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The effective Hamiltonian for cuprates at different energy scales

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Abstract

A multiband p–d model describes electronic properties of cuprates in the large energy scale $\sim U \sim 10$ eV. In the strong electron correlation (SEC) limit we project out double occupied intra-atomic states and obtain the singlet–triplet $t-t'-t''-J^*$ model at scale $\sim\Omega \approx 0.5$ eV, where Ω is the excitation energy between two-hole singlet and triplet states. At smaller energies $\sim J$ one gets the usual $t-t'-t''-J^*$ model. At energies $\sim\omega_D$ one has to add electron–phonon interaction, and the low-energy effective Hamiltonian with magnetic and phonon mechanisms of pairing is constructed in SEC limit with parameters calculated from the ab initio approach. Magnetic mechanism of pairing results in a very high value of the critical temperature T_c while electron–phonon interaction suppresses d-pairing to the $T_c \sim 100$ K.

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During the last 20 years, a lot of theoretical studies of the electronic properties and phase diagram of cuprates have been published. Due to the effects of strong electron correlations (SEC), the conventional single electron ab initio approach like LDA cannot be used, and typically single-band Hubbard model or three-band p–d model have been used with model parameters considered as fitting or calculated separately [1,2]. Beyond these models are $(d_{z^2}-p)-\sigma$ bonds of a_{1g} symmetry that gives quite noticeable contribution to the density of states (DOS) near Fermi energy. A multiband p–d model [3] incorporates all relevant p-oxygen and d-copper orbital. To account for SEC, a generalized tight binding (GTB) method has been developed, and the electronic structure of undoped La_2CuO_4 has been calculated in the multiband p–d model in the energy scale $\sim U \sim 10$ eV [4]. By projecting out double occupied states due to SEC, usually the single-band Hubbard model or three-band p–d model result in the $t-t'-t''-J^*$ Hamiltonian as the low-energy effective model. Here $t-J^*$ means the t–J model plus the three cite correlated hopping term H_3. Nevertheless, similar unitary transformation of the multiband p–d model results in a two-band singlet–triplet t–J model [5] with an energy scale of spin exaction $\Omega = E(^3B) - E(^1A)$, where ^1A is a two-hole state of a CuO_6 cluster with dominant contribution of Zhang–Rice singlet and ^3B is its triplet partner. In the three-band p–d model Ω is rather large and typically triplet state is omitted in the low-energy effective Hamiltonian. Nevertheless, in realistic multiband model, Hund coupling and some other interactions decrease Ω up to 0.5 eV. The configuration interaction calculations [6] predicts possible crossover of singlet and triplet states. Recent analysis of ARPES data in strongly underdoped $BiSr_2Ca_{1-x}Y_xCu_2O_8$ proves the decreasing Ω with x and large contribution of triplet band in the low-energy ARPES [7]. Only at smaller energy scale $E \sim J \ll \Omega$, the $t-t'-t''-J^*$ model is the adequate low-energy model, which provides magnetic mechanism of pairing. The three cite correlated hopping term H_3 results in strong renormalization of T_c in magnetic mechanism of pairing [8,9]. Recently developed hybrid LDA+GTB method allows to calculate ab initio parameters of the

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$t-t'-t''-J^*$ Hamiltonian [10] by projecting out LDA basis functions to the set of Wannier functions of the GTB calculations. The derivation of the effective Hamiltonian and the calculation of T_c have been done in cluster perturbation theory with exact diagonalization of the multiband p–d model in the CuO_6 unit cell and perturbation treatment of inter cell hopping in X-operator representation.

