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On the Superconducting Gap Dispersion in Hole-Doped Cuprates

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Solutions of the equation for the superconducting gap including superexchange, spin–fluctuation, plasmon, and phonon pairing mechanisms are obtained. Solutions of the Bardeen–Cooper–Schrieffer equation are approximated by the expression $\Delta_{\mathbf{k}} = \Delta_0(B\cos(2\phi) + (1 - B)\cos(6\phi))$ at a carrier concentration close to optimal. It is found that the dependence proportional to $\cos(6\phi)$ is due to the spin–fluctuation and phonon-mediated interactions.

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The dependence of the superconducting gap on the wave vector contains important information on the pairing mechanism. It is apparently established that this gap for hole-doped cuprates is approximately described by the expression $\Delta_{\mathbf{k}} = \Delta_1(\cos(k_x a) - \cos(k_y a))/2$. Recent measurements with increasing accuracy provide grounds for the inclusion of higher order harmonics with the d symmetry in the gap dispersion relation of the form $\Delta_2(\cos(2k_x a) - \cos(2k_y a)) + \Delta_3(\cos(2k_x a)\cos(k_y a) - \cos(2k_y a)\cos(k_x a)) + \ldots$. The behavior of the gap along the Fermi contour is described by the phenomenological formula $\Delta_{\mathbf{k}} = \Delta_0(B\cos(2\phi) + (1 - B)\cos(6\phi))$, where the angle is measured from the antinodal direction in the Brillouin zone [1–3]. The relevant theoretical works were carried out within separate possible pairing mechanisms. In the pioneering work [4], only the spin-fluctuation mechanism with a phenomenological expression for the spin susceptibility was considered, which later was no longer used as too rough an approximation. In the recent work [5], the calculations of the dependence of the superconducting gap on the wave vector in the Hubbard model with the parameter of the Coulomb interaction between electrons at one site were generalized. The calculations with the additional inclusion of the Coulomb interaction between electrons at neighboring lattice sites are reviewed in [6]. In principle, higher harmonics were obtained in solutions [5, 6], but they were not analyzed and were not compared with experimental data for hole cuprates. One of the main aims of this work is to propose a possible scenario of the origin of the correction term in the gap with the harmonic $\cos(6\phi)$. Another aim of ours is to show that the usage of microscopically substantiated expressions for the spin and charge susceptibilities proposed in [7–10] and [11–13], respectively, makes it possible to obtain the observed values of the quantities Δ_0 and B at realistic parameters of Coulomb, superexchange, electron–phonon, and spin–fluctuation coupling. The latter parameter in our calculations was approximately one quarter of the width of the conduction band. This result removes the problem of too large a parameter of the spin–fluctuation coupling of charge carriers. In the phenomenological or random phase approximation expression for the susceptibility [4, 14, 15], this parameter is assumed to be about the width of the band.

For the description of the band structure of CuO planes, we use the singlet-correlated conduction band model [16–18] with the parameters in agreement with photoemission data:

$$H = \sum_{ij} t_{ij}\psi_i^{pd,\sigma}\psi_j^{\sigma,pd} + \frac{1}{2}\sum_{ij} G_{ij}^{\infty}\delta_i\delta_j + \frac{1}{2}\sum_{ij} J_{ij}\left[S_i S_j - \frac{n_i n_j}{4}\right] + H_{\text{el-ph}}, \quad (1)$$

where $\psi_i^{pd,\sigma}\left(\psi_j^{\sigma,pd}\right)$ are the quasiparticle operators; J_{ij} and G_{ij}^{∞} are the parameters of the superexchange and screened Coulomb interactions, respectively; n_i and δ_i are the number operators of spins and holes per unit cell, respectively; and $H_{\text{el-ph}}$ is the operator of the electron–phonon coupling in the CuO plane.

In the Bardeen–Cooper–Schrieffer (BCS) theory, the superconducting gap is determined by the integral equation

$$\Delta_{\mathbf{q}} = -\frac{1}{N}\sum_{\mathbf{k}} V_{\mathbf{k-q}}\frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}\tanh\left(\frac{E_{\mathbf{k}}}{2k_{\mathrm{B}}T}\right). \quad (2)$$