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Electronic spectrum in a microscopical model for the Zn-doped CuO_2 plane

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Abstract. We consider a microscopical model for the Zn-doped CuO_2 plane with Zn impurities being described as vacancies for the d-states on Cu sites. A reduction of the original p-d model to an effective one-band model results in the t-J model with vacancies for the spin 1/2 d-states at the Zn-sites. By employing the T-matrix formalism for the Green functions in terms of the Hubbard operators the density of electronic states (DOS) is calculated. Symmetry analysis of the perturbation matrix shows that in the system with d-type electronic wave functions additional DOS of d-, p- and s-types appear due to the perturbation of local energy levels and the interaction between nearest neighbors around the vacancy. The local and resonant state formation caused by Zn impurities is analyzed.

PACS. 71.27.+a Strongly correlated electron systems; heavy fermions – 71.55.-i Impurity and defect levels – 74.72.-h High-T_c compounds

1 Introduction

A number of experimental and theoretical works was dedicated to the investigation of impurity problems in superconducting cuprates (see, *e.g.* [1,2]). Their main goals were to draw out some definite conclusions concerning their electronic structure and the superconducting order parameter symmetry. As an example of an inherent nonmagnetic dopant in a strongly correlated electronic system, special interest was attracted to the study of the Zn/Cu substitutions in the CuO_2 plane. In order to conceive some of the unexpected consequences caused by Zn, many theoretical models have been investigated, although without preliminary proper consideration of the corresponding electronic states.

In a number of papers, the Zn impurity in the CuO_2 plane was considered as a local nonmagnetic impurity level at high energy in the Hubbard model [3,4] or the t-J model [5,6]. Using the T-matrix description, bound impurity states within the Hubbard gap were obtained. Due to strong Coulomb correlations in the model, the bare local impurity potential becomes a dynamic one which results in the resonant scattering and bound state formation of different (p, d-wave) symmetries in the gap. Formation of local magnetic moments induced by a spin vacancy in underdoped cuprates was considered in [7–9] within the RVB theory for the two-dimensional spin liquid. Influence of the impurity local moments on magnetic and transport properties in the RVB state were studied within the slave-boson and slave-fermion mean-field theories in [10,11]. The importance of the $4s$ orbital for the Zn^{2+} impurity in charge transfer excitations between copper $3d$ and zinc $4s$ orbitals was pointed out in [12]. To investigate the influence of nonmagnetic impurities on the d-wave superconductivity, several phenomenological models of Fermi liquid type were also considered (see, *e.g.*, [13–17]). In the framework of the many-band p-d model, a general qualitative analysis of the density of state (DOS) modifications caused by Zn and Ni impurities in electron and hole doped cuprates were performed in [18].

Based on band structure calculations we proposed in our previous paper [2] a microscopical model for the Zn-doped CuO_2 plane. It was shown that in the low-energy electronic spectrum the contribution of the Zn $3d^{10}$ orbitals can be neglected in comparison with the Cu $3d$ and O $2p$ ones. That permits to consider Zn impurities as vacancies for the d-states on Cu sites with the oxygen p-states being unaffected within the p-d model with strong correlations. Using the cell-perturbation method we derived an effective two-band Hubbard model for the Zn/CuO_2 system. Further reduction to an effective one-band model results in the t-J model with impurity sites having different hopping energy and exchange interaction of ferromagnetic type.

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In the present paper we investigate the proposed t-J model for Zn/CuO_2 in order to find the perturbation in the DOS caused by the Zn-impurities. The paper is organized as follows. In Section 2, we apply the equation of motion method for the Green function (GF) in order to obtain the corresponding Dyson equation with impurity-caused perturbation matrix $\hat{V}$. In Section 3, using the irreducible representation method of group theory [19,20] the nondiagonal matrix $\hat{V}$ is transformed into block-diagonal form which corresponds to states of s-, p- and d-symmetry. In Section 4, we calculate the perturbative parts of the GF caused by the impurity and the corresponding additional DOS. The numerical results and the discussion are presented in Sections 5 and 6 respectively.

2 Model and Green function equations

We consider an effective t-J model for the CuO_2 plane with one Zn impurity [2]

$$H = H_0 + V_{\rm vac} + V_{\rm imp}, \tag{1}$$

where the host lattice without impurity is described by the t-J model

$$H_0 = H_{t-J} = \epsilon \sum_{i\sigma} X_i^{\sigma\sigma} + t \sum_{i\neq j,\sigma} X_i^{\sigma 0} X_j^{0\sigma} + \frac{1}{4} J \sum_{i\neq j,\sigma} (X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} - X_i^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}}), \tag{2}$$

written in terms of the Hubbard operators, *e.g.*, $X_i^{\sigma 0} = c_{i\sigma}^{+}(1 - n_{i\bar{\sigma}})$ where $\bar{\sigma} = -\sigma$. The vacancy contribution is given by

$$V_{\rm vac} = -\epsilon \sum_{\sigma} X_0^{\sigma\sigma} - t \sum_{\Delta\sigma} (X_0^{\sigma 0} X_\Delta^{0\sigma} + \text{h.c.}) - \frac{1}{4} J \sum_{\Delta\sigma} (X_0^{\sigma\bar{\sigma}} X_\Delta^{\bar{\sigma}\sigma} - X_0^{\sigma\sigma} X_\Delta^{\bar{\sigma}\bar{\sigma}} + \text{h.c.}), \tag{3}$$

where the summations are performed over the nearest neighbor (n.n.) Cu-sites of the host square lattice, and the Zn-impurity is at the $i = 0$ site with $\Delta = 1, 2, 3, 4$ denoting its n.n. sites as shown in Figure 1. The Hamiltonian (1–3) is applicable both for electron ($0 < n < 1$) and hole ($1 < n < 2$) doping. In the former case ϵ and t are the on-site energy and the hopping integral for the lowest one-hole state $|D\rangle$ of the CuO_4 plaquette, whereas in the latter one they are those of the Zhang-Rice singlet state $|\psi\rangle$, as outlined in [2]. For the sake of simplicity we consider in the following analysis only the electron doping, since the transformation to the hole doping is quite straightforward. In what follows we neglect in (1) the uncoupled impurity oxygen state given by $V_{\rm imp}$ at the $i = 0$ site since its energy is much higher than the chemical potential μ [2].