To study both magnetic and phonon pairings in the energy scale of the phonon frequency ω_D, a new low-energy Hamiltonian is

$$H = H_{t-t'-t''-J^*} + H_{e-ph-e} \tag{1}$$

with H_{e-ph-e} given by

$$H_{e-ph-e} = \sum_{kk'q}\sum_{\sigma\sigma'} V_{kk'q} X^{\sigma 0}_{k+q} X^{\sigma' 0}_{k'-q} X^{0\sigma'}_{k'} X^{0\sigma}_{k}. \tag{2}$$

Here $X^{0\sigma}_k$ is the Hubbard operator creating a hole with spin σ, and momentum k, $V_{kk'q}$ is the matrix element, calculated in Ref. [11] for the three phonon modes: breathing, apical breathing and buckling, that are known to have the largest electron–phonon interaction. Hamiltonian (1) is adequate to study superconductivity in strongly correlated electronic system of cuprates, as it contains only one external parameter (the effective electron–phonon coupling), and all the electronic parameters have been calculated in the LDA-GTB scheme [10]. A mean field theory of superconductivity in the regime of strong correlations is developed for d-type pairing. We should emphasize that our mean field theory differs from the standard mean field treatment of the Coulomb interaction like $Un_1n_2 \to Un_1\langle n_2\rangle$. In the GTB and LDA + GTB methods, the cluster perturbation theory is used that combines the exact diagonalization treatment of the multiband p–d model Hamiltonian inside the unit cell (here it is the CuO_6 octahedron), construction of the Hubbard X-operators based on the exact intracell multielectron eigenstates and perturbation treatment of the intercell hopping in the X-operator representation. For the normal state this mean field approach is just a cluster generalization of the Hubbard I approximation. For superconducting state, the mean field theory in the X-operator representation that is reliable in the strong correlation regime has been developed in Ref. [12]. Double occupation is prohibited in this approach by the local constraint formulated in the X-operator representation similar to the local constraint in the slave boson approach. Contrary to the slave boson mean field theory where the local constraint is violated in our mean field theory, the X-operator algebra provides the local constraint in all stages of calculations. Our mean field theory considers both magnetic and phonon contributions for pairing generated by Hamiltonian (1). A self-consistent equation determining the superconducting transition temperature has the form following:

$$1 = \frac{1}{N}\sum_q \left\{ J\frac{1-x}{2} + G\left(\frac{-3c_{01}}{4(1+x)} + \frac{(1+x)}{8}\right) \times \theta\left(|\xi_q - \mu| - \omega_D\right)\right\} \frac{\left(\cos q_x - \cos q_y\right)^2}{\xi_q - \mu} \tan h \frac{\xi_q - \mu}{2T_c}, \tag{3}$$

where $\xi_{\mathbf{q}}$ is the normal state dispersion taking into account spin correlation functions and tree-center interactions [9], μ is the chemical potential and c_{01} is the spin correlation function of the nearest Cu–Cu neighbors calculated self-consistently in [13] for different doping. The first term in Eq. (3) results from magnetic pairing with coupling J, and the rest stems from phonons with coupling G. The θ- function appears because the phonon contribution is significant only in a narrow layer ω_D near the Fermi surface. A product $c_{01}G$ corresponds to the interference of the magnetic (in spin liquid state c_{01} is not small) and phonon mechanism. Eq. (3) was solved together with the equation for the chemical potential for hole concentration $1+x$, which corresponds to $La_{2-x}Sr_xCuO_4$. It appears that magnetic mechanism of pairing (if $G=0$) results in very large values of $T_c \sim 250$ K (with ab initio parameters). We would like to emphasize that all electronic structures and magnetic pairing parameters have been calculated from ab initio calculations in Ref. [10] and the only fitting parameter in Eq. (3) the effective electron–phonon coupling at G. The dominant contribution of the breathing phonon mode provides negative value of G and suppression of d-pairing. Therefore, T_c decreases to a realistic value $T_c \sim 100$ K at $G/J = -0.5$.

In conclusion, different microscopic models should be used at different energy scales depending on the characteristic energy of the problem to study. For the low-energy effective Hamiltonian we have shown that magnetic mechanism is dominant. The phonon mechanism is also very important, as it decreases from a very high magnetic T_c to the realistic value.

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