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**RESONANT STATES IN HIGH-TEMPERATURE
SUPERCONDUCTORS WITH IMPURITIES**

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1 Introduction

A lot of experimental and theoretical works were dedicated to investigation of Zn impurity influence on properties of cuprate compounds [1]-[20]. A special attention attracted recent scanning tunneling microscope (STM) study of spatial variation of the local density of states (LDOS) around the nonmagnetic impurity (Zn,Ni) in a cuprate superconductor, as $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (Bi-2212) compound [5]-[8]. There was shown that nonmagnetic impurities cause appearance of localized low-energy excitations in their close vicinity.

Such impressive experimental results inspired many theoretical investigations [9] - [16]. In spite of the important findings concerning space variation of the LDOS around an impurity and implicit information about corresponding superconducting condensate symmetry, one should stress that the proposed models were of a phenomenological character. In particular, in [9, 10, 15] the ' \mathcal{T} -matrix' formalism for the Green functions (GF) was used with an impurity scattering potential modeled by a phenomenological 2×2 matrix. Off-diagonal terms in the matrix was given by a local supression of the gap function at the impurity site [10, 11]. The Bogoliubov - de Gennes (BdG) formalism was considered for a model impurity potential [14] where only s-wave scattering was taken into account and solution was obtained by a variational ansatz for the $u(\mathbf{r})$ and $v(\mathbf{r})$ parameters. In [17] spatial dependence of the spin-dependent part of the scattering potential $K(\mathbf{r})$ was modeled in accordance with nuclear magnetic resonance experimental results.

In our recent papers [3, 4] a microscopic model of the CuO_2 plane with Zn impurities has been proposed based on band structure calculations for corresponding compounds using the original p - d model for the CuO_2 plane. Using cell-perturbation scheme and Schrieffer-Wolf transformation, we derived an effective one-band t - J model in terms of the Hubbard operators [4]. That Hamiltonian was further used to study s -, p - and d - wave contributions to the density of state (DOS) in the normal phase for the CuO_2 plane with Zn impurities [4].

Main goal of the present paper is to generalize our calculations for a superconducting phase of the proposed model. Applying the projection technique in the equation of motion method for the normal and anomalous GF, we obtain the corresponding \mathcal{T} -scattering matrix. It contains frequency dependent diagonal and off-diagonal parts of the scattering

potential. Finally, we calculate s -, p - and d -wave contributions to the on-site LDOS $D(\omega, \mathbf{r})$ which is proportional to the differential conductivity dI/dV [1],[11] measured in STM experiments [5]-[8].

The paper is organized as follow. In the next, Section 2, we introduce the model Hamiltonian and derive equations for the Green functions. In Sec. 3 we present the results: symmetry analysis (Sec. 3.1), density of electronic states (Sec. 3.2) and local density of electronic states (Sec. 3.3) for s -, p - and d -wave symmetry. Conclusions are given in the Section 4.

2 Green functions

In order to investigate influence of Zn impurity on the superconducting state, we consider an effective t - J model for the CuO_2 plane with Zn impurities [3, 4]

$$H = H'_{t-J} + V_{\text{imp}} = H_0 + V_{\text{vac}} + V_{\text{imp}}. \quad (1)$$

The Hamiltonian H'_{t-J} for the host lattice with a vacancy at the impurity site $i = 0$ can be written as the t - J model for an ideal lattice H_0 :

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

with the vacancy contribution V_{vac} given by

$$V_{\text{vac}} = -\epsilon \sum_{\sigma} X_0^{\sigma\sigma} - t \sum_{a\sigma} (X_0^{\sigma 0} X_a^{0\sigma} + \text{H.c.}) - \frac{1}{4} J \sum_{a\sigma} (X_0^{\sigma\bar{\sigma}} X_a^{\bar{\sigma}\sigma} - X_0^{\sigma\sigma} X_a^{\bar{\sigma}\bar{\sigma}} + \text{H.c.}). \quad (3)$$

Here $\epsilon = \epsilon_d - \mu$ is the energy of the hole, $t_{ij} = t$ is the hopping parameter for the nearest neighbors ($n.n.$) sites i, j in a square lattice and μ is the chemical potential. The summations in Eq.(3) are performed over the Cu-sites of the host square lattice, where the Zn-impurity is at the $i = 0$ site and $a = 1(a_x), 2(a_y), 3(-a_x), 4(-a_y)$ denoting its $n.n.$ sites. In what follows we neglect in (1) the impurity potential V_{imp} at the $i = 0$ site since its energy is much higher than the chemical potential μ [3] and impurity levels rest unoccupied in the low energy transitions.