In order to calculate the DOS for one-electron excitations in the system, we consider the equation of motion

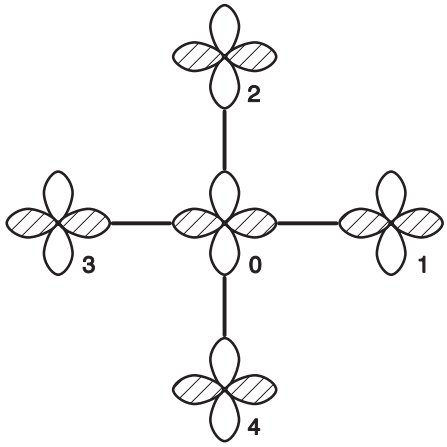

Fig. 1. Schematic picture of the impurity influenced cluster.

for the GF in terms of Hubbard operators:

$$\mathcal{G}_{ij\sigma}(t,t') = \langle\langle X_i^{0\sigma}(t); X_j^{\sigma 0}(t')\rangle\rangle = -\mathrm{i}\theta(t-t')\langle\{X_i^{0\sigma}(t), X_j^{\sigma 0}(t')\}\rangle, \tag{4}$$

where the Zubarev notation [21] is used. By employing the projection technique [22] for the GF we write down the corresponding Dyson equation. Neglecting the self-energy contribution in the generalized mean-field approximation (GMFA) we obtain

$$\omega G_{ij\sigma}(\omega) = \delta_{ij} + \sum_l E_{il} G_{lj\sigma}(\omega) + \sum_l V_{il} G_{lj\sigma}(\omega), \tag{5}$$

where we introduced the normalized GF:

$$G_{ij\sigma}(\omega) = Q_i^{-1} \mathcal{G}_{ij\sigma}(\omega), \qquad \int_{-\infty}^{\infty} \mathrm{d}\omega \left\{ \frac{1}{\pi} \mathrm{Im}\, G_{ij\sigma}(\omega - \mathrm{i}0^+) \right\} = \delta_{ij} \tag{6}$$

with the correlation function $Q_i = \langle X_i^{00} + X_i^{\sigma\sigma}\rangle = 1 - n_i/2$. In the paramagnetic state it depends only on the average number of holes

$$n_i = \sum_\sigma \langle X_i^{\sigma\sigma}\rangle = Q_i \int_{-\infty}^{\infty} \frac{2\,\mathrm{d}\omega}{\mathrm{e}^{(\omega-\mu)/T} + 1} \left\{ \frac{1}{\pi} \mathrm{Im}\, G_{ii\sigma}(\boldsymbol{\omega}) \right\}, \tag{7}$$

where $n_i \simeq n$ for $i \neq 0, \Delta$. In (7) and later on we use the notation $\boldsymbol{\omega} = \omega - \mathrm{i}0^+$. The equation for the frequency matrix E_{il} of the host lattice reads

$$E_{il} = \langle\{[X_i^{0\sigma}, H_0], X_l^{\sigma 0}\}\rangle\, Q_l^{-1}, \tag{8}$$

and the perturbation matrix is given by

$$V_{il} = \langle\{[X_i^{0\sigma}, V_{\rm vac}], X_l^{\sigma 0}\}\rangle\, Q_l^{-1} = \delta_{i0}\delta_{l0} V_{00} + \delta_{i0} \sum_\Delta \delta_{l\Delta} V_{01} + \delta_{l0} \sum_\Delta \delta_{i\Delta} V_{10} + V_{11} \sum_\Delta \delta_{i\Delta}\delta_{l\Delta}. \tag{9}$$

Equation (5) can be written in the form of the Dyson equation (in the matrix notation)

$$\hat{G} = \hat{G}^0 + \hat{G}^0 \hat{V} \hat{G} = \hat{G}^0 + \hat{G}^0 \hat{M} \hat{G}^0, \tag{10}$$

where the scattering matrix is

$$\hat{M} = \hat{V}\frac{1}{1-\hat{G}^0\hat{V}}, \tag{11}$$

and the zero-order GF for the host lattice is given by:

$$\hat{G}^0(\omega) = [\omega - \hat{E}]^{-1}. \tag{12}$$

Introducing the **q**-representation for the ideal host lattice the zero-order GF can be written in the form

$$G^0_{ij\sigma}(\omega) = \frac{1}{N}\sum_{\mathbf{q}} \mathrm{e}^{\mathrm{i}\mathbf{q}(\mathbf{R}_i-\mathbf{R}_j)}\frac{1}{\omega - E(\mathbf{q})}, \tag{13}$$

