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Electron–phonon interaction in cuprates with T and T′-structure in strongly correlated limit

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Abstract

Electron–phonon interaction in cuprate oxides is consistently determined from realistic multi band p–d model in strong correlations limit. We consider the momenta dependence matrix elements of the EPI for modes which most coupled to electrons and analyze a possible mechanism of kink formation. By unitary transformation we obtain an effective low-energy single-band Hamiltonian that includes only electron–electron interactions renormalized by the electron–phonon coupling and depends on occupation factors.

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The nature of high-temperature superconductivity (HTSC) is far from being understood. While strong correlations and d-wave pairing suggested the importance of a spin-based pairing interaction there has been a resent accumulation of experimental results indicating the electron–phonon interaction (EPI) must play an important role in HTSC oxides. This evidence has come from Raman spectroscopy, neutron scattering, penetration depth measurements, ARPES and something else [see special issue Physica Status Solidi 242(1) 2005]. Evidently for description both superconducting pairing and normal state properties of HTSC compounds it is necessary to take into account electron interaction with phonons and spin fluctuations simultaneously.

Therefore the purpose of the present work was the consistent determination of the EPI in cuprate oxides starting from realistic multi band p–d model in strong correlations limit with consideration of phonon modes which are most coupled to electrons. To describe EPI in cuprates the atoms in the p–d model are displaced and the changes of Hamiltonian parameters are calculated to linear order in the displacements. In frame of the GTB method [1] we obtain

$$H_{\mathrm{el-ph}} = \sum_{\mathbf{k}\mathbf{q}\nu} \sum_{mm'} g^{(\nu)}_{mm'}(\mathbf{k},\mathbf{q})\, \overset{+}{X}{}^{m}_{\mathbf{k}+\mathbf{q}} X^{m'}_{\mathbf{k}} (b_{\mathbf{q},\nu} + b^{+}_{-\mathbf{q},\nu}),$$

$$g^{(\nu)}_{mm'}(\mathbf{k},\mathbf{q}) = \delta_{mm'} g^{(\nu)}_{\mathrm{dia},m}(\mathbf{q}) + g^{(\nu)}_{\mathrm{off},mm'}(\mathbf{k},\mathbf{q}),$$

where Hubbard operator $X^{m}_{\mathbf{k}}$ describe the m-kind of hole quasiparticle with wave vector $\mathbf{k}$; the operator $b^{+}_{\mathbf{q},\nu}$ creates a phonon with wave vector $\mathbf{q}$, index ν and frequency $\omega_{\nu}(\mathbf{q})$; total matrix element of EPI is presented as a sum of diagonal part $g^{(\nu)}_{\mathrm{dia},m}(\mathbf{q})$ depending on $\mathbf{q}$-scattering momentum of electron and off-diagonal part $g^{(\nu)}_{\mathrm{off},mm'}(\mathbf{k},\mathbf{q})$ depending on $\mathbf{k}$-initial momentum also (see detail in Ref. [2]).

Further we restrict our consideration by three phonon modes which have the greatest coupling strength [3], i.e., the vibration of the in-plane oxygens along Cu–O-plane and along the z-axis (breathing mode and buckling mode) and the vibration of the apex oxygen in the z direction (apex breathing mode). Explicit dependence of matrix elements on $\mathbf{k}$ and $\mathbf{q}$ was obtained taking into consideration the symmetry of atomic displacements for each mode. Plots of the EPI coupling for breathing and buckling modes are shown in Fig. 1 as a function of scattered momentum $\mathbf{q}$ for initial state in the nodal $\mathbf{k}_{\mathrm{n}}$ and antinodal $\mathbf{k}_{\mathrm{nod}}$ points accordingly. (Matrix elements of the apex breathing mode

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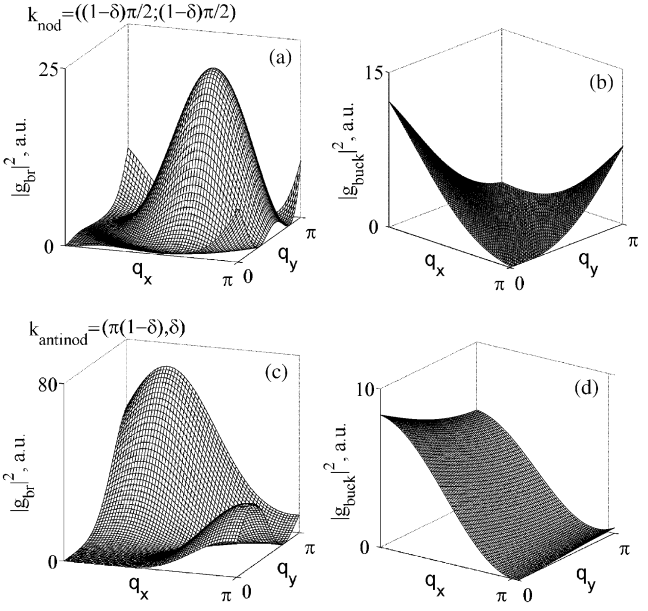

