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SPIN BIPOLARON IN THE FRAMEWORK OF EMERY MODEL FOR HIGH-Tc COPPER OXIDE SUPERCONDUCTORS.

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The high-Tc oxide compounds discovered recently exhibit a number of interesting physical properties.Two-dimensional antiferromagnetic spin order has been observed in these materials at the oxygen deficiency.This fact can be explained by strong correlation of the spins,situated on Cu sites in the conducting planes of the oxide superconductors.The doping or the oxygen deficiency lead to the occurence of holes,occupying the oxygen p-orbitals according to Emery model.At the small hole concentration they can move along the antiferromagnetic lattice of spins,localized on Cu sites.

We consider two holes situation and describe in what way their behaviour depends on the antiferromagnetic exchange interaction J .It is known that in the framework of Hubbard model with strong on-site Coulomb repulsion a single hole can form spin polaron of the large radius [1] .It is reasonable to admit that two holes with parallel spins(triplet) form the spin bipolaron complex owing to the hole excitations' capability to polarize Cu spin surrounding.Such an excitation was considered in the fenomenological way in [2] .

Here the problem is discussed on the basis of the microscopic approach in the framework of the variational principle.The special kind of wave function is used for such a purpose.The wave function is constructed by generalizing the trial functions proposed in [3,4] over two holes excitation situation (triplet) and then the region of spin bipolaron existance in the framework of Emery model is studied.

In this model the Hamiltonian [3,4] can be easily rewritten by forming the oxygen states transforming as the irreducible representations of the group D_4 .This transformation can be performed by using the matrix B :

$$B = \frac{1}{2}\begin{pmatrix} 1 & 1 & -\sqrt{2} & 0 \\ 1 & -1 & 0 & \sqrt{2} \\ 1 & 1 & \sqrt{2} & 0 \\ 1 & -1 & 0 & -\sqrt{2} \end{pmatrix} \qquad (1)$$

where every column determines the basis of the representations A_1, B_1, E of the group D_4 .

Finally, the Hamiltonian has the following form:

$$H = H_t + H_J \quad ; \quad H_J = J \sum_{i_1 i_2} \vec{S}_{i_1} \vec{S}_{i_2}$$

$$H_t = 2t \sum_{j \in A} a^{+(1)}_{j\sigma} \left(1 + 2\vec{S}_j \vec{\sigma}\right) a^{(1)}_{j\sigma'} + \frac{t}{2} \sum_{\substack{\gamma\gamma' \\ \alpha\alpha'}} \sum_{j \in A} a^{+(\alpha)}_{j\sigma} \cdot \qquad (2)$$

$$\cdot \left(1 + 2\vec{S}_{j+2\hat{x}-\tau_\gamma} \vec{\sigma}\right) a^{(\alpha')}_{j+\tau_{\gamma'}-\tau_\gamma} B_{\gamma\alpha} B_{\gamma'\alpha'}$$

where σ_α are Pauli matrices, $\vec{S}_j$ is a spin operator on Cu site

$$a^{+(\delta)}_{j\sigma} = \sum_{\alpha} B_{\alpha\delta} \hat{p}^{+(\alpha)}_{j\sigma} \quad ; \quad \hat{p}^{+}_{j\sigma} = \left(p^{+}_{j+\hat{y}}, p^{+}_{j-\hat{x}}, p^{+}_{j-\hat{y}}, p^{+}_{j+\hat{x}}\right) \qquad (3)$$

$$\tau_1 = 2\hat{x} - 2\hat{y} \quad ; \quad \tau_2 = 4\hat{x} \quad ; \quad \tau_3 = 2\hat{x} + 2\hat{y} \quad ; \quad \tau_4 = 0$$

the translation τ is expressed in a units (a is a distance between Cu and O sites), J is an antiferromagnetic exchange interaction, $p^{+}_{j\sigma}$'s describe $p_{x,y}$ oxygen states.

The representation of the Hamiltonian in the form (2) is rather convenient, because the summation is taken only over the sublattice A (the lattice parameter is equal to 2) and $a^{(\alpha)}_{j\sigma}$'s satisfy commutation relations for fermion operators. It is worth mentioning that only spin operators $\vec{S}_{i+\tau_\gamma}$ are connected with the sites of another sublattice B.