To study the superconducting phase within the proposed model Hamiltonian (1-3) we introduce the following matrix Green function (GF) in

the Nambu representation

$$\hat{\mathcal{G}}_{ij\sigma}(t-t') = \langle\langle \hat{\Psi}_{i\sigma}(t); \hat{\Psi}_{j\sigma}^+(t') \rangle\rangle = -i\theta(t-t') \langle\{ \hat{\Psi}_{i\sigma}(t), \hat{\Psi}_{j\sigma}^+(t') \}\rangle.$$

with Nambu operators in terms of the Hubbard operators [21]-[25]

$$\hat{\Psi}_{i\sigma} = \begin{pmatrix} X_i^{0\sigma} \\ X_i^{\bar{\sigma}0} \end{pmatrix}, \quad \hat{\Psi}_{i\sigma}^+ = (X_i^{\sigma 0} \ X_i^{0\bar{\sigma}}),$$

where Zubarev's notation [26] for the GF is used. Corresponding time-Fourier component can be written in the following way

$$\hat{\mathcal{G}}_{ij\sigma}(\omega) = \begin{pmatrix} \mathcal{G}_{ij\sigma}^{11}(\omega) & \mathcal{G}_{ij\sigma}^{12}(\omega) \\ \mathcal{G}_{ij\sigma}^{21}(\omega) & \mathcal{G}_{ij\sigma}^{22}(\omega) \end{pmatrix}. \quad (4)$$

where $\mathcal{G}_{ij\sigma}^{11}(\omega) \equiv \langle\langle X_i^{0\sigma} | X_j^{\sigma 0} \rangle\rangle_\omega$ is the normal and $\mathcal{G}_{ij\sigma}^{21} \equiv \langle\langle X_i^{\bar{\sigma}0} | X_j^{\sigma 0} \rangle\rangle_\omega$ is the anomalous components of GF. The GF components (4) obey the following symmetry relations $\mathcal{G}_{ij\bar{\sigma}}^{12} = -\mathcal{G}_{ij\sigma}^{12}$; $\mathcal{G}_{ij\sigma}^{12}(-\omega) = \mathcal{G}_{ij\sigma}^{12}(\omega)$. The equation of motion for the Nambu operator $\hat{\Psi}_{i\sigma}$ can be written in the form

$$i \frac{d}{dt} \hat{\Psi}_{i\sigma} \equiv \hat{Z}_{i\sigma} = [\hat{\Psi}_{i\sigma}, H] \simeq \sum_l (\hat{E} + \hat{V})_{il\sigma} \hat{\Psi}_{l\sigma} + \hat{Z}_{i\sigma}^{irr},$$

where linear in $\hat{\Psi}_{i\sigma}$ part define the frequency matrix \hat{E} for the ideal lattice and static perturbation \hat{V} . The irreducible part $\hat{Z}_{i\sigma}^{irr}$ caused by the inelastic scattering processes is defined by the following orthogonality condition $\langle\{ \hat{Z}_{i\sigma}^{irr}, \hat{\Psi}_{j\sigma}^+ \}\rangle = 0$. It results in the following definitions of the frequency matrix

$$\hat{E}_{ij\sigma} = \langle\langle [\hat{\Psi}_{i\sigma}, H_0], \hat{\Psi}_{j\sigma}^+ \rangle\rangle \hat{Q}_\sigma(j)^{-1} = \begin{pmatrix} E & \Delta \\ \Delta^+ & -E \end{pmatrix}_{ij\sigma}$$

and the perturbation potential

$$\hat{V}_{ij\sigma} = \langle\langle [\hat{\Psi}_{i\sigma}, V_{vac}], \hat{\Psi}_{j\sigma}^+ \rangle\rangle \hat{Q}_\sigma(j)^{-1} = \begin{pmatrix} V & \phi \\ \phi^+ & -V \end{pmatrix}_{ij\sigma} \quad (5)$$

where $\langle\{ \hat{\Psi}_{i\sigma}, \hat{\Psi}_{i\sigma}^+ \}\rangle = \hat{Q}_\sigma(i) = \begin{pmatrix} Q_\sigma(i) & 0 \\ 0 & Q_{\bar{\sigma}}(i) \end{pmatrix}$ with $Q_\sigma(i) = \langle X_i^{00} + X_i^{\sigma\sigma} \rangle$. Since we consider the paramagnetic state, the correlation function $Q_\sigma(i) = Q_i = 1 - n_i/2$ depends only on the average number of the holes

n_i at lattice site i . In what follows we neglect here lattice site dependence of n_i and introduce $Q_i = Q = 1 - n/2$.

Introducing the normalized GF, $\hat{G}_{ij\sigma} = \hat{\mathcal{G}}_{ij\sigma} Q_j^{-1}$, we obtain the following equation:

$$\omega \hat{G}_{ij\sigma}(\omega) = \delta_{ij} \hat{\tau}_0 + \sum_l (\hat{E}_{il\sigma} + \hat{V}_{il\sigma}) \hat{G}_{lj\sigma}(\omega),$$

where $\hat{\tau}_0$ is the unit matrix. From this matrix equation we get the following linear system

$$\omega G_{ij}(\omega) = \delta_{ij} + \sum_l (E_{il} + V_{il}) G_{lj}(\omega) + \sum_l (\Delta_{il}^\sigma + \phi_{il}^\sigma) F_{lj\sigma}(\omega), \quad (6)$$

$$\omega F_{ij\sigma}(\omega) = \sum_l (\Delta_{il}^{\sigma+} + \phi_{il}^{\sigma+}) G_{lj}(\omega) - \sum_l (E_{il} + V_{il}) F_{lj\sigma}(\omega), \quad (7)$$

for the normal $G_{ij} = G_{ij\sigma}^{11}$ and the anomalous $F_{ij\sigma} = G_{ij\sigma}^{12}$ components of GF.

