Mechanism of hole attraction in the extended Hubbard model

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The expansion in the Cu-O hybridization energy, t, usually used for the simplification of the extended Hubbard Hamiltonian, is shown to meet with difficulties for the known parameters of CuO_2 planes of cuprate perovskites. An expansion in a power series in λt, $\lambda \approx 0.1$, is suggested, which is applicable for these values of parameters and in which the Hubbard repulsion and the Cu-O hybridization are considered on an equal footing. A Hamiltonian obtained with the help of the expansion for the lower part of the energy spectrum, is equivalent to the t-J Hamiltonian and the corresponding states are some generalizations of the Zhang-Rice singlets. The Hamiltonian contains terms describing a static attraction between holes and for reasonable sets of parameters the attraction is approximately equal to a half of the superexchange constant.

The extended Hubbard model[1] is widely accepted for the description of CuO_2 planes of high-T_c perovskite superconductors. The main demand to any model claiming such description is the existence of a superconducting pairing mechanism. And, indeed, a number of computer experiments in different versions of the model in small lattices indicates the existence of such a mechanism connected with an attraction between holes (see, e.g., Ref. 2). However, it is not easy to elucidate the role of different terms of the Hamiltonian and different processes in the results of these experiments. Besides, sometimes the influence of a comparatively small lattice size also remains unrevealed. As a result, there is still no generally accepted point of view of the attraction mechanism.

In this Brief Report it is shown that even the simplest version of the extended Hubbard model, containing the Cu-O hybridization and the Hubbard repulsion on copper, can explain the attraction for an infinite lattice. With some modifications the mechanism is retained in model generalizations, which gives grounds for hoping that at least a part of the attractive potential between holes in CuO_2 planes is connected with this mechanism. In some respect it is similar to the bond-breaking mechanism of the static hole attraction in the t-J model.[3] Moreover, it is shown that in a wide range of material parameters, including the ones presumably realized in La_2CuO_4, the considered model can be reduced to the one-band t-J model and the corresponding hole states, forming the low-energy part of the spectrum, are some generalizations of Zhang-Rice singlets.[4]

The Hamiltonian for the model is given by

$$H = U\sum_{\mathbf{m}} n_{\mathbf{m},+1}n_{\mathbf{m},-1} + \frac{\Delta}{2}\sum_{\mathbf{m}\delta} n_{\mathbf{m}+\delta} + t\sum_{\mathbf{m}\delta\sigma}(d^{\dagger}_{\mathbf{m}\sigma}p_{\mathbf{m}+\delta,\sigma} + \text{H.c.}), \tag{1}$$

where $d^{\dagger}_{\mathbf{m}\sigma}$ and $p^{\dagger}_{\mathbf{m}+\delta,\sigma}$ are the creation operators of electrons in the $3d_{x^2-y^2}$ orbitals of copper and the $2p_\sigma$ orbitals of oxygen, respectively, with spin $\sigma = \pm 1$; $\Delta > 0$ is the Cu-O promotion energy; U is the Hubbard repulsion on copper; t is the Cu-O hybridization; $n_{\mathbf{m}\sigma} = d^{\dagger}_{\mathbf{m}\sigma}d_{\mathbf{m}\sigma}$, $n_{\mathbf{m}+\delta} = \sum_\sigma p^{\dagger}_{\mathbf{m}+\delta,\sigma}p_{\mathbf{m}+\delta,\sigma}$, $\delta = (\pm a/2, 0)$, $(0, \pm a/2)$; and a is the copper lattice spacing. The Hubbard repulsion on oxygen is supposed to be incorporated by the Hartree approximation.

The values of parameters usually cited in the literature for La_2CuO_4 are as follows: $U \approx 8 - 10\,\text{eV}$, $\Delta \approx 1$–$5\,\text{eV}$, and $|t| \approx 1$–1.5 eV.[5] Because of the smallness of $|t|$, the usual way for the simplification of the Hamiltonian consists in the usage of some version of perturbation theory with an expansion in t (and in Δ, if $\Delta \approx t$). This procedure gives effective Hamiltonians which are some generalizations of the t-J Hamiltonian.[6,7] However, an analysis of these series shows that for the values of parameters cited above these expansions meet with the following difficulty. Because of large numeric factors, terms of higher order appear to be comparable to, or even larger than, the lower-order terms. In particular, at $U - \Delta$, $\Delta \gg |t|$, when the expansion starts from second-order terms, one of these terms describing the interaction of spins on copper and surrounding oxygen sites was supposed to be responsible for the formation of the Zhang-Rice singlets as the lowest hole states of the energy spectrum.[4] However, among the fourth-order terms there is an analogous term with the coefficient $-64t^4[\Delta^{-3}+(U-\Delta)^{-3}+(U-\Delta)^{-2}\Delta^{-1}+(U-\Delta)^{-1}\Delta^{-2}]$ which is larger in absolute value than the coefficient in the second-order term $8t^2[\Delta^{-1} + (U-\Delta)^{-1}]$ for the parameter values mentioned. Besides, the terms have opposite signs, which makes questionable the results of Ref. 4. In this approach terms of various orders contribute to the interaction of holes. Under such conditions it is practically impossible to elucidate the sign of the interaction. The difficulty is certainly connected with the fact that the hybridization is actually not small.