where

$$E(\mathbf{q}) = \tilde{\epsilon} + 2\tilde{t}(\cos q_x + \cos q_y). \tag{14}$$

In the GMFA, according to (8), the hopping energy $\tilde{t}$ and the on-site energy $\tilde{\epsilon} = \epsilon + \delta\epsilon$ are renormalized due to the kinematic and exchange interactions [22]:

$$\begin{aligned}\tilde{t} = {} & \frac{t}{Q}[\langle(1-n_0/2)(1-n_\Delta/2)\rangle + \langle \mathbf{S}_0\mathbf{S}_\Delta\rangle] \\ & - \frac{2J}{Q}\langle X_0^{\sigma 0}|X_\Delta^{0\sigma}\rangle; \end{aligned} \tag{15}$$

$$\begin{aligned}\delta\epsilon = {} & \frac{2J}{Q}[\langle(1-n_0/2)(1-n_\Delta/2)\rangle + \langle \mathbf{S}_0\mathbf{S}_\Delta\rangle - Q] \\ & - \frac{4t}{Q}\langle X_0^{\sigma 0}|X_\Delta^{0\sigma}\rangle, \end{aligned} \tag{16}$$

where Q is the correlation function for $n_i = n$. In the same approximation we obtain for the perturbation potential

$$V_{00} = -\tilde{\epsilon}, \quad V_{01} = V_{10} = -\tilde{t}, \quad V_{11} = -\delta\epsilon/4, \tag{17}$$

if the correlation functions for the number n_i and spin $\mathbf{S}_i$ operators in (9) are calculated for the host ideal lattice. Later on we measure the energy ω in units of the half-bandwidth $w = 4\tilde{t}$ (it means $V_{01} = V_{10} = -1/4$) from the renormalized on-site energy ($V_{00} = -\tilde{\epsilon} = 0$).

3 Symmetry analysis

The perturbation matrix has the following form:

$$\hat{V} = \begin{pmatrix} V_{00} & V_{01} & V_{01} & V_{01} & V_{01} \\ V_{10} & V_{11} & 0 & 0 & 0 \\ V_{10} & 0 & V_{11} & 0 & 0 \\ V_{10} & 0 & 0 & V_{11} & 0 \\ V_{10} & 0 & 0 & 0 & V_{11} \end{pmatrix}, \tag{18}$$

where its elements are given in (17). The notation used throughout the paper takes into account the d-type symmetry of the impurity wave function shown in Figure 1.

One can diagonalize the perturbation matrix (18) by the unitary transformation ($\hat{U}^+\hat{U} = 1$)

$$\hat{U} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ 1/2 & 1/\sqrt{2} & 0 & 0 & 1/2 \\ -1/2 & 0 & 1/\sqrt{2} & 0 & 1/2 \\ 1/2 & -1/\sqrt{2} & 0 & 0 & 1/2 \\ -1/2 & 0 & -1/\sqrt{2} & 0 & 1/2 \end{pmatrix}: \tag{19}$$

$$\hat{U}^+\hat{V}\hat{U} = \left(\begin{array}{c|c|c} V_s & 0 & 0 \\ \hline 0 & \hat{V}_p & 0 \\ \hline 0 & 0 & \hat{V}_d \end{array}\right), \tag{20}$$

where the s-, p- and d-symmetry matrices are

$$V_s = V_{11}, \quad \hat{V}_p = \begin{pmatrix} V_{11} & 0 \\ 0 & V_{11} \end{pmatrix}, \quad \hat{V}_d = \begin{pmatrix} V_{00} & 2V_{01} \\ 2V_{10} & V_{11} \end{pmatrix}. \tag{21}$$

The corresponding s-, p- and d-symmetry wave functions for the impurity cluster are defined by

$$\begin{aligned} |s\rangle &= \sum_{l=0}^{4} U(l,0)|l\rangle = \frac{1}{2}\Big\{|1\rangle - |2\rangle + |3\rangle - |4\rangle\Big\}; \\ |p_x\rangle &= \sum_{l} U(l,1)|l\rangle = \frac{1}{\sqrt{2}}\Big\{|1\rangle - |3\rangle\Big\}; \\ |p_y\rangle &= \sum_{l} U(l,2)|l\rangle = \frac{1}{\sqrt{2}}\Big\{|2\rangle - |4\rangle\Big\}; \\ |d_1\rangle &= \sum_{l} U(l,3)|l\rangle = |0\rangle; \\ |d_2\rangle &= \sum_{l} U(l,4)|l\rangle = \frac{1}{2}\Big\{|1\rangle + |2\rangle + |3\rangle + |4\rangle\Big\}. \end{aligned} \tag{22}$$

Using the rectangular $\hat{T}$-matrices [20] which are the columns of the unitary matrix (19)

$$\hat{T}_s = \frac{1}{2}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}; \; \hat{T}_p = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \\ -1 & 0 \\ 0 & -1 \end{pmatrix}; \; \hat{T}_d = \begin{pmatrix} 1 & 0 \\ 0 & 1/2 \\ 0 & 1/2 \\ 0 & 1/2 \\ 0 & 1/2 \end{pmatrix},$$

we can write the Dyson equation (10) for the GF in the form[1]

$$\hat{G} = \hat{G}^0 + \sum_{\mu=s,p,d} \hat{G}^0\hat{T}_\mu\hat{M}_\mu\hat{T}_\mu^+\hat{G}^0\,, \tag{23}$$

[1] Everywhere the argument of a function is omitted it is assumed to be ω.

where

$$\hat{M}_\mu = \hat{T}_\mu^+ \hat{V} \frac{1}{1-\hat{G}^0\hat{V}} \hat{T}_\mu = \hat{V}_\mu \left[1 - \hat{G}^0_\mu \hat{V}_\mu\right]^{-1}. \quad (24)$$