The diagonal components of the frequency matrix can be written in the following way

$$E_{ij\sigma}^{11} = E_{ij} = \tilde{\epsilon} \delta_{ij} + \tilde{t} \delta_{j,i+a},$$

where the on-site energy $\tilde{\epsilon} = \epsilon + \delta\epsilon$, and the effective hopping energy \tilde{t} in the generalised mean field approximation (GMFA) are renormalized due to the kinematic and exchange interactions [23],[4]

$$\delta\epsilon = \frac{J}{2Q} \sum_a [\langle (1 - n_i/2)(1 - n_{i+a}/2) \rangle + \langle \mathbf{S}_i \mathbf{S}_{i+a} \rangle - Q] - \frac{t}{Q} \sum_a \langle X_i^{\sigma 0} X_{i+a}^{0\sigma} \rangle,$$

$$\tilde{t} = \frac{t}{Q} [\langle (1 - n_i/2)(1 - n_{i+a}/2) \rangle + \langle \mathbf{S}_i \mathbf{S}_{i+a} \rangle] - \frac{J}{2Q} \langle X_i^{\sigma 0} X_{i+a}^{0\sigma} \rangle.$$

Off-diagonal components of the frequency matrix can be written as follows

$$\Delta_{ij}^\sigma = \delta_{ij} \frac{2t}{Q} \sum_a \langle X_i^{0\sigma} X_{i+a}^{0\bar{\sigma}} \rangle + \delta_{j,i+a} \frac{J}{Q} \langle X_i^{0\sigma} X_{i+a}^{0\bar{\sigma}} \rangle, \quad (8)$$

where $a = (\pm a_x, \pm a_y)$. In what follows we consider only d -wave symmetry of the gap Δ_{ij}^σ and therefore disregard the first term in Eq. (8), which is zero for this symmetry, i.e. $\sum_a \langle X_i^{0\sigma} X_{i+a}^{0\bar{\sigma}} \rangle = 0$. Diagonal and off-diagonal components of the perturbation matrix have respectively the following nonzero elements

$$V_{ij} = V_{00} \delta_{i0} \delta_{j0} + V_{01} \delta_{i0} \sum_a \delta_{ja} + V_{01} \delta_{j0} \sum_a \delta_{ia} + V_{11} \sum_a \delta_{ia} \delta_{ja}, \quad (9)$$

with $V_{00} = -\tilde{\epsilon}$, $V_{01} = -\tilde{t}$, $V_{11} = -(1/4)\delta\epsilon$, and

$$\phi_{ij}^\sigma = -\delta_{i,0}\Delta_{0a}^\sigma - \delta_{j0}\Delta_{0a}^\sigma - \delta_{ia}\delta_{ja}(2t/J)\Delta_{0a}^\sigma, \quad (10)$$

where $\Delta_{0a}^\sigma = \Delta_{01}^\sigma(\delta_{a,\pm a_x} - \delta_{a,\pm a_y})$ and $\Delta_{01}^\sigma = (J/Q)\langle X_0^{0\sigma} X_{a_x}^{0\bar{\sigma}} \rangle$. Solving the system of equations (6), (7) for the GF as the $N \times N$ matrices in the cell sites representation, one obtains the following equation

$$\{\omega I - (E + V) - (\Delta^\sigma + \phi^\sigma)[\omega I + E + V]^{-1}(\Delta^\sigma + \phi^\sigma)^\dagger\}G = I, \quad (11)$$

where I is the $N \times N$ unit matrix. For the ideal lattice ($V = 0$), we introduce the corresponding zero-order GF in the superconducting state

$$G^0 = \{\omega I - E - \Delta^\sigma(\omega I + E)^{-1}\Delta^{\sigma\dagger}\}^{-1}. \quad (12)$$

Then one can write the equation (11) in the following form

$$G = G^0 + G^0(V + \Phi)G, \quad (13)$$

where

$$\Phi = (\Delta^\sigma + \phi^\sigma)\frac{1}{\omega I + E + V}(\Delta^\sigma + \phi^\sigma)^\dagger - \Delta^\sigma\frac{1}{\omega I + E}\Delta^{\sigma\dagger} \quad (14)$$

After simple algebraic transformations, one obtains the following formal solution of the Dyson equation (13)

$$G = \frac{1}{I - G^0(V + \Phi)}G^0 = G^0 + G^0MG^0,$$

where we introduced the scattering matrix

$$M = (V + \Phi)\frac{1}{I - G^0(V + \Phi)}. \quad (15)$$

In the linear in ϕ approximation, one obtains

$$\Phi \simeq -\{\Delta^\sigma G_n^0(-\omega)\phi^{\sigma\dagger} + H.c.\} - \Delta^\sigma G_n^0(-\omega)V G_n^0(-\omega)\Delta^{\sigma\dagger}, \quad (16)$$

where the zero-order GF for the host lattice in the normal state is given by

$$G_n^0(\omega) = \frac{1}{\omega I - E}.$$

3 Results and discussion

3.1 Symmetry analysis

Scattering of quasiparticle electron excitations on an impurity potential results in the additional contribution δG to zero-order GF. In accordance with the irreducible representations (IR) of the corresponding lattice group transformations, δG can be separated in different s -, p - and d -parts [27], i.e.