To overcome the difficulty let us represent Hamiltonian (1) in the form

$$H = \sum_{\mathbf{m}} H_{\mathbf{m}} + 2t\lambda_{\mathbf{a}}\sum_{\mathbf{ma}\sigma}(d^{\dagger}_{\mathbf{m}\sigma}\phi_{\mathbf{m}+\mathbf{a},\sigma} + \text{H.c.}),$$
$$H_{\mathbf{m}} = Un_{\mathbf{m},+1}n_{\mathbf{m},-1} + \Delta\sum_\sigma \phi^{\dagger}_{\mathbf{m}\sigma}\phi_{\mathbf{m}\sigma} + 2t\lambda_0\sum_\sigma(d^{\dagger}_{\mathbf{m}\sigma}\phi_{\mathbf{m}\sigma} + \text{H.c.}) \tag{2}$$

$\phi_{\mathbf{m}\sigma}$ is the Fourier transform of the operator $\phi_{\mathbf{k}\sigma} = (\beta_{\mathbf{k}}/2\sqrt{N})\sum_{\mathbf{m}\delta}\exp(i\mathbf{k}\cdot\mathbf{m})p_{\mathbf{m}+\delta,\sigma}$;[4] the factor $\beta_{\mathbf{k}} = \{1+[\cos(k_x a)+\cos(k_y a)]/2\}^{-1/2}$ ensures the fulfillment of the commutation relations for the Fermi operators, $\lambda_{\mathbf{m}} = N^{-1}\sum_{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{m})\beta_{\mathbf{k}}^{-1}$, $\lambda_0 \approx 0.96$, $\lambda_{\mathbf{a}} \approx 0.14$, $\mathbf{a}$ being one of the vectors of primitive translations; other components of $\lambda_{\mathbf{m}}$ are small and, therefore, omitted. The operators $\phi_{\mathbf{m}\sigma}$ do not form a complete set of oxygen operators for CuO_2 planes; however, the complementary operators form a conservative subsystem and are omitted in (2). It is clear that the one-site part of the Hamiltonian should be taken as the zero-order Hamiltonian and the two-site part as perturbation in the perturbation expansion. The characteristic energy scales of these two parts of the Hamiltonian are $2t\lambda_0 \approx 2\,\mathrm{eV}$ and $2t\lambda_{\mathbf{a}} \approx 0.3$ eV, respectively. Thus the applicability conditions for the perturbation theory expansion are much better than for the expansion in powers in t. Actually, the former expansion is applicable for the entire range of the parameters cited above. Another merit of the expansion is the possibility of limiting it to first- and second-order terms, while to obtain relevant terms the usual expansion has to be prolonged up to fourth-order terms.

Let us introduce the following notation for the relevant eigenfunctions of $H_{\mathbf{m}}$:

$$|\mathbf{m}1s\sigma\rangle = (a_{1s1}\phi^{\dagger}_{\mathbf{m}\sigma} + a_{1s2}d^{\dagger}_{\mathbf{m}\sigma})|v_{\mathbf{m}}\rangle,$$

$$|\mathbf{m}2s\rangle = \left[a_{2s1}\frac{1}{\sqrt{2}}(\phi^{\dagger}_{\mathbf{m},+1}d^{\dagger}_{\mathbf{m},-1} - \phi^{\dagger}_{\mathbf{m},-1}d^{\dagger}_{\mathbf{m},+1}) + a_{2s2}\phi^{\dagger}_{\mathbf{m},-1}\phi^{\dagger}_{\mathbf{m},+1} + a_{2s3}d^{\dagger}_{\mathbf{m},-1}d^{\dagger}_{\mathbf{m},+1}\right]\Big|v_{\mathbf{m}}\Big\rangle,$$