The trial function is chosen in the following form:

$$|\psi^+\rangle = \frac{A}{N_R} \sum_{\substack{i \le N_R \\ \tau}} f_i \varphi^{+}_{i+\tau} \exp\left[-\frac{\pi}{\lambda}\left(\quad + \quad\right)\right] \qquad (4)$$

where N_R - the number of atoms inside the circle with radius $\frac{\sqrt{N}}{\pi}$, λ is a variational parameter, the constant A is determined by the normalizing condition $\langle\psi|\psi^+\rangle = 1$. The summation is taken over the sublattice A (i is expressed in the lattice parameter units). $|G\rangle$ describes the spin state of the copper sublattice (the ferromagnetic one at $i \le N_R$ and the antiferromagnetic one otherwise).

$$\varphi^{+}_i = a^{+(1)}_{i\uparrow} \sqrt{1 - z} - \sqrt{\frac{z}{2}}\, a^{+(1)}_{i\downarrow} b^{+}_i - \frac{1}{2}\sqrt{\frac{z}{2}} \sum_{\hat{x}} B_{\gamma\alpha}\, a^{+(\alpha)}_{i\downarrow} b^{+}_{i+2\hat{x}-\tau_\gamma}$$

$$f(\tau) = -f(-\tau) \quad ; \quad f(\tau_1) f(\tau_2) = \frac{(\vec{\tau}_1, \vec{\tau}_2)}{|\vec{\tau}_1| \cdot |\vec{\tau}_2|} \qquad (5)$$

$$b^{+}_i = S^{+}_i \quad ; \quad b^{+}_{i+2\hat{x}} = \begin{cases} S^{+}_{i+2\hat{x}} & ; \; i \le N_R \\ S^{-}_{i+2\hat{x}} & ; \; i > N_R \end{cases}$$

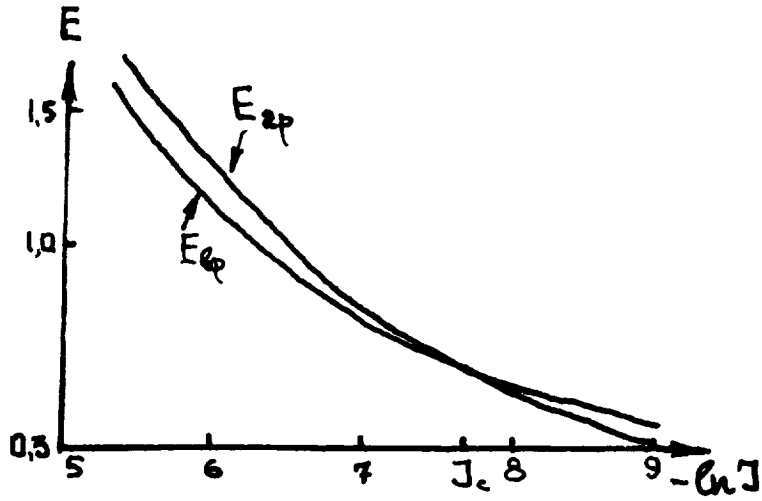
The results obtained below show that the region of the spin bipolaron existance corresponds to the small value of the exchange interaction J .Therefore,one can choose $z = 0.46$ (this value is obtained in $J \to 0$ limit in [3,4]) and consider only two variational parameters (α , N_R).Using the trial function (4)-(5) ,the energy of the system is calculated:

$$E_{bp} = -10.36 + 6.05 \frac{\alpha \exp(-\alpha)}{(1-\exp(-\alpha))\sqrt{N_R}} \cdot \frac{1}{\sqrt{N_R}} + \frac{\alpha}{N_R}\left(2.8t + 0.11 t \ln\frac{N_R}{2}\right) + 4N_R J \quad (6)$$

The calculation for two separate polarons can be performed in the analogous way:

$$E_{2p} = -10.36 + 7.98 \frac{\alpha \exp(-\alpha)}{(1-\exp(-\alpha))\sqrt{N_R}} \cdot \frac{1}{\sqrt{N_R}} + 4.45 \frac{\alpha}{N_R} + 8 N_R J \quad (7)$$

Minimizing E_{bp} E_{2p} with respect to α and N_R ,one finds that the region of the spin bipolaron existance-as it follows from the plot-is determined by the following condition: $J > J_c = 4.42 \cdot 10^{-2} t$



The energy versus exchange coupling (all the quantities are expressed in t units,the energy origin is -10.36)

It is worth mentioning that in $J \to 0$ limit the extended state($\alpha \to 0$ $\varphi(r) \to 1/\sqrt{N_R}$ in(4)) is the most advantageous one,providing the energy minimum.Therefore,the localized state is absent in this limit.

References
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