$$G = G^0 + \sum_{\mu=s,p,d} \delta G_{\mu}, \quad (17)$$

where

$$\delta G_{\mu} = G^0 T_{\mu} M_{\mu} T_{\mu}^+ G^0 \quad (18)$$

and

$$M_{\mu} = T_{\mu}^+ M T_{\mu} = (V_{\mu} + \Phi_{\mu}) [1 - G_{\mu}^0 (V_{\mu} + \Phi_{\mu})]^{-1}, \quad (19)$$

with $V_{\mu} = T_{\mu}^+ V T_{\mu}$, $G_{\mu}^0 = T_{\mu}^+ G^0 T_{\mu}$ and

$$\Phi_{\mu} = T_{\mu}^+ \Phi T_{\mu} = -\{\Delta_{\mu}^{\sigma} G_{n,\mu}^0(-\omega) \phi_{\mu}^{\sigma+} + H.c.\} - \Delta_{\mu}^{\sigma} G_{n,\mu}^0(-\omega) V_{\mu} G_{n,\mu}^0(-\omega) \Delta_{\mu}^{\sigma+}. \quad (20)$$

Explicit forms of the T_{μ} and the perturbation V and ϕ matrices are given in the Appendix (A1),(A2).

The s -, p - and d -symmetry block-diagonal parts of the perturbation matrices V_{μ} and ϕ_{μ} (9), (10) are given by the equations

$$V_s = V_{11}, \quad V_p = V_{11} \hat{\tau}_0, \quad V_d = \begin{pmatrix} V_{00} & 2V_{01} \\ 2V_{01} & V_{11} \end{pmatrix}, \quad (21)$$

$$\phi_s = 0, \quad \phi_p^{\sigma} = -(2t/J) \Delta_{01}^{\sigma} \hat{\tau}_3, \quad \phi_d = 0 \quad (22)$$

Applying the unitary transformations (A1) on the G^0 , Δ_{σ} and G_n^0 matrices, one obtains respectively the following equations

$$G_s^0 = G_{11}^0 - 2G_{12}^0 + G_{13}^0 \equiv \gamma_s, \quad (23)$$

$$G_p^0 = \gamma_p \hat{\tau}_0, \quad \gamma_p = G_{11}^0 - G_{13}^0, \quad (24)$$

$$G_d^0 = \begin{pmatrix} d_{00} & d_{01} \\ d_{10} & d_{11} \end{pmatrix} = \begin{pmatrix} G_{00}^0 & 2G_{01}^0 \\ 2G_{01}^0 & \sum_a G_{a1}^0 \end{pmatrix} \quad (25)$$

$$\Delta_s = 0, \quad \Delta_p = 0, \quad \Delta_d^\sigma = 2\Delta_{01}^\sigma \hat{\tau}_1 \quad (26)$$

$$G_{n,s}^0 = G_{11}^{0,n} - 2G_{12}^{0,n} + G_{13}^{0,n} \equiv \gamma_{n,s}, \quad (27)$$

$$G_{n,p}^0 = \gamma_{n,p} \hat{\tau}_0, \quad \gamma_{n,p} = G_{11}^{0,n} - G_{13}^{0,n}, \quad (28)$$

$$G_{n,d}^0 = \begin{pmatrix} d_{00}^n & d_{01}^n \\ d_{10}^n & d_{11}^n \end{pmatrix} = \begin{pmatrix} G_{00}^{0,n} & 2G_{01}^{0,n} \\ 2G_{01}^{0,n} & \sum_a G_{a1}^{0,n} \end{pmatrix}, \quad (29)$$

where $\hat{\tau}_1, \hat{\tau}_3$ are Pauli matrices.

3.2 Density of states

Impurity scattering causes the additional contribution to DOS, which can be separated in s -, p - and d -wave parts according to the symmetry [27, 4]

$$\delta g = \sum_{\mu} \delta g_{\mu} = -\frac{1}{\pi} \sum_{\mu} \text{Im}\{\delta G_{\mu}(\omega + i\varepsilon)\} = -\frac{1}{\pi} \sum_{\mu} \frac{d}{d\omega} \arg\{D_{\mu}(\omega)\},$$

where

$$I_{\mu} = 1 - G_{\mu}^0(V_{\mu} + \Phi_{\mu}) \quad (30)$$

is symmetrized denominator of the scattering matrix M (15) and D_{μ} is the determinant of I_{μ} .

According to the Eqs. (20) and (26), one obtains that $\Phi_s = 0$ and $I_s = D_s = 1 - \gamma_s V_{11}$, where γ_s is defined in (23) in terms of the GF G^0 (12) for the superconducting phase and V_{11} is given in Eqs. (9),(10).

In accordance with the Eqs. (20), (A1) one obtains that Φ_p is 2×2 zero matrix, so that Eq. (30) gives the following expression for the p -wave part of the perturbation matrix 'denominator'

$$I_p = (1 - \gamma_p V_{11}) \hat{\tau}_0 \quad \text{with} \quad D_p = \det\{I_p\} = (1 - \gamma_p V_{11})^2,$$

where γ_p is given by (24).