$$|\mathbf{m}2\rangle = \frac{1}{\sqrt{2}}(\phi^{\dagger}_{\mathbf{m},+1}d^{\dagger}_{\mathbf{m},-1} + \phi^{\dagger}_{\mathbf{m},-1}d^{\dagger}_{\mathbf{m},+1})|v_{\mathbf{m}}\rangle,\ |\mathbf{m}2\sigma\rangle = \phi^{\dagger}_{\mathbf{m}\sigma}d^{\dagger}_{\mathbf{m}\sigma}|v_{\mathbf{m}}\rangle, \tag{3}$$

$$|\mathbf{m}3s\sigma\rangle = (a_{3s1}\phi^{\dagger}_{\mathbf{m}\sigma}\phi^{\dagger}_{\mathbf{m},-\sigma}d^{\dagger}_{\mathbf{m}\sigma} + a_{3s2}\phi^{\dagger}_{\mathbf{m}\sigma}d^{\dagger}_{\mathbf{m},-\sigma}d^{\dagger}_{\mathbf{m}\sigma})|v_{\mathbf{m}}\rangle,$$

$$|\mathbf{m}4\rangle = \phi^{\dagger}_{\mathbf{m},-1}\phi^{\dagger}_{\mathbf{m},+1}d^{\dagger}_{\mathbf{m},-1}d^{\dagger}_{\mathbf{m},+1}|v_{\mathbf{m}}\rangle,$$

where $|v_{\mathbf{m}}\rangle$ is the site vacuum state. The eigenenergies of the two-electron triplets $|\mathbf{m}2\rangle$, $|\mathbf{m}2\sigma\rangle$, E_{2t}, and of the four-electron state $|\mathbf{m}4\rangle$, E_4, are equal to Δ and $U+2\Delta$, respectively. The eigenenergies E_{ns} of $H_{\mathbf{m}}$ and the amplitudes a_{nsi} for other eigenfunctions (3) are found from the corresponding systems of two (one- and three-electron functions) and three (two-electron functions) linear equations. In this notation, n, s, and i are the number of electrons in the state, the solution, and the component numbers, respectively. For $n = 2, 3$ the solutions with $s = 1$ are the corresponding ground states. For the mentioned values of parameters the degenerate ground state of the zero-order Hamiltonian consists of different products of these two site states.

Apparently the state $|\mathbf{m}2, s = 1\rangle$ is the generalization of the Zhang-Rice singlet state.[4] The latter is obtained from the former if a_{212} and a_{213} are set to be equal to zero. For the considered values of parameters these coefficients are not small, which leads to a marked difference between the two states.

It is easy to express Hamiltonian (2) in terms of vectors (3). The application of the operator perturbation theory[8] to it gives the effective Hamiltonian acting in the subspace of the ground states of the zero-order Hamiltonian and describing the low-energy part of the spectrum,

$$\begin{aligned}
H_{\mathrm{eff}} = {} & 2t\lambda_{\mathbf{a}}\alpha_{411}\sum_{\mathbf{ma}\sigma}|\mathbf{m}+\mathbf{a},31\sigma\rangle\langle\mathbf{m}+\mathbf{a},21||\mathbf{m}21\rangle\langle\mathbf{m}31\sigma| + \frac{J}{2}\sum_{\mathbf{ma}}\mathbf{s}_{\mathbf{m}}\mathbf{s}_{\mathbf{m}+\mathbf{a}} \\
& - \sum_{\mathbf{ma}}(\gamma_1 n_{\mathbf{m}3}n_{\mathbf{m}+\mathbf{a},3} + \gamma_2 n_{\mathbf{m}3}n_{\mathbf{m}+\mathbf{a},2} + \gamma_3 n_{\mathbf{m}2}n_{\mathbf{m}+\mathbf{a},2}) \\
& - \widetilde{\sum_{\mathbf{maa}'}}\sum_{\sigma\sigma'}\gamma_{4\sigma\sigma'}|\mathbf{m}31\sigma'\rangle\langle\mathbf{m}31\sigma||\mathbf{m}+\mathbf{a}',21\rangle\langle\mathbf{m}+\mathbf{a}',31\sigma'||\mathbf{m}+\mathbf{a},31\sigma\rangle\langle\mathbf{m}+\mathbf{a},21| \\
& - \widetilde{\sum_{\mathbf{maa}'}}\sum_{\sigma\sigma'}\gamma_{5\sigma\sigma'}|\mathbf{m}31,-\sigma'\rangle\langle\mathbf{m}31,-\sigma||\mathbf{m}+\mathbf{a}',21\rangle\langle\mathbf{m}+\mathbf{a}',31\sigma||\mathbf{m}+\mathbf{a},31\sigma'\rangle\langle\mathbf{m}+\mathbf{a},21| \\
& - \widetilde{\sum_{\mathbf{maa}'}}\sum_{\sigma}\gamma_6 n_{\mathbf{m}2}|\mathbf{m}+\mathbf{a}',21\rangle\langle\mathbf{m}+\mathbf{a}',31\sigma||\mathbf{m}+\mathbf{a},31\sigma\rangle\langle\mathbf{m}+\mathbf{a},21|,
\end{aligned} \tag{4}$$

