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Bound states in models of high-T_c superconductors

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Abstract

It is widely believed that the essential low-energy physics of the high-T_c CuO_2 based systems is described by the t–J-like model, which contains in itself the strong interaction of local spins with mobile holes. We have studied the problem of the hole–hole interaction in an antiferromagnetic background using recently developed analytical method. Spin-wave exchange and an effective interaction due to minimization of the number of broken antiferromagnetic bonds have been taken into consideration. The bound state of the $d_{x^2-y^2}$ symmetry has been found to be the groundstate of the system in the wide region of parameters. Possible relation of the obtained results to the problem of superconductivity in real systems is discussed.

Keywords: t–J; model; Spin polaron; Pairing mechanism

The t–J model reads

$$H_{t-J} = t \sum_{\langle ij\rangle,\alpha} \tilde{c}^{\dagger}_{i,\alpha}\tilde{c}_{j,\alpha} + J \sum_{\langle ij\rangle} \left(\boldsymbol{S}_i\boldsymbol{S}_j - \frac{1}{4}N_i N_j\right), \qquad (1)$$

in the standard notation of the constrained fermion operators $\tilde{c}^{\dagger}_{i,\alpha}(\tilde{c}_{i,\alpha})$, $\langle ij\rangle$ denotes the nearest neighbor sites, $\boldsymbol{S}_i$ is a local spin operator, and N_i is the operator of the number of spins.

Theoretical studies of the t–J model have resulted in the clear understanding of the nature of the low-energy excitations for the system near half-filling. The charge carrier created by the hole introduced in an AF background is described as the spin polaron, i.e. as a quasiparticle consisting of the hole and the cloud of the spin excitations. AF spin-polaron conception has been put forward in the earlier work [1] and then developed in a number of works [2–5] using different techniques.

To be more specific, the wave function of the spin polaron in an AF background can be written as

$$\tilde{h}^{\dagger}_{k}|0\rangle = \Bigg[a_k h^{\dagger}_k + \sum_q b_{k,q} h^{\dagger}_{k-q}\alpha^{\dagger}_q + \sum_{q,q'} c_{k,q,q'} h^{\dagger}_{k-q-q'}\alpha^{\dagger}_q\alpha^{\dagger}_{q'} + \cdots \Bigg]|0\rangle \qquad (2)$$

in terms of the AF magnon and spinless hole creation operators $\alpha^{\dagger}_q$ and $h^{\dagger}_k$, respectively. On the way from the t–J Hamiltonian Eq. (1) to Eq. (2) we used the spinless-fermion Schwinger-boson representation of the constrained electron operators, which has been shown to be adequate to the problem, or,

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in other words, is able to treat properly the nonlinear feature of the kinetic energy term of Eq. (1). $a_k^2 = Z_k < 1$ is the quasiparticle residue. An explicit expression of an exact spin-polaron wave function within the self-consistent Born approximation (SCBA) in the form Eq. (2) has been written in Ref. [5]. Direct correspondence of the wave function Eq. (2) to the string picture [3] is evident.

Investigations of the interaction of such quasiparticles is the subject of prime interest in the context of the magnetic pairing mechanism. Studies of this problem show much less convergence of the results than the single-hole problem. One of the analytical problems on this way is that the SCBA approach, which has been successfully used for the single-hole problem, cannot be directly applied to the two-hole case. Nevertheless, two key mechanisms leading to the pairing were intensively studied. One of them is the effective hole–hole static attraction due to minimization of the number of broken bonds by placing two holes at the nearest-neighbor sites. Another one is the spin-wave exchange which leads to the dipolar-type interaction between holes [6].