For d -wave symmetry Eqs.(19),(20), (21),(25) lead to the following solution for the Φ matrix

$$\Phi_d = \begin{pmatrix} \Phi_d^{11} & \Phi_d^{12} \\ \Phi_d^{21} & \Phi_d^{22} \end{pmatrix},$$

where its matrix elements are given in the Appendix, (A3)-(A6). Introducing the following denotations

$$\begin{aligned} V'_{00} &= V_{00} + \Phi_d^{11}; & 2V'_{01} &= 2V_{01} + \Phi_d^{12}, \\ 2V'_{10} &= 2V_{01} + \Phi_d^{21}; & V'_{11} &= V_{11} + \Phi_d^{22}, \end{aligned} \quad (31)$$

d -wave part of the perturbation matrix denominator (30) can be written as follows

$$I_d = 1 - G_d^0(V_d + \Phi_d) \equiv \begin{pmatrix} I_d^{11} & I_d^{12} \\ I_d^{21} & I_d^{22} \end{pmatrix},$$

where the corresponding matrix elements are

$$\begin{aligned} I_d^{11} &= 1 - G_{00}^0 V'_{00} - 4G_{01}^0 V'_{10}, & I_d^{12} &= 2G_{00}^0 V'_{01} + 2G_{01}^0 V'_{11}, \\ I_d^{21} &= 2G_{01}^0 V'_{00} + 2 \sum_a G_{a1}^0 V'_{10}, & I_d^{22} &= 1 - 4G_{01}^0 V'_{01} - \sum_a G_{a1}^0 V'_{11}. \end{aligned}$$

Its determinant can be written in the following way

$$\begin{aligned} D_d &= I_d^{11} I_d^{22} - I_d^{12} I_d^{21} = \\ &1 - V'_{00} G_{00}^0 - V'_{11} \sum_a G_{a1}^0 - 4V'_{01} G_{01}^0 - 4V'_{10} G_{01}^0 + \det\{V_d'\} \det\{G_d^0\}, \end{aligned}$$

where the matrix elements $V_d' = V_d + \Phi_d$ and G_d^0 are given in Eqs.(31) and (24), respectively.

3.3 Local density of states

As a consequence of the impurity scattering there appears the following additional contribution to the on-site local density of state (LDOS), which can be also separated in s -, p - and d -wave parts

$$\delta D^{(\mu)}(\omega, i) = -\frac{1}{\pi} \text{Im}\{\delta G_{ii}^{(\mu)}(\omega + i\varepsilon)\}, \quad (32)$$

where symmetrized GF matrix is given in Eqs.(17)-(19).

For s -wave part, one have $M_s = V_{11}/I_s$ and $I_s = 1 - \gamma_s V_{11}$ and γ_s is given in Eq.(23) and

$$\delta G_{ii}^{(s)} = \frac{1}{4} \sum_{aa'} (-1)^{a+a'} G_{ia}^0 G_{a'i}^0 M_s = \frac{1}{4} \left\{ \sum_a (-1)^a G_{ia}^0 \right\}^2 M_s. \quad (33)$$

In particular, for the impurity site $i = 0$ and $i = a_2 = \pm(a_x \pm a_y)$ - the next nearest neighbour to the impurity site, one has $\sum_a (-1)^a G_{ia}^0 = 0$ which causes zero contribution to LDOS of s -wave part at sites 0 and a_2 for any ω , i.e.

$$\delta D^{(s)}(\omega, 0) = \delta D^{(s)}(\omega, a_2) = 0.$$

For sites $i = 1 (a_x)$, $2 (a_y)$, one has nonzero LDOS (32) where

$$\delta G_{11}^{(s)} = \frac{1}{4} \{2G_{12}^0 - G_{11}^0 - G_{13}^0\}^2 M_s,$$

with

$$\delta D^{(s)}(\omega, \pm a_x) = \delta D^{(s)}(\omega, \pm a_y) = -\frac{1}{\pi} \text{Im} \{ \delta G_{11}^{(s)}(\omega + i\varepsilon) \}.$$

For p -wave, one has the following corresponding equations

$$M_p = \frac{V_{11}}{1 - \gamma_p V_{11}} \hat{\tau}_0, \quad (34)$$

and

$$\delta G_{ii}^{(p)} = \frac{V_{11}}{1 - \gamma_p V_{11}} \frac{1}{2} \{ (G_{i1}^0 - G_{i3}^0)^2 + (G_{i2}^0 - G_{i4}^0)^2 \}.$$

In particular, for the site $i = 0$, one has $G_{01}^0 = G_{03}^0 = G_{02}^0 = G_{04}^0$ and $\Delta G_{00}^p = 0$, which causes zero contribution to LDOS of p -wave part at 0 site for any ω value, i.e. $\delta D^{(p)}(\omega, 0) = 0$.

