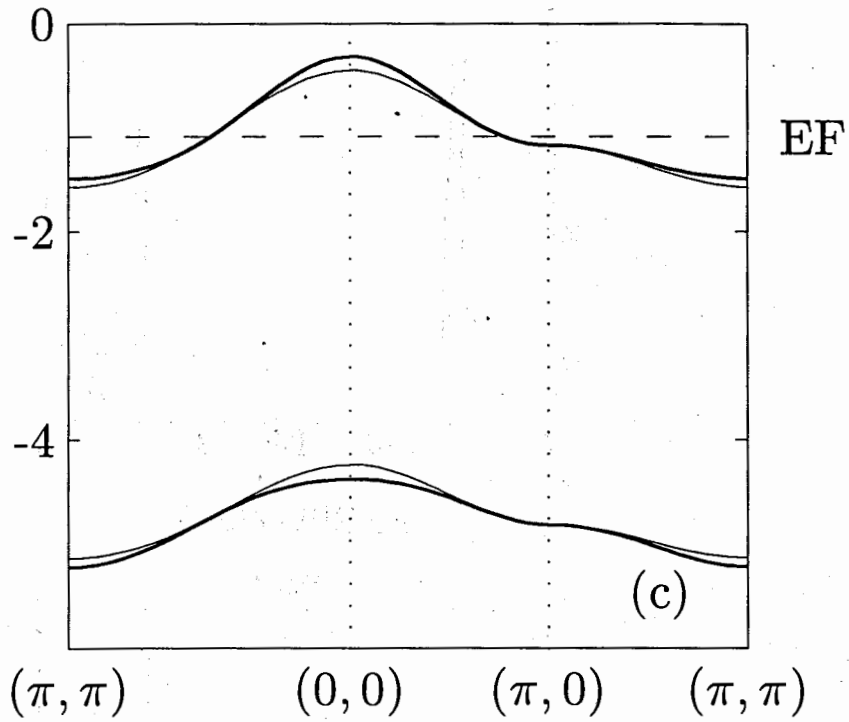

Fig. 1c.

FIG. 1: The band structure (thick line) in the undoped (a) $n = 1$, doped (b) $n = 1.2$ and overdoped (c) $n = 1.4$ case for $\Delta = 3eV$ and $t = 1.5eV$. For comparison we show also the result without hybridization (thin line). The zero of energy corresponds to the position of the nonbonding oxygen band and the EF denotes the Fermi level.

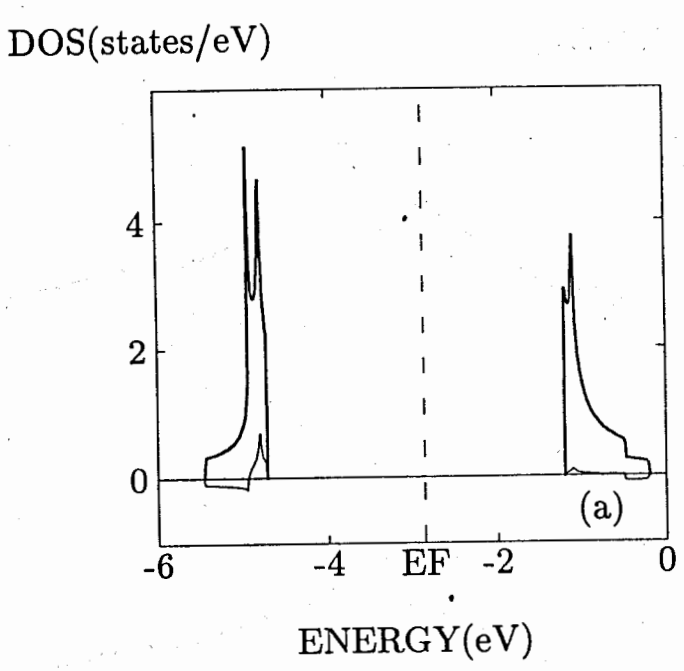

Fig. 2a.

