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

Anna E. Myasnikova
dept. of physics
Southern federal university
Rostov-on-Don, Russia
myasnikova67@yandex.ru

Stanislava V. Doronkina
dept. of physics
Southern federal university
Rostov-on-Don, Russia
doronkina1234@gmail.com

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. Employing method reminiscent of finite elements one, we show that CO potential transforms Bloch QPs into distributed wave packets with different momentums in areas with different potential. Modeling the dispersion of the hole-doped cuprates and constructing numerically 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. Variation of the obtained PG width and PG onset temperature with doping is in consent with one observed in cuprates.

Keywords—pseudogap, cuprates, charge ordering, dispersion topology

I. INTRODUCTION

Hole-doped cuprate superconductors keep two main enigmas for researchers: pairing mechanism and pseudogap (PG) nature [1], here we model the second one. The term PG is ordinarily used to denote absence of the carrier states with momentums near antinodes (i.e. in the vicinity of points $(0,\pm\pi)$, $(\pm\pi,0)$ in the First Brillouin zone (FBZ)) in some interval of energies under Fermi surface (FS). PG is observed at temperatures up to T^* which is higher than the temperature of superconducting transition, except overdoped systems. Two existing models of the PG emergence in cuprates are conventional charge density wave model and recent pair density wave scheme [2]. However, they both have discrepancies with experiments. The first cannot describe the so-called Fermi momentum misalignment, or particle-hole symmetry [2,3], the second leads to superconductivity due to pairing of the antinodal carriers [2] which does not occur in cuprates.

We model the third mechanism of the PG emergence in cuprates. It is neither scattering of Bloch carriers on each other (as in conventional charge density wave model) nor their pairing (as in pair density wav0e scheme). Charge ordering (CO) with short coherence length is well known phenomenon in cuprates. In systems with strong long-range (Frohlich) electron-phonon coupling such CO is formed by large bipolarons [4]. They create potential that influences the delocalized carriers which coexist with autolocalized ones provided they are of the large radius. Here we model this influence and demonstrate how it results in antinodal PG appearance.

II. THE MODEL AND METHODS

A. Charge ordering potential

As experiments show, in the CO phase of cuprates charge density is proportional to the a sum $cos(K_{COx}x)+cos(K_{Coy}y)$ [5]. Together with the known total charge of a bipolaron $2e/\varepsilon_0$, where ε_0 is static dielectric constant, this allows calculating the CO potential amplitude U_0. It is naturally to suppose that CO potential is also quasi-periodic function with the same period as CO, $C=2\pi/K_{CO}$ and short coherence length. One of the considered CO potentials is shown in Fig.1(a).

B. Method reminiscent of finite elements one to solve Shroedinger equation with CO potential

To solve the Shroedinger equation with additional CO potential we use a method reminiscent of finite elements one [6]. Namely, we divide the conducting plane into so small stripes or squares that the CO potential can be considered constant inside. Then we solve Shroedinger equation in each stripe or square with constant CO potential U_j and obtain Bloch function with the wave vector determined by the equation

$$\varepsilon(\mathbf{k}_j)=E-U_j, \qquad (1)$$

where $\varepsilon(\mathbf{k})$ is Bloch electron dispersion, E is the quasiparticle energy. This equation together with the boundary conditions for the wave vector projections (we suppose boundaries parallel to coordinate axes as is illustrated by Fig.1(b)) completely determine the QP.

C. Modeling carrier dispersion near Fermi surface in hole-doped cuprates

We model carrier dispersion near FS in hole-doped cuprates with a function that provides arc-shaped FS, shown by inset of Fig.1(c), and sufficiently flat dispersion near antinodes. It is presented in Fig.1(c).