where

$$J = 4(2t\lambda_{\mathbf{a}})^2\left(\sum_s\frac{\alpha_{1s}^2}{E_4+E_{2s}-2E_{31}} - \frac{1}{2}\frac{\alpha_2^2}{E_4+E_{2t}-2E_{31}}\right),$$

$$\gamma_1 = (2t\lambda_{\mathbf{a}})^2\left(\frac{1}{2}\sum_s\frac{\alpha_{1s}^2}{E_4+E_{2s}-2E_{31}} + \frac{3}{4}\frac{\alpha_2^2}{E_4+E_{2t}-2E_{31}}\right),$$

$$\gamma_2 = (2t\lambda_{\mathbf{a}})^2\left(\sum_s\frac{\alpha_{3s}^2}{E_4+E_{1s}-E_{31}-E_{21}} + \widetilde{\sum_{ss'}}\frac{\alpha_{4ss'}^2}{E_{3s}+E_{2s'}-E_{31}-E_{21}} + \frac{3}{2}\sum_s\frac{\alpha_{5s}^2}{E_{3s}+E_{2t}-E_{31}-E_{21}}\right),$$

$$\gamma_3 = 2(2t\lambda_{\mathbf{a}})^2 \sum_{ss'} \frac{\alpha^2_{6ss'}}{E_{3s} + E_{1s'} - 2E_{21}},$$

$$\gamma_{4\sigma\sigma'} = (2t\lambda_{\mathbf{a}})^2 \left(\sum_{s\neq 1} \frac{\alpha^2_{41s}}{E_{2s} - E_{21}} + \frac{1}{2}\sigma\sigma' \frac{\alpha^2_{51}}{E_{2t} - E_{21}} \right),$$

$$\gamma_{5\sigma\sigma'} = (2t\lambda_{\mathbf{a}})^2 \left(\frac{\alpha^2_{51}}{E_{2t} - E_{21}} \delta_{\sigma\sigma'} - \sigma\sigma' \frac{\alpha^2_{11}}{E_4 + E_{21} - 2E_{31}} \right),$$

$$\gamma_6 = (2t\lambda_{\mathbf{a}})^2 \left(\sum_{s} \frac{\alpha^2_{61s}}{E_{31} + E_{1s} - 2E_{21}} - \frac{\alpha^2_{421}}{E_{32} - E_{31}} \right),$$

$$\alpha_{1s} = \frac{1}{\sqrt{2}} a_{2s1} - a_{311}a_{312}(a_{2s2} + a_{2s3}),\ \alpha_2 = a^2_{312} - a^2_{311}, \tag{5}$$

$$\alpha_{3s} = a_{312}\left(\frac{1}{\sqrt{2}} a_{211}a_{1s1} - a_{213}a_{1s2} \right) - a_{311}\left(\frac{1}{\sqrt{2}} a_{211}a_{1s2} - a_{212}a_{1s1} \right),$$

$$\alpha_{4ss'} = \left(\frac{1}{\sqrt{2}} a_{211}a_{3s2} - a_{212}a_{3s1} \right)\left(a_{312}a_{2s'3} - \frac{1}{\sqrt{2}} a_{311}a_{2s'1} \right) + \left(a_{213}a_{3s2} - \frac{1}{\sqrt{2}} a_{211}a_{3s1} \right)\left(\frac{1}{\sqrt{2}} a_{312}a_{2s'1} - a_{311}a_{2s'2} \right),$$

$$\alpha_{5s} = a_{311}\left(\frac{1}{\sqrt{2}} a_{211}a_{3s2} - a_{212}a_{3s1} \right) - a_{312}\left(a_{213}a_{3s2} - \frac{1}{\sqrt{2}} a_{211}a_{3s1} \right),$$