The matrices $\hat{V}_\mu \equiv \hat{T}_\mu^+ \hat{V} \hat{T}_\mu$ are given by (21). The matrices $\hat{G}^0_\mu(\omega) \equiv \hat{T}_\mu^+ \hat{G}^0(\omega)\hat{T}_\mu$, $\hat{I}_\mu(\omega) = 1 - \hat{G}^0_\mu(\omega)\hat{V}_\mu$ and the determinants $D_\mu(\omega) = \det \hat{I}_\mu(\omega)$ are obtained as follows:

$$G^0_s(\omega) = G^0_{11}(\omega) - 2G^0_{12}(\omega) + G^0_{13}(\omega) \equiv \gamma_s(\omega)\ , \quad (25)$$

$$I_s = D_s = 1 - V_{11}\gamma_s\ ; \quad (26)$$

$$\hat{G}^0_p(\omega) = \begin{pmatrix} \gamma_p & 0 \\ 0 & \gamma_p \end{pmatrix}; \quad \gamma_p(\omega) = G^0_{11}(\omega) - G^0_{13}(\omega), \quad (27)$$

$$\hat{I}_p = \begin{pmatrix} 1 - V_{11}\gamma_p & 0 \\ 0 & 1 - V_{11}\gamma_p \end{pmatrix}; \quad D_p = (1 - V_{11}\gamma_p)^2; \quad (28)$$

$$\hat{G}^0_d(\omega) = \begin{pmatrix} G^0_{00} & 2G^0_{01} \\ 2G^0_{01} & \sum_\Delta G^0_{\Delta 1} \end{pmatrix} \equiv \begin{pmatrix} d_{00}\ d_{01} \\ d_{10}\ d_{11} \end{pmatrix}, \quad (29)$$

$$\hat{I}_d \ = \ \begin{pmatrix} 1 - V_{00}d_{00} - 2V_{10}d_{01} & -2V_{01}d_{00} - V_{11}d_{01} \\ -V_{00}d_{10} - 2V_{10}d_{11} & 1 - 2V_{01}d_{10} - V_{11}d_{11} \end{pmatrix},$$

$$\begin{aligned} D_d &= 1 - V_{00}d_{00} - V_{11}d_{11} - 2V_{01}d_{10} - 2V_{10}d_{01} \\ &\quad + (V_{00}V_{11} - 4V_{01}V_{10})(d_{00}d_{11} - d_{01}d_{10}) \\ &= (\omega - V_{00})(G^0_{00} - 4V_{11}G^0_{01}) - (1 + 4V_{10})(1 + 4V_{01})G^0_{01}, \end{aligned} \quad (30)$$

where we used the relations $d_{11} = 4\omega G^0_{01}$, $G^0_{01} = \omega G^0_{00} - 1$. Substituting in (30) the perturbation potential given by (17) we obtain

$$D_d(\omega) = \omega[G^0_{00}(\omega) - 4V_{11}G^0_{01}(\omega)]. \quad (31)$$

In (25, 27, 29) we have used the symmetry of the zero-order GF $G^0_{ij}(\omega)$ given by (13) for the impurity cluster. Finally, for the partial scattering matrices $\hat{M}_\mu = \hat{V}_\mu \hat{I}^{-1}_\mu$ we derive:

$$M_s(\omega) = \frac{V_{11}}{1 - V_{11}\gamma_s}\ ; \quad (32)$$

$$\hat{M}_p(\omega) = \frac{V_{11}}{1 - V_{11}\gamma_p} \begin{pmatrix} 1\ 0 \\ 0\ 1 \end{pmatrix}\ ; \quad (33)$$

$$\hat{M}_d(\omega) = \frac{1}{D_d} \begin{pmatrix} V_{00} - |V|d_{11} & 2V_{01} + |V|d_{01} \\ 2V_{10} + |V|d_{10} & V_{11} - |V|d_{00} \end{pmatrix}, \quad (34)$$

where $|V| = V_{00}V_{11} - 4V_{01}V_{10}$ is the determinant of $\hat{V}_d$ and we used the identity

$$|1 - AB|\,(1 - AB)^{-1} = 1 - |A|\,|B|\,B^{-1}A^{-1}$$

valid for 2×2 matrices A and B.

4 Green functions and DOS

We can write the GF (23) in the form

$$G_{ij}(\omega) = G^0_{ij}(\omega) + \sum_{\mu=s,p,d} \Delta G^{(\mu)}_{ij}(\omega). \quad (35)$$

To calculate the perturbation parts, we need the following products $\hat{T}^+_\mu \hat{G}^0$:

$$\begin{aligned} &\Big(0\ \ 1/2\ \ -1/2\ \ 1/2\ \ -1/2\ \ 0\ \ ...\Big)_N \hat{G}^0(\omega) = \\ &\Big(... \textstyle\sum_l (\hat{T}^+_s)_l G^0_{lj}\ ...\Big)_N = \frac{1}{2}\Big(... \textstyle\sum_\Delta (-1)^{1+\Delta} G^0_{\Delta j}\ ...\Big)_N, \end{aligned} \quad (36)$$

$$\begin{pmatrix} 0 & 1/\sqrt{2} & 0 & -1/\sqrt{2} & 0 & 0 & ... \\ 0 & 0 & 1/\sqrt{2} & 0 & -1/\sqrt{2} & 0 & ... \end{pmatrix}_N \hat{G}^0(\omega) =$$