For sites $i = 1, 2$, one has

$$\delta G_{11}^{(p)} = \frac{V_{11}}{1 - \gamma_p V_{11}} \frac{1}{2} (G_{11}^0 - G_{13}^0)^2,$$

and for site $i = a_2 = \pm(a_x \pm a_y)$ one has

$$\delta G_{a_2 a_2}^{(p)} = \frac{V_{11}}{1 - \gamma_p V_{11}} (G_{a_2 1}^0 - G_{a_2 3}^0)^2,$$

which leads to corresponding nonzero values for LDOS for p -wave part at the sites 1, 2 and a_2

$$\delta D^{(p)}(\omega, \pm a_x) = \delta D^{(p)}(\omega, \pm a_y) = -\frac{1}{\pi} \text{Im} \{ \delta G_{11}^{(p)}(\omega + i\varepsilon) \}$$

and

$$\delta D^{(p)}(\omega, a_2) = -\frac{1}{\pi} \text{Im} \left\{ \delta G_{a_2 a_2}^{(p)}(\omega + i\varepsilon) \right\},$$

respectively. For d -wave, one has

$$M_d = V'_d I_d^{-1} = \frac{1}{D_d} \begin{pmatrix} \tilde{M}_d^{11} & \tilde{M}_d^{12} \\ \tilde{M}_d^{21} & \tilde{M}_d^{22} \end{pmatrix}, \quad (35)$$

where

$$\begin{aligned} \tilde{M}_d^{11} &= V'_{00} - d_{00} V'^2_{00} - 2d_{01} V'_{10} V'_{00} + 2d_{01} V'_{01} V'_{00} + 4d_{11} V'_{01} V'_{10}, \\ \tilde{M}_d^{12} &= 2V'_{00} d_{00} V'^2_{01} + d_{01} V'_{11} V'_{00} + 2V'_{01} - (2V'_{01})^2 d_{10} - 2d_{11} V'_{01} V'_{11}, \\ \tilde{M}_d^{21} &= 2V'_{10} - 2d_{00} V'^2_{10} V'_{00} - (2V'_{10})^2 d_{01} + d_{10} V'_{11} V'_{00} + 2d_{11} V'_{11} V'_{10}, \\ \tilde{M}_d^{22} &= 2V'_{00} d_{10} V'^2_{10} + V'_{11} - 2d_{10} V'_{01} V'_{11} - d_{11} (V'_{11})^2, \end{aligned}$$

and

$$\delta G_{ii}^{(d)} = \frac{1}{D_d} \left\{ \tilde{M}_d^{11} (G_{0i}^0)^2 + \frac{1}{2} (\tilde{M}_d^{12} + \tilde{M}_d^{21}) G_{i0}^0 \sum_a G_{ai}^0 + \frac{1}{4} \tilde{M}_d^{22} \sum_{aa'} G_{ia}^0 G_{a'i}^0 \right\},$$

where

$$\sum_{aa'} G_{ia}^0 G_{a'i}^0 = \sum_a (G_{ai}^0)^2 + 2G_{1i}^0 \sum_a G_{ai}^0 + 2G_{2i}^0 (G_{3i}^0 + G_{4i}^0) + 2G_{3i}^0 G_{4i}^0.$$

In particular, for the impurity site $i = 0$ one has $\sum_a G_{a0}^0 = 4G_{01}^0$ and $\sum_{aa'} G_{0a}^0 G_{a'0}^0 = 18(G_{01}^0)^2$, so that one obtains

$$\delta G_{00}^{(d)} = \frac{1}{D_d} \left\{ \tilde{M}_d^{11} (G_{00}^0)^2 + 2(\tilde{M}_d^{12} + \tilde{M}_d^{21}) G_{00}^0 G_{01}^0 + \frac{9}{2} \tilde{M}_d^{22} (G_{01}^0)^2 \right\},$$

with

$$\delta D^{(d)}(\omega, 0) = -\frac{1}{\pi} \text{Im} \left\{ \delta G_{00}^{(d)}(\omega + i\varepsilon) \right\}.$$

For the $i = 1, 2$ sites, one has

$$\begin{aligned} \delta G_{11}^{(d)} &= \\ & \frac{1}{D_d} \left\{ \tilde{M}_d^{11} (G_{01}^0)^2 + \frac{1}{2} (\tilde{M}_d^{12} + \tilde{M}_d^{21}) G_{01}^0 (G_{11}^0 + 2G_{12}^0 + G_{13}^0) + \frac{1}{4} \tilde{M}_d^{22} \sum_{aa'} G_{1a}^0 G_{a'1}^0 \right\}, \end{aligned}$$

with

$$\delta D^{(d)}(\omega, \pm a_x) = \delta D^{(d)}(\omega, \pm a_y) = -\frac{1}{\pi} \text{Im} \left\{ \delta G_{11}^{(d)}(\omega + i\varepsilon) \right\}.$$

And for the $i = a_2$, one has

$$\begin{aligned} \sum_a G_{aa_2}^0 &= 2(G_{1a_2}^0 + G_{3a_2}^0), \\ \sum_{aa'} G_{a_2a}^0 G_{a'a_2}^0 &= 6(G_{1a_2}^0)^2 + 4(G_{3a_2}^0)^2 + 4G_{1a_2}^0 G_{3a_2}^0 + 4G_{2a_2}^0 G_{3a_2}^0, \end{aligned}$$

which are contained in the following expression

$$\delta G_{a_2a_2}^{(d)} = \frac{1}{D_d} \left\{ \tilde{M}_d^{11} (G_{0a_2}^0)^2 + (\tilde{M}_d^{12} + \tilde{M}_d^{21}) G_{0a_2}^0 (G_{1a_2}^0 + G_{3a_2}^0) + \frac{1}{4} \sum_{aa'} G_{a_2a}^0 G_{a'a_2}^0 \right\},$$

with

$$\delta D^{(d)}(\omega, a_2) = -\frac{1}{\pi} \text{Im} \left\{ \delta G_{a_2a_2}^{(d)}(\omega + i\varepsilon) \right\}.$$

