Modeling Quasiparticles and Pseudogap in Cuprates in Presence of Charge Ordering Potential

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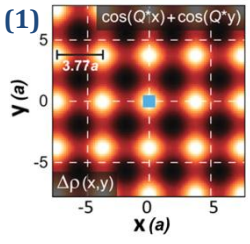
Abstract

We are modeling quasiparticles (QP) that emerge in cuprates in additional charge ordering (CO) potential. At *strong Frohlich electron-phonon interaction* autolocalized carriers form CO and coexist with delocalized ones [1]. We show that CO potential transforms Bloch QPs into distributed wave packets (DWP) with different momentums in areas with different potential. Modeling the dispersion of the hole-doped cuprates and constructing the momentum space trajectories of the new QPs we found that topology of the cuprates dispersion forbid QPs with average momentum near antinode. Modeling photoemission of carriers from the permitted QPs, we demonstrate that antinodal photoemission (ARPES) spectra have all the features characteristic of the pseudogap (PG) behavior in cuprates.

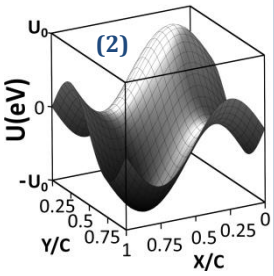
The Model and Methods

(1)

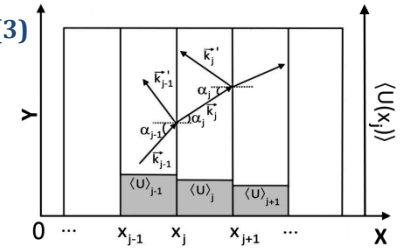


In the CO phase of cuprates charge density is proportional to the sum $\cos(K_{COx}x) + \cos(K_{COy}y)$ [2] (Fig. 1). This (together with the bipolaron charge e/ε_0, where ε_0 is static dielectric constant) allows calculating the CO potential. It is naturally to suppose that CO potential is also quasi-periodic function with the same period as CO, $C=2\pi/K_{CO}$. One of the considered CO potentials is shown in Fig. 2.

(2)



(3)



To solve the Shroedinger equation with additional CO potential we develop a method reminiscent of finite elements one [3]. We divide the conducting plane into so small stripes or squares that the CO potential Uj can be considered constant inside. In the 1st case boundaries between constant potential areas are supposed to be parallel to y-axis as shown in Fig. 3, so that the y-projection of the wave vector ky is conserved on each boundary. In the 2nd case a boundary is parallel to y or x axes and the corresponding projection (ky or kx) is conserved. The solution of Shroedinger equation in each stripe (or square) is Bloch function with projections of the wave vector satisfying the following system of equations (in the case of stripes, a boundary of a square parallel to y and x axes, respectively).

$$\begin{cases} \varepsilon(\mathbf{k_j}) = E - U_j \\ k_y = const \end{cases} \quad \begin{cases} \varepsilon(\mathbf{k_j}) = E - U_j \\ k_{y_{j-1}} = k_{y_j} \end{cases} \quad \begin{cases} \varepsilon(\mathbf{k_j}) = E - U_j \\ k_{x_{j-1}} = k_{x_j} \end{cases} \qquad (1)$$

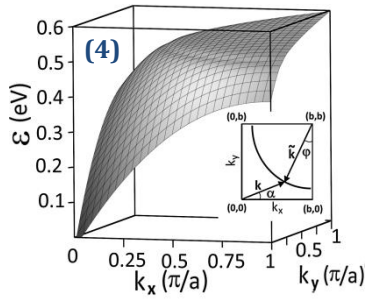
where $\varepsilon(\mathbf{k})$ is Bloch electron dispersion, E is the QP energy.

We model carrier dispersion near FS in hole-doped cuprates with following function (Fig.4) that provides arc-shaped FS (shown in the inset) and flat band near it:

$$\varepsilon(\mathbf{k}) = 0.5 - c * \left(\sqrt{(k_{j,x} - b)^2 + (k_{j,y} - b)^2} - \tilde{k}_0 \right)^d, \varepsilon \le 0.5$$

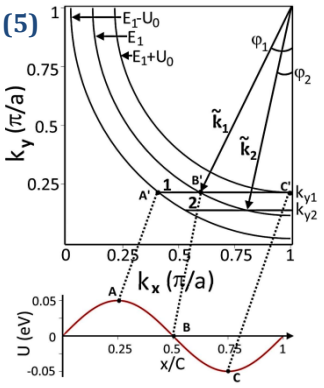
$$\varepsilon(\mathbf{k}) = 0.5 + c' * \left(\tilde{k}_0 - \sqrt{(k_{j,x} - b)^2 + (k_{j,y} - b)^2} \right)^{d'}, \varepsilon(\mathbf{k}) > 0.5$$

