The Hole Excitation Spectrum in CuO_2 Plane

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Abstract. The hole spectrum $e(\vec{k})$ that is studied in the framework of Emery model is shown to be strongly dependent on direct $O-O$ hopping h and on doping n, the latter being modeled through the frustration α in Cu spin subsystem. The $e(\vec{k})$ demonstrates non-rigid-band behavior, its minimum value and band bottom position are changed with doping.

The CuO_2 plane hole motion is studied in the framework of strong coupling limit of Emery model with the Hamiltonian [1,2]:

$$\hat{H} = \tau \sum_{\vec{R},\vec{a}_1,\vec{a}_2,\sigma} Z^{\sigma_1\sigma_2}_{\vec{R}} c^{+}_{\vec{R}+\vec{a}_2,\sigma_2} c_{\vec{R}+\vec{a}_1,\sigma_1} - h \sum_{\vec{R},\vec{a}=\vec{a}_x,\vec{a}_y,\vec{b},\sigma} c^{+}_{\vec{R}+\vec{a},\sigma} c_{\vec{R}+\vec{a}+\vec{b},\sigma} + \hat{H}_J \quad (1)$$

$$\hat{H}_J = \hat{J}_1 + \hat{J}_2,\ \hat{J}_1 = J \sum_{\vec{R},\vec{a}} \hat{S}_{\vec{R}} \hat{S}_{\vec{R}+2\vec{a}},\ \hat{J}_2 = \alpha J \sum_{\vec{R},\vec{b}} \hat{S}_{\vec{R}} \hat{S}_{\vec{R}+2\vec{b}}$$

here $\vec{R}+\vec{a}$ are four vectors of O sites nearest to Cu site $\vec{R}$; $\vec{b}$ — nearest neighbor vectors for the oxygen sublattice; $Z^{\sigma_1\sigma_2}_{\vec{R}}$ are Hubbard projection operators for Cu sites.

We believe that the influence of finite but small doping may be modeled by including the frustration $\hat{J}_2$ in $Cu-Cu$ spin interaction.

It was earlier shown [2] that the carrier spectrum can be obtained by variational approach in the framework of the concept of magnetic polaron. The variational ansatz is:

$$\theta_{\vec{R}} = \tfrac{1}{2} \sum_{\vec{a}=\pm\vec{a}_x,\pm\vec{a}_y} \beta_{\vec{a}} (c^{+}_{\vec{R}+\vec{a}_2,+1} Z^{--}_{\vec{R}} - c^{+}_{\vec{R}+\vec{a}_2,-1} Z^{+-}_{\vec{R}}) |G\rangle;\ |\beta_{\vec{a}}| = 1 \quad (2)$$

where $|G\rangle$— the singlet wave function of Cu spin subsystem, which is described by $\hat{H}_J$. The properties of the state $|G\rangle$ for various values of α are discussed in [3] in detail.

In the simplest approximation $\beta_{\vec{a}} = 1$ the spectrum can be found analytically ($h = 0$):

$$e(\vec{k}) = -3.5\tau - [4J(A_3 + \alpha A_4) + (4.5A_1\tau - A_3 J)\gamma_{\vec{k}} + A_2\tau(1 - 4\gamma^2_{\vec{k}})][1 + A_1\gamma_{\vec{k}}]^{-1} \quad (3)$$

$$A_1 = 0.25 + K_1;\ A_2 = 0.125 - K_1 + 0.5K_2;\ A_3 = 2K_1;\ A_4 = 2K_2;\ K_1 = \langle \hat{S}_{\vec{R}} \hat{S}_{\vec{R}+2a} \rangle;$$

$$K_2 = \langle \hat{S}_{\vec{R}} \hat{S}_{\vec{R}+2a_1+2a_2} \rangle;\ \langle \ldots \rangle \equiv \langle G| \ldots |G\rangle;\ \gamma_{\vec{k}} \equiv 0.5(\cos 2k_x a + \cos 2k_y a)$$

For $\alpha = 0,\ 0.2$ the correlations are $K_1 = -0.324,\ -0.297$; $K_2 = 0.221,\ 0.169$ respectively. The spectrum (3) reaches its minimum at line $\gamma_{\vec{k}} = const \approx 0$, which leads to a pronounced peak in the density of states (DOS) near the band bottom.

The results of $e(\vec{k})$ calculations with the general ansatz (2) are shown in fig. 1 a,b. To allow for direct hopping $h \neq 0$ term we add the functions $c^{+}_{\vec{R}+\vec{a},+1}|G\rangle$ to the basis set (see fig.2).

As we see from Fig. 1, 2 the $e(\vec{k})$ minimum position and Fermi surface topology strongly depend on α and h values. The DOS has a sharp peak near the band bottom. The inclusion of frustration enhances the spectrum anisotropy and DOS peak intensity. Let us note that the frustration shifts the spectrum $e(\vec{k})$ downward the energy axes. If we take into account that the increase of α is roughly proportional to the doping n, then the Fermi energy shift with doping is much less in magnitude then the shift predicted by rigid band model. Moreover the shift can have an opposite sign.

We see also that the general shape of the Fermi surface qualitatively coincides with

the numerical results on $t - J$ model: the increase of doping changes its hole character to the electronic one.