3.4 Host lattice Green functions

To study DOS and LDOS one needs the zero-order GF for normal phase $G_{ij}^{0,n}(\omega)$ and for superconducting phase $G_{ij}^0(\omega)$. The normal phase GF $G_{ij}^{0,n}(\omega)$ obeys the following equations [4]

$$\sum_a G_{a1}^{0,n}(\omega) = 4\omega G_{01}^{0,n}(\omega), \quad G_{01}^{0,n}(\omega) = \omega G_{00}^{0,n}(\omega) - 1$$

where

$$G_{00}^0(\omega) = \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{\omega - \varepsilon(\mathbf{q})},$$

where the quasiparticle spectrum in normal phase is given by $\varepsilon(\mathbf{q}) = \gamma(\mathbf{q})$, $\gamma(\mathbf{q}) = (1/2)(\cos q_x + \cos q_y)$, where the energy is measured in units of the half bandwidth $w = 4t$ and we take $\tilde{\varepsilon} = 0$.

For the superconducting phase, the zero-order normal GF $G_{ij}^0(\omega)$ can be calculated using the Fourier transformation

$$G_{ij}^0(\omega) = \frac{1}{N} \sum_{\mathbf{q}} G^0(\mathbf{q}, \omega) \cos \mathbf{q}(\mathbf{i} - \mathbf{j}). \quad (36)$$

The corresponding host lattice GF in $\{\mathbf{q}\}$ -representation can be written as follows

$$G^0(\mathbf{q}, \omega) = \frac{\omega + \varepsilon(\mathbf{q})}{\omega^2 - E_\sigma^2(\mathbf{q})} = u_{\mathbf{q}}^2 \frac{1}{\omega - E_\sigma(\mathbf{q})} + v_{\mathbf{q}}^2 \frac{1}{\omega + E_\sigma(\mathbf{q})}. \quad (37)$$

where we introduce the quasiparticle energy $E_\sigma(\mathbf{q}) = \sqrt{\varepsilon(\mathbf{q})^2 + \Delta_\sigma(\mathbf{q})^2}$ and the Bogoliubov parameters

$$u_{\mathbf{q}}^2 = \frac{1}{2} \left(1 + \frac{\varepsilon(\mathbf{q})}{E_\sigma(\mathbf{q})} \right); \quad v_{\mathbf{q}}^2 = \frac{1}{2} \left(1 - \frac{\varepsilon(\mathbf{q})}{E_\sigma(\mathbf{q})} \right).$$

The superconducting gap $\Delta_\sigma(\mathbf{q})$ obeys the following equation

$$\Delta_\sigma(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{q}} J(\mathbf{k} - \mathbf{q}) \frac{\Delta_\sigma(\mathbf{q})}{2E_\sigma(\mathbf{q})} \tanh \left(\frac{E_\sigma(\mathbf{q})}{2T} \right),$$

with $J(\mathbf{q}) = 4J\gamma(\mathbf{q})$. Solution of the gap equation for the d -wave pairing is analyzed in a number of papers, see e.g., [21]-[24].

4 Conclusions

In the present paper we considered the microscopical model for the Zn-doped CuO_2 plane [3] and generalize the calculations of the electron spectrum [4] to the superconducting phase. Applying the projection technique in the equation of motion method for the normal and anomalous Green functions (GF), we obtained the corresponding \mathcal{T} -scattering matrix. As scattering potential, in addition to the diagonal V elements of the perturbation matrix (5),(9), it contains also the ω -dependent part $\Phi(\omega)$, given by Eq.(16), which has the off-diagonal element of the perturbation matrix (5),(10). This ω -dependent perturbation was not considered in earlier investigations [9]-[17].

Performing the symmetry analysis, in Section 4 we fully took into account the d -symmetry of the wave functions at the Cu-sites of the host lattice, that resulted in special forms for the $\mu = (s, p, d)$ symmetry of the wave functions [4], partial scattering potentials V_μ, ϕ_μ (21)(22), scattering matrix M_μ (33),(34),(35) and Φ_μ (A4)-(A7) and GF (23)-(29). In such a way, we derived the analytical expressions for the total (DOS) and local (LDOS) density of states, separated to s -, p - and d -wave contributions.

The ω -dependences of these expressions are given through zero-order GF in the superconducting phase and for d -symmetry also for the GF in the normal phase. It can be calculated using the Fourier transformation (36) and known corresponding Fourier transforms $G^0(\mathbf{q}, \omega)$ in (37). Numerical calculation can be greatly simplified by using corresponding analytical forms for Green functions in terms of the elliptic integrals [4] and it will be given elsewhere. One could expect that for different ω values (or bias voltage in the experiments with scanning tunneling microscope $\omega = eV$), different partial contributions of s -, p -, d -symmetry will dominate in measured LDOS and DOS. Such separate contributions also were not considered in [9]-[17]. Finally, we stress that our calculation were performed without fitting parameters, contrary to phenomenological approaches in [9]-[17].