Fig. 1. Plots of the EPI coupling for the breathing (a, c) and buckling (b, d) modes at nodal (a, b) and antinodal (c, d) initial $\mathbf{k}$ states.

does not depend on $\mathbf{k}$ and $\mathbf{q}$.) For a nodal fermion initial state, the coupling is largest to the breathing mode for $\mathbf{q} = (\pi, 0)$ (Fig. 1a) and to the buckling mode with small value of $\mathbf{q}$ (Fig. 1b) since such phonons connect electrons with initial states $\mathbf{k} \sim \mathbf{k}_F$ to the final states on the Fermi surface. For an antinodal fermion initial state, the breathing coupling is weak (Fig. 1c) while the buckling interaction has a maximal value for small $\mathbf{k}$ (Fig. 1d).

To analyze a possible kink formation [4] we take into account plots of coupling and consider conservation of energy and momentum assuming electron energy in superconducting phase is given by BCS theory $E(\mathbf{k}) = \pm\sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$ and order parameter has d-wave symmetry.

In the nodal point $\mathbf{k}_n = ((1-\delta)\pi/2, (1-\delta)\pi/2)$, $\delta \leqslant 0,1$ the breathing mode has maximum coupling to scattering momentum $\mathbf{q}_1 = (\pi, \pi)$ and $\mathbf{q}_2 = (\pi, 0)$. At the same time we have $E(\mathbf{k}_n - \mathbf{q}_1) \approx \Delta(\mathbf{k}_n - \mathbf{q}_1) = 0$ from this a kink energy is $\varepsilon(\mathbf{k}_n) = |E(\mathbf{k}_n - \mathbf{q}) - \omega_{\mathbf{q}}^{(1)}| = 70\,\text{meV}$. This energy corresponds to breathing mode frequency at $\mathbf{q}_1 = (\pi, \pi)$. Similarly, the mode with $\mathbf{q}_2$ also satisfies a conservation of energy. In that way we obtain that contribution to electron spectra renormalization comes from coupling to breathing mode with $\mathbf{q}_1 = (\pi, \pi)$, $\mathbf{q}_2 = (\pi, 0)$ at the nodal point and from coupling to buckling mode with small value of $\mathbf{q}$ at the antinodal point.

The difference in the EPI for n-type cuprates with T′-structure results from the absence of apical oxygen ion. Transverse vibrations of apical ion strongly modulate the Madelung potential. Hence the very strong EPI with apex breathing mode is absent.

For construction of superconducting theory it is of interest to obtain an effective Hamiltonian where EPI was excluded in the manner of Fröhlich transformation [5]. For low-energy single-band t−J* model (t–J plus three site correlated hopping term) this transformation is not quite trivial. To perform it we neglect by interband excitations and apply Hubbard-I-type approximation. As a result effective Hamiltonian can be written in the following form:

$$H_{\text{eff}} = H_{\text{t-J}^*} + H_{\text{el-ph-el}},$$

$$H_{\text{el-ph-el}} = \sum_{\mathbf{kk'q}} \sum_{m} V^{mm}_{\mathbf{kk'q}} \overset{+}{X}{}^{m}_{\mathbf{k+q}} \overset{+}{X}{}^{m}_{\mathbf{k'-q}} X^{m}_{\mathbf{k'}} X^{m}_{\mathbf{k}},$$

$$V^{mm}_{\mathbf{kk'q}} = \frac{g^{(v)}_{mm}(\mathbf{k}, \mathbf{q}) g^{(v)}_{mm}(\mathbf{k}, -\mathbf{q}) \omega_{\mathbf{q},v}}{[t_m(\mathbf{k}) - t_m(\mathbf{k}+\mathbf{q})]^2 F_m^2 - \omega^2_{\mathbf{q},v}},$$

where $H_{\text{t-J}^*}$ is low-energy single-band t−J* model, quasiparticle index m is different for cuprates with hole or electron doping type, $t_m(\mathbf{k})$ is dispersion of free electrons, and $V^{mm}_{\mathbf{kk'q}}$ is effective electron–electron interaction which depends on occupation factors F_m and hence on doping concentration, temperature and magnetic field in contrast to theory of weak coupling electrons.

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