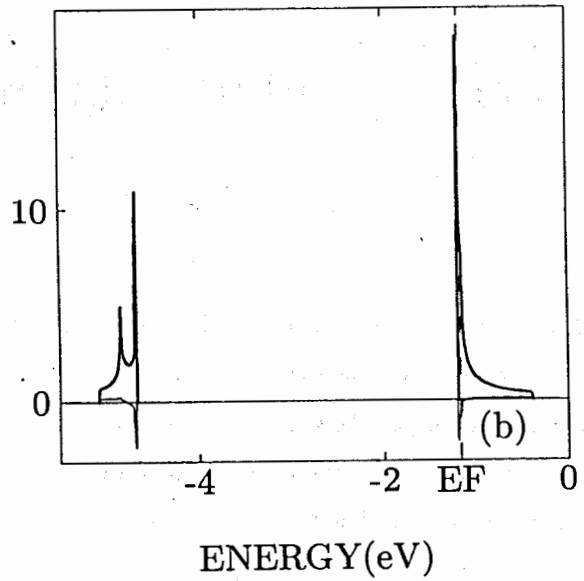

Fig. 2b.

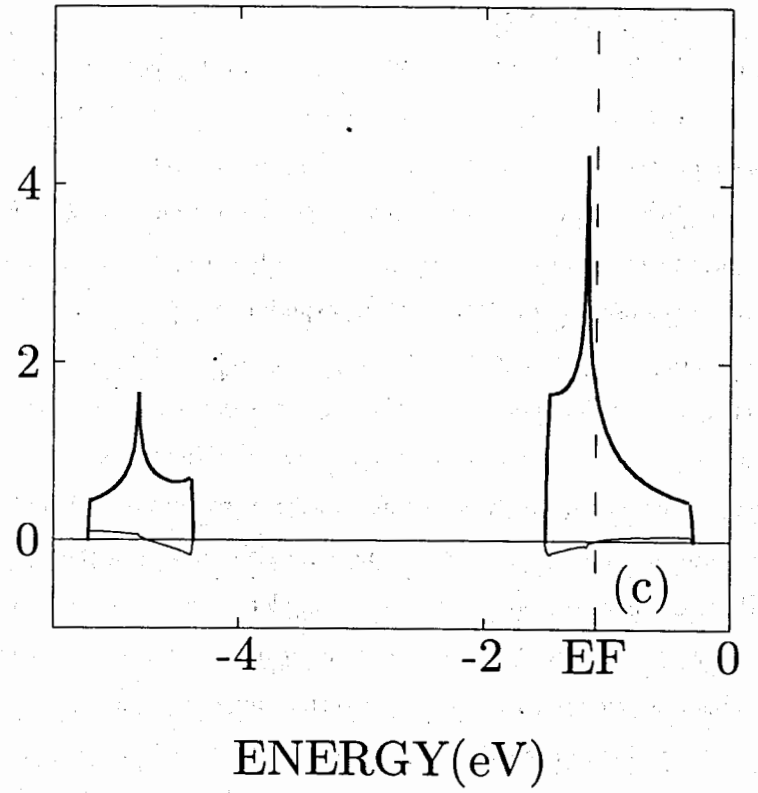

Fig. 2c.

FIG. 2: The density of states corresponding to Fig. 1 (thick line). The thin line shows the imaginary part of the mixed Green's function $G^{\psi D}$.

with only short-range antiferromagnetic correlations. In that case, however, the degeneracy between (π,π) and $(0,0)$ is lifted and one finds (π,π) to be higher in energy (see Fig. 1a).

It is clearly visible in Fig. 1 that the change of the dispersion for the singlet band with doping occurs mainly at the point (π,π) and not at the Γ-point. It results mainly due to the suppression of χ_q at the point (π,π) by decreasing ξ in (58). Furthermore, there is a flat dispersion region around $(\pi,0)$ which is even enhanced in the doped case (Fig. 1b). Interestingly, such a flat dispersion region was observed recently, both in experiment [28] and in a Monte Carlo calculation [29]. In agreement with the experiment [28] we find the Fermi level in the singlet band below the band position at $(\pi,0)$ (Fig. 1b). The energy difference, however, is too small, only $5meV$ in contrast to the measured $30meV$. But to find all these details in agreement with experiment is beyond the scope and the accuracy of the present calculation. Another disagreement is the position of the point (π,π) in the singlet band above the Fermi level for $n = 1.2$. That gives also rise to a wrong feature in the Fermi surface shape. Besides this wrong detail, the Fermi surface for $n = 1.2$ has some similarities to the large Fermi surface of the usual bandstructure calculations within the local density approximation. It should be noted, however, that our approach does not fulfill the Luttinger theorem, i.e. there are only 33 percent occupied k-values for $n = 1.2$ in contrast to 60 percent from the Luttinger sum rule. Even for $n = 1.4$ we find less occupied k-values (57 percent) as it should be (70 percent).