$$\alpha_{6ss'} = \left(\frac{1}{\sqrt{2}} a_{211}a_{3s2} - a_{212}a_{3s1} \right)\left(\frac{1}{\sqrt{2}} a_{211}a_{1s'2} - a_{212}a_{1s'1} \right) + \left(a_{213}a_{3s2} - \frac{1}{\sqrt{2}} a_{211}a_{3s1} \right)\left(\frac{1}{\sqrt{2}} a_{211}a_{1s'1} - a_{213}a_{1s'2} \right),$$

$$n_{\mathbf{m}3\sigma} = |\mathbf{m}31\sigma\rangle\langle\mathbf{m}31\sigma|,\ n_{\mathbf{m}3} = \sum_{\sigma} n_{\mathbf{m}3\sigma},\ n_{\mathbf{m}2} = |\mathbf{m}21\rangle\langle\mathbf{m}21|,$$

$$s^{\sigma}_{\mathbf{m}} = s^x_{\mathbf{m}} + i\sigma s^y_{\mathbf{m}} = |\mathbf{m}31\sigma\rangle\langle\mathbf{m}31, -\sigma|,\ s^z_{\mathbf{m}} = \frac{1}{2}\sum_{\sigma} \sigma n_{\mathbf{m}3\sigma}.$$

The tildes near the sums over $\mathbf{a}$, $\mathbf{a}'$ and over s, s' mean that $\mathbf{a} \neq \mathbf{a}'$ and the term with $s = s' = 1$ is omitted.

The first two terms in the right-hand side of Eq. (4) are the transport and the Heisenberg term of the t-J Hamiltonian written in terms of the Hubbard operators which are built from the vectors of the considered basis $|\mathbf{m}31\sigma\rangle$ and $|\mathbf{m}21\rangle$. The three last terms in (4), describing the conditional hole transport, also resemble the so-called pair-hopping terms sometimes included in the t-J Hamiltonian.[3]

If for a moment the first term in Hamiltonian (4) is neglected, it can be shown that the second and third terms of the Hamiltonian provide a static interaction between holes. The interaction can be elucidated with the following broken-bond arguments in some respect analogous to the ones adduced for explaining the static hole attraction in the t-J model[3]. Two holes on adjacent sites remove seven bonds connecting sites with the site states $|\mathbf{m}31\sigma\rangle$ and introduce six bonds connecting sites with the states $|\mathbf{m}31\sigma\rangle$, $|\mathbf{m}21\rangle$, and a bond connecting sites with the states $|\mathbf{m}21\rangle$. When the holes are far from each other, the respective numbers of the bonds are 8, 8, and 0. The difference in the energies between these two cases is

$$E_B = -J/4 - 2\gamma_1 + 2\gamma_2 - 2\gamma_3. \tag{6}$$

$E_B < 0$ and $E_B > 0$ correspond to attraction and repulsion, respectively, between holes.

The dependences of E_B, J, and $t' = 2t\lambda_{\mathbf{a}}\alpha_{411}$ on Δ at $U = 6\lambda_0 t$ and on U at $\Delta = 2\lambda_0 t$ are shown in Figs. 1 and 2. In the entire range of Δ in Fig. 1 $E_B < 0$ and $|E_B| \approx (0.3 - 0.5)J$. A static attraction close in value is experienced by the holes in the t-J model, if the term $-(J/8)\sum_{\mathbf{ma}} n_{\mathbf{m}} n_{\mathbf{m+a}}$ is included in the t-J Hamiltonian. Together with the above-mentioned identity of the transport and Heisenberg terms and the similarity of the static attraction mechanisms, it means that for the range of parameters presumably realized in cuprate perovskites the extended Hubbard model with Hamiltonian (4) and the t-J model are very close.

From Figs. 1 and 2 it can be seen that E_B may become positive for smaller values of Δ and larger values of U, and the similarity of the two models disappears (the static interaction in the t-J model is always negative). The interaction is mainly determined by the terms proportional to α^2_{11} in J and γ_1, and to α^2_{51} in γ_2 [see (5)]. The first terms are connected with the virtual transitions $|\mathbf{m}31\sigma\rangle + |\mathbf{m}+\mathbf{a}, 31, -\sigma\rangle \rightarrow |\mathbf{m}21\rangle + |\mathbf{m}+\mathbf{a}, 4\rangle$. Their contribution into E_B is always negative, since the configuration with holes on adjacent sites enlarges the number of bonds connecting the three-electron states,