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Appendix

Rectangular T_μ -matrices are columns of the corresponding unitary matrix (see [4] for details), i.e. have the following form

$$T_s = \frac{1}{2} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}; \quad T_p = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \\ -1 & 0 \\ 0 & -1 \end{pmatrix}; \quad T_d = \begin{pmatrix} 1 & 0 \\ 0 & 1/2 \\ 0 & 1/2 \\ 0 & 1/2 \\ 0 & 1/2 \end{pmatrix}. \quad (A1)$$

The nonzero submatrix of the perturbation V and ϕ matrices have the following form

$$V = \begin{pmatrix} V_{00} & V_{01} & V_{01} & V_{01} & V_{01} \\ V_{01} & V_{11} & 0 & 0 & 0 \\ V_{01} & 0 & V_{11} & 0 & 0 \\ V_{01} & 0 & 0 & V_{11} & 0 \\ V_{01} & 0 & 0 & 0 & V_{11} \end{pmatrix}, \quad \phi = \Delta_{01}^{\sigma} \begin{pmatrix} 0 & -1 & 1 & -1 & 1 \\ -1 & -\theta & 0 & 0 & 0 \\ 1 & 0 & \theta & 0 & 0 \\ -1 & 0 & 0 & -\theta & 0 \\ 1 & 0 & 0 & 0 & \theta \end{pmatrix}, \quad (A2)$$

where $\theta = 2t/J$ and the matrix elements V_{ij} are given in the Eq. (9).

The elements of the d -wave part of the ω -dependent perturbation are as follows

$$\begin{aligned} \Phi_d^{11} &= -4\Delta_{01}^2 \{8G_{01}^{0,n}(-\omega) \\ &\times V_{01} \sum_a G_{a1}^{0,n}(-\omega) + 4[G_{01}^{0,n}(-\omega)]^2 V_{00} + V_{11} [\sum_a G_{a1}^{0,n}(-\omega)]^2\}, \quad (A4) \end{aligned}$$

$$\begin{aligned} \Phi_d^{12} &= -8\Delta_{01}^2 \{V_{00}G_{01}^{0,n}(-\omega)G_{00}^{0,n}(-\omega) + 4V_{01}[G_{01}^{0,n}(-\omega)]^2 + V_{01}G_{00}^{0,n}(-\omega) \\ &\times \sum_a G_{a1}^{0,n}(-\omega) + V_{11} \sum_a G_{a1}^{0,n}(-\omega)G_{01}^{0,n}(-\omega)\}, \quad (A5) \end{aligned}$$

$$\begin{aligned} \Phi_d^{21} &= -16\phi_{01}\Delta_{01}G_{a1}^{0,n}(-\omega) - 8\Delta_{01}^2 \{V_{00}G_{01}^{0,n}(-\omega)G_{00}^{0,n}(-\omega) + V_{01}G_{00}^{0,n}(-\omega) \times \\ &\sum_a G_{a1}^{0,n}(-\omega) + 4V_{01}[G_{01}^{0,n}(-\omega)]^2 + V_{11}G_{01}^{0,n}(-\omega) \sum_a G_{a1}^{0,n}(-\omega)\}, \quad (A6) \end{aligned}$$

$$\begin{aligned} \Phi_d^{22} &= -4\Delta_{01}^2 \{8V_{01}G_{00}^{0,n}(-\omega)G_{01}^{0,n}(-\omega) + V_{00}[G_{00}^{0,n}(-\omega)]^2 + 4V_{11}[G_{01}^{0,n}(-\omega)]^2\}. \quad (A7) \end{aligned}$$

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Ковачевич Ж., Плакида Н. М., Хайн Р.
Резонансные состояния в высокотемпературных
сверхпроводниках с примесями

E17-2002-203

Предложена микроскопическая теория резонансных состояний для плоскости CuO_2 с примесями Zn в сверхпроводящей фазе в рамках эффективной t - J -модели. В предложенной модели, выведенной из p - d -модели, примеси Zn рассматриваются как вакансии d -состояний на узлах Cu. В сверхпроводящей фазе дополнительно к статическому возмущению за счет вакансии появляется динамический вклад, в результате чего матрица возмущений становится частотно-зависимой. На основе метода функций Грина от операторов Хаббарда вычислена локальная плотность электронных состояний, имеющих d -, p - и s -симметрию.

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Kovačević Ž., Plakida N. M., Hayn R.
Resonant States in High-Temperature Superconductors
with Impurities

E17-2002-203

A microscopic theory of resonant states for the Zn-doped CuO_2 plane in superconducting phase is formulated within the effective t - J model. In the model derived from the original p - d model Zn impurities are considered as vacancies for the d states on Cu sites. In the superconducting phase in addition to the local static perturbation induced by the vacancy a dynamical perturbation appears which results in frequency-dependent perturbation matrix. By employing the T -matrix formalism for the Green functions in terms of the Hubbard operators the local density of electronic states with d -, p - and s -symmetry is calculated.

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

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