$$\begin{pmatrix} ... \sum_l (\hat{T}^+_p)_{1l} G^0_{lj}\ ... \\ ... \sum_l (\hat{T}^+_p)_{2l} G^0_{lj}\ ... \end{pmatrix}_N = \frac{1}{\sqrt{2}} \begin{pmatrix} ... \ G^0_{1j} - G^0_{3j}\ ... \\ ... \ G^0_{2j} - G^0_{4j}\ ... \end{pmatrix}_N, \quad (37)$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & ... \\ 0 & 1/2 & 1/2 & 1/2 & 1/2 & 0 & ... \end{pmatrix}_N \hat{G}^0(\omega) =$$

$$\begin{pmatrix} ... \sum_l (\hat{T}^+_d)_{1l} G^0_{lj}\ ... \\ ... \sum_l (\hat{T}^+_d)_{2l} G^0_{lj}\ ... \end{pmatrix}_N = \begin{pmatrix} ... & G^0_{0j} & ... \\ ... & \frac{1}{2}\sum_\Delta G^0_{\Delta j} & ... \end{pmatrix}_N. \quad (38)$$

The corresponding elements $\sum_l G^0_{il}(\hat{T}_\mu)_{lm}$ can be obtained by transposition of the matrix given in (36–38). Therefore, for the GF in (35) we have

$$\Delta G^{(s)}_{ij} = \frac{V_{11}}{1 - V_{11}\gamma_s} \frac{1}{4} \sum_{\Delta'\Delta} (-1)^{\Delta' + \Delta} G^0_{i\Delta'} G^0_{\Delta j}, \quad (39)$$

$$\begin{aligned} \Delta G^{(p)}_{ij} &= \frac{V_{11}}{1 - V_{11}\gamma_p} \frac{1}{2}\Big\{(G^0_{i1} - G^0_{i3})(G^0_{1j} - G^0_{3j}) \\ &\quad + (G^0_{i2} - G^0_{i4})(G^0_{2j} - G^0_{4j})\Big\}, \end{aligned} \quad (40)$$

$$\begin{aligned} \Delta G^{(d)}_{ij} &= M^d_{00} G^0_{i0} G^0_{0j} + M^d_{01} \frac{1}{2} \sum_\Delta G^0_{i0} G^0_{\Delta j} \\ &\quad + M^d_{10} \frac{1}{2} \sum_{\Delta'} G^0_{i\Delta'} G^0_{0j} + M^d_{11} \frac{1}{4} \sum_{\Delta'\Delta} G^0_{i\Delta'} G^0_{\Delta j}, \end{aligned} \quad (41)$$

where M^d_{ij} are given by (34). The expression (41) can be simplified further using the relation $\sum_\Delta G^0_{i\Delta} = 4(\omega G^0_{i0} - \delta_{i0})$. For the perturbation potential (17) we obtain:

$$\begin{aligned} \Delta G^{(d)}_{ij} &= \frac{1}{D_d}\Big[\omega(4V_{11}\omega - 1)G^0_{i0}G^0_{0j} \\ &\quad - 4V_{11}\omega(G^0_{i0}\delta_{0j} + \delta_{i0}G^0_{0j}) + (4V_{11} + G^0_{00})\delta_{i0}\delta_{0j}\Big]. \end{aligned} \quad (42)$$

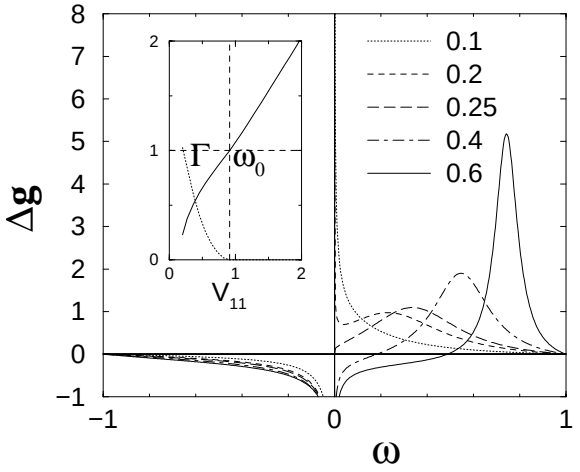

Fig. 2. $\Delta g_s(\omega)$ for different scattering potential $V_{11} < V_s^c$. The inset shows the position ω_0 and the inverse height Γ of the peak.

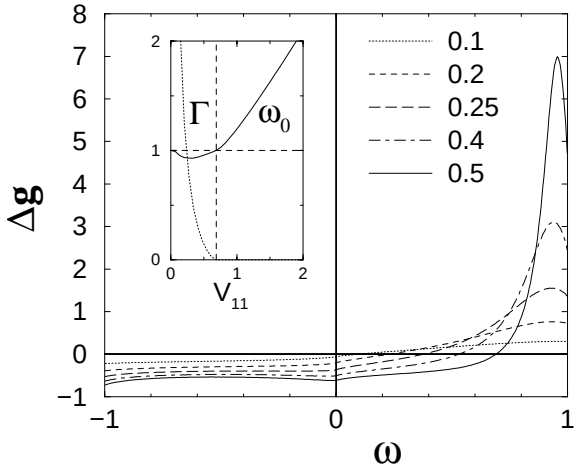

Fig. 3. $\Delta g_p(\omega)$ for different scattering potential $V_{11} < V_p^c$. The inset shows the position ω_0 and the inverse height Γ of the peak.