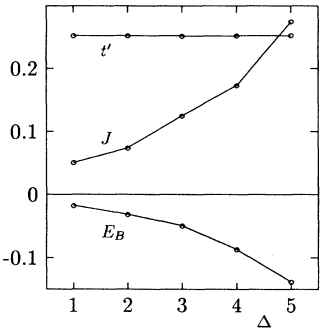

FIG. 1. Dependences of the static interaction energy of holes, E_B, the superexchange constant J, and the effective hopping constant of holes, t', on the Cu-O promotion energy Δ when the Hubbard repulsion on copper $U = 6$. Here and in Fig. 2 the value $\lambda_0 t$ is taken as the unit of energy, $\lambda_0 = 0.96$, and t is the Cu-O hybridization.

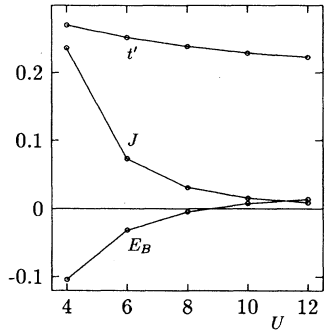

FIG. 2. Dependences of E_B, J, and t' on U at $\Delta = 2$.

the initial states of the transition. The term proportional to α_{51}^2 is connected with the virtual transitions $|\mathbf{m}31\sigma\rangle + |\mathbf{m}+\mathbf{a},21\rangle \rightarrow |\mathbf{m}2\rangle + |\mathbf{m}+\mathbf{a},31\sigma\rangle$ or $|\mathbf{m}2\sigma\rangle + |\mathbf{m}+\mathbf{a},31,-\sigma\rangle$. Its contribution is always positive, as the adjacent arrangement of the holes reduces the number of bonds connecting sites with three and two electrons.

Thanks to the pointed-out similarity of the extended Hubbard and the t-J models for the parameter range of interest, the results obtained for the latter can be transferred to the former. In particular, it can be concluded that the static hole attraction leads to the coupling of holes at least in the region of large and intermediate values of J/t'. Since this conclusion is mainly based on the results obtained on small lattices and the finite-size effect reveals itself apparently in the coupling energy (see Ref. 9 and references therein), an attempt has been undertaken to calculate the energy for an infinite lattice. The calculations employ the spin-wave approximation[10,11] and the Lanczos procedure with selecting the largest wave function components.[11] The procedure gives the lower estimate for the coupling energy. As a preliminary information on the obtained results it can be said that at least in the range $J/t' \gtrsim 1$ and at least for the function of d orbital symmetry with zero wave vector there is a coupling of holes with the coupling energy approximately equal to $|E_B|$.

In conclusion, let us discuss possible limitations of the considered expansion and its connection with earlier results obtained with the help of the expansion in a power series in t. For parameter values close to those of interest there are two regions where the considered expansion fails. The first is determined by the inequality $20|t| \lesssim \Delta$ when the denominators $E_{22}-E_{21}$, $E_{2t}-E_{21}$ in the second-order terms (5) become of the order of $2\lambda_{\mathbf{a}}|t|$. This case has been considered in Ref. 7 where it has been shown that the case cannot be described by the one-band t-J model. The second region is the case $\Delta \approx U$ and the possible failure of the expansion manifests itself in the large value of the second-order quantity J which becomes comparable to, or even larger than, the first-order quantity t' in the region (Figs. 1 and 2). This behavior is connected with a small value of the denominators $E_4 + E_{21} - 2E_{31}$ in J and γ_1.

From the obtained results it can be seen that the lowest hole state has a large admixture of the Zhang-Rice singlet and the first excited hole states are triplets. Thus, in spite of the difficulties mentioned, the expansion in powers in t gives a qualitatively correct description of the one-hole spectrum. However, the quantitative differences may be considerable for the La_2CuO_4 parameter values. For example, at $U = 6\lambda_0 t$ and $\Delta = 3\lambda_0 t$ the formulas $t' = 4t^2\lambda_0\lambda_{\mathbf{a}}[2\Delta^{-1} + (U-\Delta)^{-1}]$ (Ref. 7) and $J = 4t^4(U-\Delta)^{-2}[U^{-1} + (U-\Delta)^{-1}]$,[6,7] obtained from the expansion in t, give $t' = 0.6\lambda_0 t$, $J = 0.26\lambda_0 t$, the values which are more than 2 times larger than those in Fig. 1. Of course, the main defect of the expansion in t lies not in quantitative inaccuracy but in the difficulties on describing the hole interaction in the considered parameter range.

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