Quite recently a new approach to the two-hole problem in the t–J model has been developed [7]. It has used a generalization of the canonical transformation approach of the Lang–Firsov type. An effective Hamiltonian for the spin polarons Eq. (2), which includes in itself both types of the hole–hole interaction in the natural way, has been obtained during these studies:

$$\mathscr{H}_{\text{eff}} = \sum_k E_k \tilde{h}_k^\dagger \tilde{h}_k + \sum_q \omega_q \alpha_q^\dagger \alpha_q + \sum_{k,k',q} V_{k,k',q} \tilde{h}_{k-q}^\dagger \tilde{h}_{k'+q}^\dagger \tilde{h}_{k'} \tilde{h}_k + \sum_{k,q} F_{k,q} M_{k,q} (\tilde{h}_{k-q}^\dagger \tilde{h}_k \alpha_q^\dagger + \text{h.c.}), \quad (3)$$

where E_k and ω_q are the polaron and magnon energies, respectively. Polaron energy E_k and weights of the components of the polaron's wave function have been compared with the results of the other works, especially SCBA ones, and an excellent agreement has been found. Since the way of derivation of the polaron energy and the polaron–polaron interaction in the framework of the canonical transformation approach is the same, one can hope that the effective Hamiltonian Eq. (3) properly describes interaction between the low-energy excitations of the t–J model. "Direct" interaction term contains the "sharing the common link" interaction renormalized by the hole movement and the short-range spin-wave exchange. The last term treating perturbatively gives the dipolar interaction.

Two-hole problem has been considered using Hamiltonian Eq. (3). The bound state of the $d_{x^2-y^2}$ symmetry has been found for all $0 < t/J < 5$. Because the analytical treatment of the problem allows one to consider the role of the interactions separately, some conclusions about their roles can be done. Briefly, the nearest-neighbor attraction is too weak to provide a bound state at $t/J > 2$ because of the evident loss of the kinetic energy ($\sim t$) due to the close hole location. Spin-wave exchange lead to the very shallow and large-size bound state at any t/J. Cumulative effect of both interactions shows a kind of the strong interference: resulting bound state is relatively deep $\sim (0.1 - 0.05)J$ at $2.5 < t/J < 5$ and the average distance between polarons is 2–3 lattice constants. The results are shown in Fig. 1.

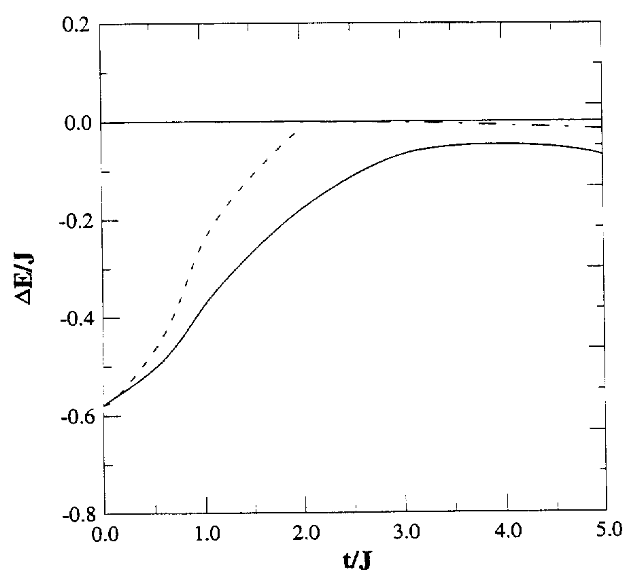

Fig. 1. Energies of the d-wave bound states versus t/J. Dashed curve is the result for the nearest-neighbor attraction, dashed-dotted curve is for the spin-wave exchange. Solid curve corresponds to the resulting bound state.

The wave function of the d-wave bound state with the total momentum $P = 0$ can be written as:

$$|2\rangle = |\Psi^{(d)}_{P=0}\rangle = \sum_{k} \Delta^{(d)}(\boldsymbol{k})\tilde{h}^{\dagger}_{k}\tilde{h}^{\dagger}_{-k}|0\rangle, \qquad (4)$$

$\Delta^{(d)}(\boldsymbol{k})$ is the solution of an analog of the Schrödinger equation for the two-body problem. The form of $\Delta^{(d)}(\boldsymbol{k})$ ensures the d-wave symmetry of the state and that the centers of the polarons are always at the different sublattices, which in its turn guarantees $S^z = 0$ for the system.

Finally, a strong tendency to the d-wave pairing has been found for the two holes in the AF background. The hole–hole interactions of different nature have been taken into consideration. Interference of the two types of the pairing interactions has been found. Retardation effect for the long-range spin-wave exchange has been carefully taken into account.

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