The general representation for the DOS is [19,20]

$$g(\omega) = g_0(\omega) + \frac{1}{N}\Delta g(\omega);\ \Delta g(\omega) = \frac{1}{\pi}\mathrm{Im}\frac{D'(\boldsymbol{\omega})}{D(\boldsymbol{\omega})} \quad (43)$$

with

$$D = \det(1 - \hat{G}^0\hat{V}) = D_s D_p D_d, \quad (44)$$

where $g_0(\omega)$ is the corresponding DOS for the host lattice and $D_\mu(\omega)$ are given by equations (26, 28, 31).

5 Numerical results

The additional DOS according to (43, 44) is given by:

$$\Delta g(\omega) = \frac{1}{\pi}\mathrm{Im}\frac{\mathrm{d}}{\mathrm{d}\omega}\ln D(\boldsymbol{\omega}) = \frac{1}{\pi}\frac{\mathrm{d}}{\mathrm{d}\omega}\arg D(\boldsymbol{\omega})$$
$$= \sum_\mu \frac{1}{\pi}\frac{\mathrm{d}}{\mathrm{d}\omega}\arg D_\mu(\boldsymbol{\omega}) = \sum_\mu \Delta g_\mu(\omega). \quad (45)$$

The zero-order GF involved in the expressions for $D_\mu(\omega)$ can be reduced to elliptical integrals (see Appendix) which is used in the numerics. The additional DOS Δg_s and Δg_p are shown in Figures 2 and 3 for $V_{11} < V_\mu^c$ with

$$V_s^c = \frac{\pi}{4(4-\pi)}, \quad V_p^c = \frac{\pi}{4(\pi-2)},$$

respectively, when there are resonant states in the band of the host lattice. For V_{11} larger than the critical values, $V_{11} > V_{s(p)}^c$, $\Delta g_{s(p)}(\omega)$ has a δ-peak outside the band. The additional p-states are doubly degenerated. The additional d-states have two modes. However the mode situated at the $i = 0$ site with $\Delta g_d(\omega) \propto \delta(\omega)$ should be excluded from the consideration since there is no state at the vacancy site and the mode has no physical meaning [20].

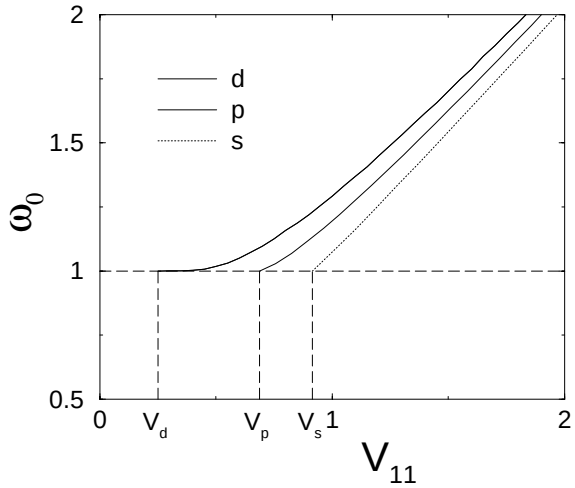

Fig. 4. The position of the local state in the additional DOS $\Delta g_\mu = \delta(\omega - \omega_0^\mu)$ outside the band for $V_{11} > V_\mu^c$ ($\mu = s, p, d$).

The other mode has no resonant states but logarithmic divergences at the center and boundaries of the band. At $V_{11} > V_d^c = 0.25$ it has a δ-peak outside the band. The energy dependences of the s-, p- and d- local modes on the interaction V_{11} are shown in Figure 4.

Let us estimate the value of the dimensionless perturbation potential V_{11}. For small doping one can neglect the last terms in (15) and (16) which are proportional to the correlation function $\langle X_0^{\sigma 0}|X_\Delta^{0\sigma}\rangle \propto (1-n) = \delta$. In this approximation we obtain:

$$V_{11} = \frac{J}{8}\left(\frac{1}{\tilde{t}} - \frac{1}{t}\right) \simeq 0.45.$$

Here we took into account that the bandwidth in the t-J model due to spin-fluctuations is strongly renormalized and as many calculations show it becomes of the order of the exchange interaction, $w = 4\tilde{t} \simeq J = 0.4t$ (see,

e.g., [22]). For a larger doping the last term in (16) gives a positive contribution to the perturbation potential V_{11} of the order $t\delta/2\tilde{t}(1+\delta)$. However, with doping the bandwidth increases that suppresses the first term in (16) and as a crude estimation one can use the value $V_{11} \leq 0.5$.

One sees that in the present calculation V_{11} exceeds the critical value for d-states whereas the two other local modes are still well above. In contrast to this result the exact diagonalization study for a 20×20 cluster [5] found that there are bound states for all three modes for $J/t = 0.4$. It cannot be excluded that an improved treatment for the one-particle GF beyond the present Hubbard I approximation yields all three localized level.