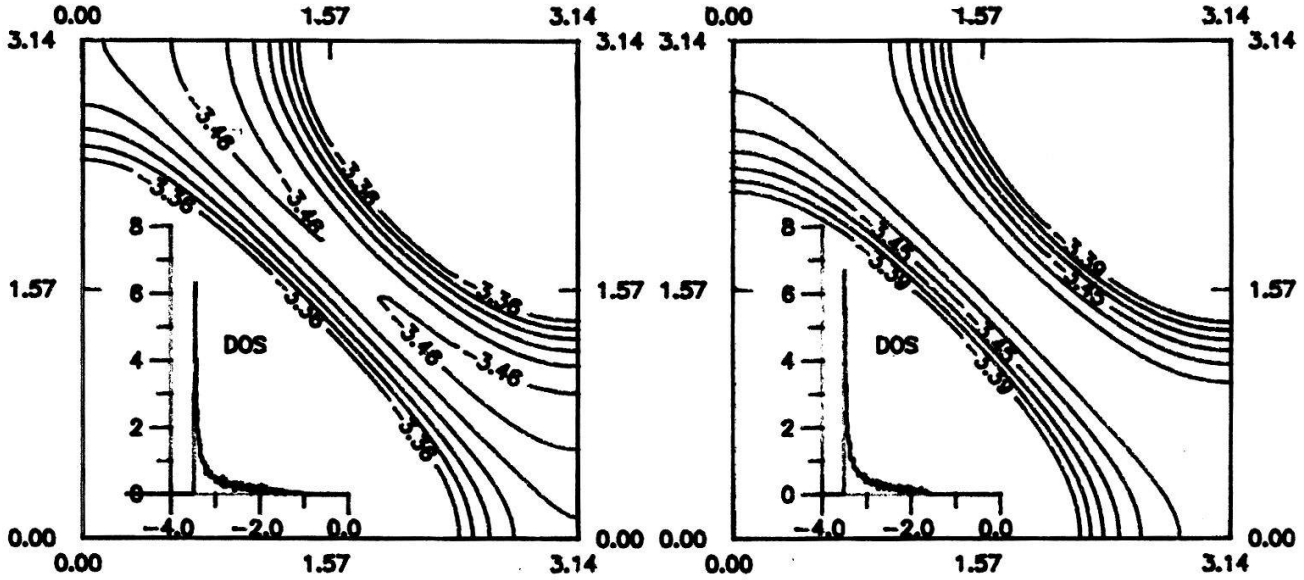

Fig.1 Equienergetic lines $e(\vec{k}) = const$, $O - O$ hopping via Cu $\tau = 1$, direct hopping $h = 0$. a) Without frustration, $\alpha = 0$. b) For $\alpha = 0.2$. Density of states is plotted in the inserts.

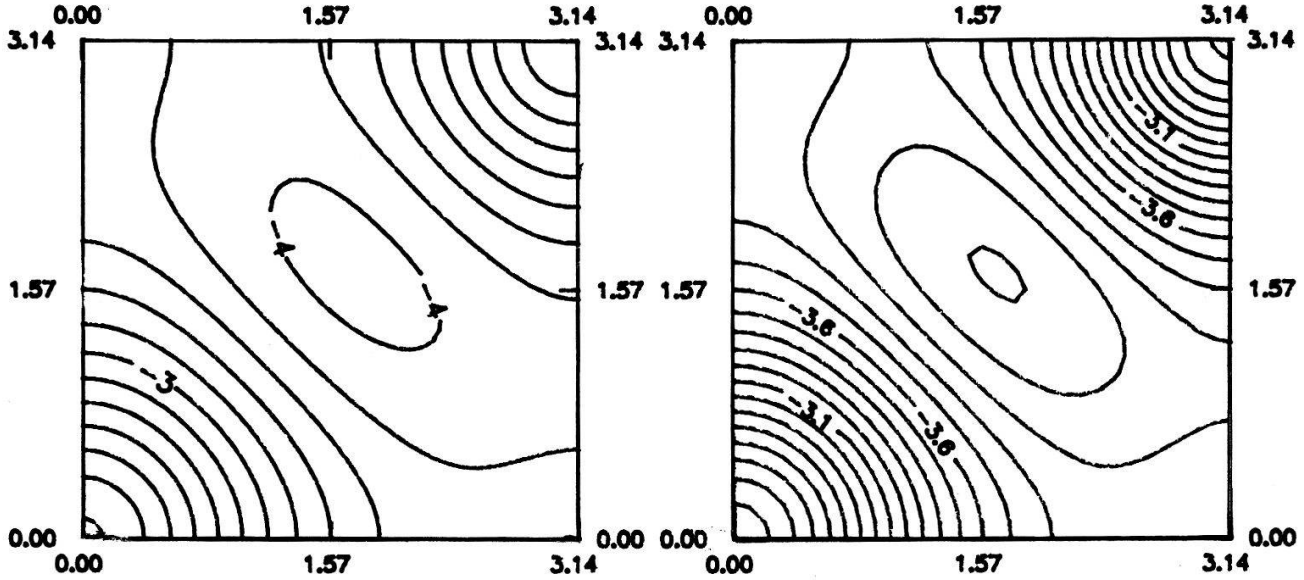

Fig.2 Equienergetic lines $e(\vec{k}) = const$ $(\tau = 1)$ for direct $O - O$ hopping $h = 0.3$. a) Without frustration, $\alpha = 0$. b) For $\alpha = 0.2$.

References

[1] V.J.Emery and G.Reiter, Phys. Rev. B38, 4547 (1988)
[2] A.F.Barabanov et al., Superconductivity: Phys. Chem. Tech. 3, 8 (1990); Sov. Phys. JETP 69(2), 371 (1989)
[3] A.F.Barabanov et al. Int. J. Mod. Phys. B4, 2319 (1990)
[4] V.Stephan and P.Horsch, Phys. Rev. Lett. 66, 2258 (1991)