6 CONCLUSION

In the present paper we proposed a new model to describe the physics both in the low energy and charge transfer excitation regions of the copper oxygen

plane of cuprate superconductors (11, 13). It describes the one-hole d-like states and the two-hole singlet states in large analogy to the original Hubbard model. We calculated all its parameters in an effective and analytical way from the more realistic p-d model by means of the cell-perturbation method. In difference to the commonly used t-J model it allows to take into account the charge fluctuations between singlet and D-hole states, describes more correctly the spectral weight transfer and has the possibility to deal with the dynamical aspects of the exchange interaction. In difference to the original Hubbard model it is an asymmetric one with different bandwidths for the singlet and the D-hole band. That may give a basis to explain the asymmetry between electron and hole doping, but that deserves further studies.

Further on, we analyzed the one-particle properties of this model. The $2 * 2$ matrix Green's function for the effective two-band model can be written in terms of a Dyson equation (34) with the self-energy operator defined by eqs. (35, 36). The zero-order GF can be obtained by the projection technique with the frequency matrix (39). To obtain a closed set of equations we decoupled the density-density correlation functions like in the Hubbard-I approximation but we kept the spin-spin correlations as parameters. The results of the numerical calculations show that the spectrum is influenced by the spin-correlations in a dramatic way: For strong antiferromagnetic correlations near to half filling we observe a next nearest neighbour dispersion very similar to known results for the one-hole motion in antiferromagnets. Our calculations within the spin-liquid ground state show, however, that the long range antiferromagnetic order is not a necessary condition for such a dispersion. Remainders of the antiferromagnetic correlations are also observed in the bandstructure of the doped case. But the overdoped system shows a simple nearest neighbour dispersion.

One should be aware of the limitations of our, quite simple calculation for

the electronic structure of the singlet band. Most importantly we neglected to calculate an additional renormalization of the singlet quasiparticle spectrum due to finite-life time effects described by the self-energy operator in the Dyson equation (34). Therefore, we cannot obtain the division of the singlet band into a rather narrow quasiparticle spin-polaron band and a broad incoherent contribution which is preserved even for finite concentration of doped holes [30]. In addition, the spin-spin correlations should be calculated self-consistently from the one-particle Green's function itself. Nevertheless, our new model and the first analysis of the one-particle properties seems to be a good starting point for further studies of the spin dynamics or exchange mediated pairing in cuprates.

7 ACKNOWLEDGEMENT

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Плакида Н.М., Хайн Р., Ричард Ж.-Л. E17-94-516

Двухзонная синглет-дырочная модель для медноксидной плоскости

Исходя из стандартной $p-d$ модели получена эффективная модель Хаббарда для однодырочных d-состояний и двухдырочных синглетных состояний для описания низкоэнергетического спектра дырок в плоскости CuO_2 купратов. На основе проекционной техники для двухвременной матричной функции Грина от хаббардовских операторов, вычислен двухзонный спектр для d-дырок и синглетов и вычислена плотность состояний для них. Обнаружена сильная перенормировка спектра, обусловленная гибридизацией d-дырок и синглетов. Дополнительно показано, что дисперсионные кривые сильно зависят от антиферромагнитных спиновых короткодействующих корреляций в спин-синглетном состоянии. При наличии сильных корреляций для низкой концентрации дырок наблюдаются дисперсионные кривые, характерные для перескоков между следующими за ближайшими соседними узлами. При увеличении допирования спиновые корреляции ослабляются и дисперсионные кривые преобразуются к виду, характерному для перескоков между ближайшими соседями.

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Plakida N.M., Hayn R., Richard J.-L. E17-94-516

Two-Band Singlet-Hole Model for the Copper Oxide Plane

An effective Hubbard model for one-hole d-like states and two-hole singlet states is derived from the original $p-d$ model to describe the low-energy electronic spectrum of the CuO_2 plane in cuprates. By using the projection technique for the two-time matrix Green's function in terms of Hubbard operators a two-band spectrum for d-like holes and singlets as well as the density of states is calculated. It is found that the hybridization between d-like holes and singlets results in a substantial renormalization of the spectrum. In addition, the dispersion relation depends strongly on the antiferromagnetic short-range spin correlations in the spin-singlet state. For large spin-correlations at small doping values one finds a next-nearest neighbour dispersion. With doping, by decreasing the spin correlations, the dispersion changes to an ordinary nearest neighbour one.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

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