6 Conclusion

In the present paper we considered the microscopical model for the Zn-doped CuO_2 plane with Zn impurities, equation (1), which are described as vacancies for the d-states on Cu sites. The perturbation potential $V_{\rm imp}$ due to the uncoupled impurity oxygen state at the Zn site has been neglected since its energy is much higher than the relevant energy region. Applying the projection technique for the Green functions in terms of the Hubbard operators we obtained the Dyson equation (5). The Hubbard operator technique has the advantage of rigorous treating the constraints of no double occupancy in the t-J model. The Dyson equation was solved by applying the standard T-matrix technique. Performing the symmetry analysis in Section 3 we fully took into account the d-symmetry of the wave functions at Cu-sites of the host lattice that resulted in special forms for the s-, p- and d-symmetry of the wave functions (22), partial scattering matrices (32, 33, 34), and Green functions (39, 40, 41). In particular, the s- and p-symmetry scattering matrices appear only due to the perturbation potential V_{11} induced by the vacancy at the nearest neighbor sites. To compute its value (16), one has to calculate the corresponding spin and electron correlation functions. The latter could be obtained from the equations (39, 40, 41) for the GF, which closes the self-consistent loop. However, in the present paper we considered this perturbation as a free parameter and studied only the additional DOS of s-, p- and d- symmetries, shown in Figures 2–4. They have either resonant peaks within the d-band of the host lattice or δ-peaks outside the band for stronger scattering potential V_{11}. Numerical calculations were greatly simplified by using the analytical forms of the GF in terms of the elliptic integrals. A self-consistent calculation of the DOS and corresponding correlation functions and the consideration of thermodynamic properties induced by the vacancy in the d-band within the t-J model will be presented in subsequent publications.

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Appendix

A.1 Zero-order Green functions

Consider the complex function of a real argument

$$J_{mn}(\omega) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \frac{\mathrm{e}^{\mathrm{i}(mx+ny)}}{\omega - \epsilon(x,y) - \mathrm{i}0^+}\mathrm{d}x\mathrm{d}y$$
$$= \frac{1}{\pi^2} \int_{0}^{\pi}\int_{0}^{\pi} \frac{\cos mx \cos ny}{\omega - \epsilon(x,y) - \mathrm{i}0^+}\mathrm{d}x\mathrm{d}y, \qquad (A.1)$$

where $\epsilon(x,y) = (\cos x + \cos y)/2$. Further we use the notation $\boldsymbol{\omega} = \omega - \mathrm{i}0^+$. Performing in the last expression the substitution $\omega \to -\omega$, $x \to \pi - x$, $y \to \pi - y$ one sees

$$J_{mn}(-\omega) = (-1)^{m+n+1} J^*_{mn}(\omega). \qquad (A.2)$$

To compute $J_{mn}(\omega)$ we integrate at first the expression $2\cos ny/(c(x) - \cos y)$ with $c(x) = 2\boldsymbol{\omega} - \cos x$ over y:

$$I_n(c) = \int_0^{\pi} \frac{2\cos ny}{c - \cos y}\,\mathrm{d}y = \int_{-\pi}^{\pi} \frac{2\mathrm{e}^{\mathrm{i}ny}}{2c - (\mathrm{e}^{\mathrm{i}y} + \mathrm{e}^{-\mathrm{i}y})}\,\mathrm{d}y$$
$$= \frac{2}{\mathrm{i}} \oint_{|z|=1} \frac{z^n\,\mathrm{d}z}{c^2 - 1 - (z-c)^2},$$

where we have substituted $z = e^{\mathrm{i}y}$. Due to the infinitesimal negative imaginary component of c one pole is inside the integration contour and the other one is outside, depending on the choice of the analytical branch of the square root. Supposing the branch to be analytically continued from the real semiaxis $[1, +\infty]$ it is $c - \sqrt{c^2-1}$. To make the branch one-valued the segment $[-1, 1]$ of the real axis is cut from the complex plane, so that c ($|c| < 1$) is at the lower bank of the cut. The residue at the pole can be easily computed giving the result

$$I_n(c) = 2\pi \frac{(c - \sqrt{c^2-1})^n}{\sqrt{c^2-1}} = 2\pi \frac{\mathrm{e}^{-n\xi}}{\sinh \xi}, \qquad (A.3)$$

where $\xi = \operatorname{arccosh} c$, the hyperbolic arccosine being a complex function of a real argument. Thus the expression for $J_{mn}(\omega)$ reads:

$$J_{mn}(\omega) = \frac{1}{\pi^2} \int_0^{\pi} I_n(c) \cos mx\,\mathrm{d}x = \frac{2}{\pi} \int_0^{\pi} \frac{\mathrm{e}^{-n\xi}\cos mx}{\sinh \xi}\,\mathrm{d}x. \qquad (A.4)$$

Substituting in (A.4) $t = \boldsymbol{\omega} - \cos x$ and neglecting the imaginary component of $\boldsymbol{\omega}$ one gets

$$J_{mn}(\omega) = \frac{2}{\pi}\int_{\omega-1}^{\omega+1} \frac{\left(\omega + t - \sqrt{(\omega+t)^2-1}\right)^n \cos m \arccos(\omega - t)}{\sqrt{(\omega+t)^2-1}\sqrt{1-(\omega-t)^2}}\,\mathrm{d}t. \tag{A.5}$$

As $\cos m \arccos x$ is a polynomial of power m in x, the expression (A.5) can be reduced to a composition of polynomials and complete elliptic integrals of the first and second kind. The easiest way to find the expressions for J_{mn} with small m, n is direct integration of (A.5), which is straightforward, especially for $\omega > 1$:

$$J_{00}(\omega) = \bar{\omega}\tilde{\mathbf{K}}(\bar{\omega}); \tag{A.6}$$

$$J_{01}(\omega) = \tilde{\mathbf{K}}(\bar{\omega}) - 1; \tag{A.7}$$

$$J_{02}(\omega) = \frac{4}{\bar{\omega}}\left[\frac{\bar{\omega}^2}{4}\tilde{\mathbf{K}}(\bar{\omega}) + \tilde{\mathbf{E}}(\bar{\omega}) - 1\right]; \tag{A.8}$$

$$J_{11}(\omega) = \frac{2}{\bar{\omega}}\left[\left(1 - \frac{\bar{\omega}^2}{2}\right)\tilde{\mathbf{K}}(\bar{\omega}) - \tilde{\mathbf{E}}(\bar{\omega})\right], \tag{A.9}$$

where $\tilde{\mathbf{K}}(k)$, $\tilde{\mathbf{E}}(k)$ are the complete elliptic integrals of the first and second kind, respectively and $\bar{\omega} = \omega^{-1}$. To simplify the expressions we have normalized the standard elliptic integrals by a factor of $2/\pi$, so that $\tilde{\mathbf{E}}(0) = \tilde{\mathbf{K}}(0) = 1$.