(4)



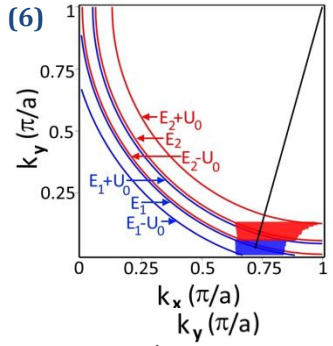
Results and their Discussion

(5)



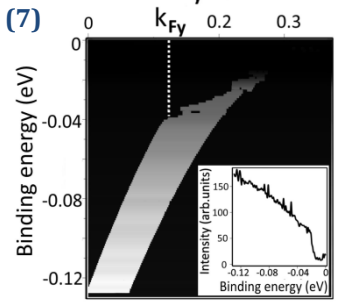
We construct numerically the *momentum-space trajectories* of the new QPs. They are shown in Fig.5 for the case of stripes and in Fig.6 for the case of squares. Consider stationary states with the energy E_1 located on the arc (Fig. 5). The 1st trajectory (line 1) reaches both the minimal and maximal kinetic energy in the layers with the maximal (point A) and minimal (point C) potential energy, respectively, thus at $\varphi \ge \varphi_1$ there exist real roots of the system of equations (1) in each layer of the CO potential. Therefore, the states with the energy E_1 and $\varphi \ge \varphi_1$ are real QPs. At $\varphi < \varphi_1$ and $E = E_1$ (line 2) there are no real roots of the system (1) in some layers with negative CO potential. Therefore, in the case of hole-like dispersion QPs with average momentums near antinode are absent [3]. Distribution of the QP state over wave vectors resembles a wave packet. However, in this distributed wave packet (DWP) the components with different wave vectors are present in different layers of the coordinate space with different CO potential.

(6)

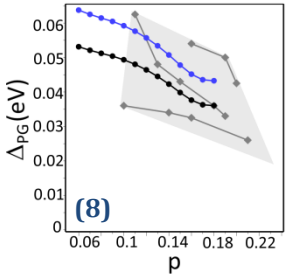


One can obtain antinodal ARPES spectrum from the QPs' momentum space trajectories that reach the First Brillouin zone boundary as one shown in Fig. 6 with red. The result is presented in Fig. 7 where intensities as functions of QP energy are inversely proportional to the area of the momentum-space trajectory (inset of Fig. 7). It demonstrates giant broadening *and shift of the spectral weight* down in the binding energies. Shift value at k_F, the Fermi momentum in the high-temperature ARPES spectrum, where PG is absent, is the PG width, and it is approximately the potential amplitude U_0. Just the same manifestations of the PG are observed in ARPES spectra of cuprates [4].

(7)

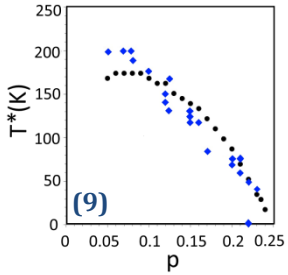


(8)



The present approach enables one to calculate doping dependences of the PG width presented in Fig. 8 ($\varepsilon_0 = 50$ and 60 for blue and black circles) together with PG width values measured in Bi2212 experimentally with STM [5] (gray diamonds) and PG onset temperature T* (Fig. 9, black circles) calculated as temperature corresponding to thermal decay of 95% of bipolarons responsible for the CO potential. To obtain this temperature we use distribution function of carriers in systems with strong long-range EPI [6] and bipolaron energy as function of doping. Calculated dependence is in good agreement with that observed in LSCO and Nd/Eu-LSCO [7] (blue diamonds).

(9)



References: [1] A. E. Myasnikova, T. F. Nazdracheva, A. V. Lutsenko, A. V. Dmitriev, A. H. Dzhantemirov, E. A. Zhileeva, and D. V. Moseykin, J. Phys.: Condens. Matter **31**, 235602 (2019); [2] R. Comin et al, Nat. Mater. **14**, 796 (2015); [3] S. V. Doronkina, A.E. Myasnikova, A. H. Dzhantemiov, A. V. Lutsenko, arXiv preprint, **arXiv:2007.16064**; [4] M. Hashimoto et al., Nat. Phys. **6**, 414 (2010). [5] Ø. Fischer, M. Kugler, I. Maggio-Aprile, C. Berthod, and C. Renner, Rev. Mod. Phys. **79**, 353 (2007); [6] A. E. Myasnikova, E. N. Myasnikov, D. V. Moseykin, and I. S. Zuev, Phys. Lett. A **379**, 458 (2015); [7] N. Doiron-Leyraud et al., Nat. Comm. **8**, 2044 (2017).