To get the explicit expression for $J_{mn}(\omega)$ with $|\omega| < 1$ one uses the following expansion for the elliptic integrals of the real argument $1/k > 1$:

$$\begin{aligned}\tilde{\mathbf{K}}\left(\frac{1}{k}\right) &= k\left[\tilde{\mathbf{K}}(k) + \mathrm{i}\tilde{\mathbf{K}}'(k)\right];\\ \tilde{\mathbf{E}}\left(\frac{1}{k}\right) &= \frac{1}{k}\left[\left\{\tilde{\mathbf{E}}(k) - k'^2\tilde{\mathbf{K}}(k)\right\} - \mathrm{i}\left\{\tilde{\mathbf{E}}'(k) - k^2\tilde{\mathbf{K}}'(k)\right\}\right],\end{aligned} \tag{A.10}$$

where $\tilde{\mathbf{K}}'(k) = \tilde{\mathbf{K}}(k')$, $\tilde{\mathbf{E}}'(k) = \tilde{\mathbf{E}}(k')$ ($k' = \sqrt{1-k^2}$) are the complementary elliptic integrals.

The GF G^0_{ij} and the integrals J_{mn} are related as follows:

$$G^0_{00} = J_{00}, \quad G^0_{01} = J_{01}, \quad G^0_{13} = J_{02}, \quad G^0_{12} = J_{11}. \tag{A.11}$$

A.2 Applications

The change in the density of states is determined as

$$\Delta g_\mu(\omega) = \frac{1}{\pi}\frac{\mathrm{d}}{\mathrm{d}\omega}\arg D_\mu(\boldsymbol{\omega}), \tag{A.12}$$

$$D_s(\omega) = 1 - V\gamma_s(\omega); \quad D_p(\omega) = \left[1 - V\gamma_p(\omega)\right]^2,$$

where V stands for V_{11} and

$$\begin{aligned}\gamma_s(\omega) &= J_{00} - 2J_{11} + J_{02}\\ &= 4\omega\left[2\tilde{\mathbf{E}}(\bar{\omega}) - (1-\bar{\omega}^2)\tilde{\mathbf{K}}(\bar{\omega}) - 1\right];\end{aligned} \tag{A.13}$$

$$\gamma_p(\omega) = J_{00} - J_{02} = 4\omega\left[1 - \tilde{\mathbf{E}}(\bar{\omega})\right]. \tag{A.14}$$

One notes that γ_s and γ_p are continuous at $\omega = 1$, in particular it means $\mathrm{Im}\,\gamma_{s(p)}(1^-) = \mathrm{Im}\,\gamma_{s(p)}(1^+) = 0$.

The critical value $V^{\mathrm{c}}_{s(p)}$ above which the density has a δ-peak outside the band ($\omega > 1$) is easy to compute noting that it is the inverse value of the real component of the function $\gamma_{s(p)}(\omega)$ at $\omega = 1$. The expressions (A.13, A.14) at $\omega = 1$ can be easily evaluated:

$$\frac{1}{V^{\mathrm{c}}_s} = 4\left(\frac{4}{\pi} - 1\right) \approx \frac{1}{0.915}, \quad \frac{1}{V^{\mathrm{c}}_p} = 4\left(1 - \frac{2}{\pi}\right) \approx \frac{1}{0.688}\cdot \tag{A.15}$$

It is also of some interest to calculate the density of states at the upper band boundary for p states (especially in the undercritical regime). From (A.12) follows that

$$\pi\Delta g_p(\omega) = \mathrm{Im}\,\frac{D'_p(\boldsymbol{\omega})}{D_p(\boldsymbol{\omega})} = \mathrm{Im}\,\frac{2\gamma'_p(\omega)}{\gamma_p(\omega) - 1/V},$$

and $\gamma'_p(\omega)$ is easily computed:

$$\frac{\mathrm{d}\gamma_p(\omega)}{\mathrm{d}\omega} = 4[1 - \tilde{\mathbf{K}}(\bar{\omega})] = 4[1 - \omega\tilde{\mathbf{K}}(\omega) - \mathrm{i}\omega\tilde{\mathbf{K}}'(\omega)], \tag{A.16}$$

where we have applied the well-known relation

$$\frac{\mathrm{d}\tilde{\mathbf{E}}(k)}{\mathrm{d}k} = \frac{1}{k}\left[\tilde{\mathbf{E}}(k) - \tilde{\mathbf{K}}(k)\right]$$

to find $\gamma'_p(\omega)$ and then (A.10) to present its components at $\omega < 1$.

As $\gamma_p(1) = 1/V^{\mathrm{c}}_p$, $\mathrm{Im}\,\gamma'_p(1^-) = -4\tilde{\mathbf{K}}'(1) = -4$, we finally get:

$$\Delta g_p(1^-) = \frac{8/\pi}{1/V - 1/V^{\mathrm{c}}_p}\cdot \tag{A.17}$$

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