III. RESULTS AND THEIR DISCUSSION

We construct numerically momentum-space trajectories of the new QPs. They are shown in Fig.2(a) for the simplified model with boundaries between constant potential areas being parallel y-axis (as is shown in Fig.1(b)) and in Fig.2(b) for boundaries parallel to both axes. In the

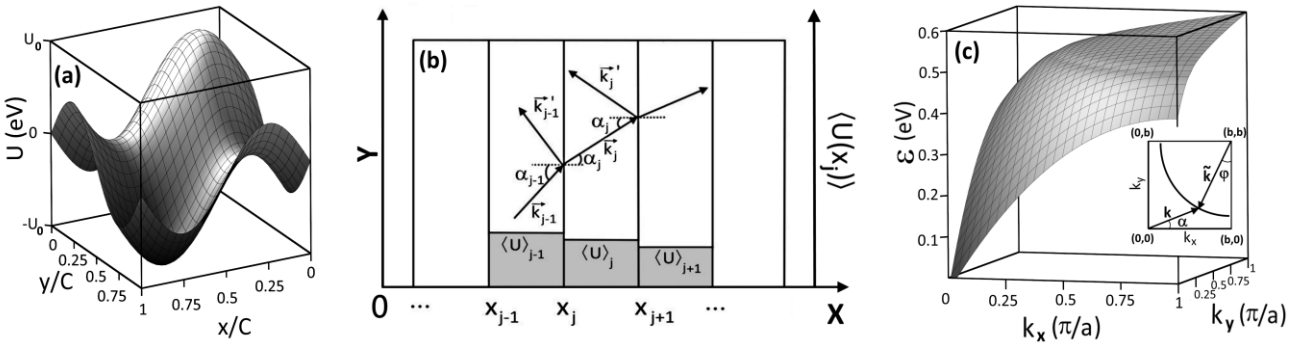

Fig.1.(a) Example of the CO potential; (b) QP momentum in layers with constant potential; (c) modeling carrier dispersion, inset – arc-shaped FS.

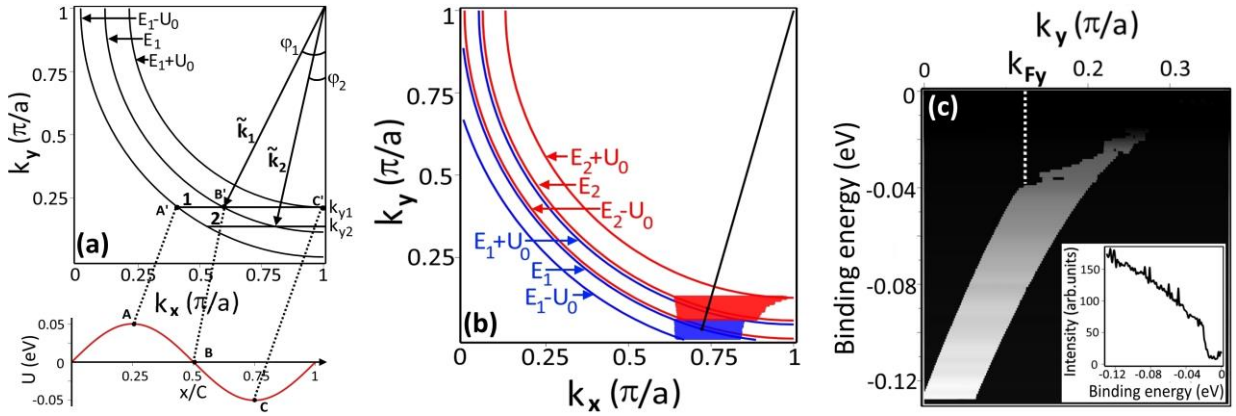

Fig.2. (a) Momentum-space trajectories of the QP in 1D CO potential and corresponding points of the potential; (b) Momentum-space trajectories of the QP in 2D CO potential; (c) calculated antinodal ARPES spectrum (image plot), inset – intensity as unction of binding energy, obtained as inverse area of the momentum-space trajectories of the QP with corresponding energy in 2D CO potential.

first case the y-projection of the wave vector k_y is conserved on each boundary:

$$k_y=\text{const.} \quad (2)$$

Geometrical analysis of compatibility of this condition and equation (1) illustrated by Fig.2(a) is the most apparent [6]. Let us consider stationary states with the energy E_1 located on the arc shown in Fig.2(a). At the QP propagation the potential U_j takes different values, so that the right-hand side of equation (1) changes from $\varepsilon=E_1-U_0$ to $\varepsilon=E_1+U_0$. Concurrently k_x value in the left-hand side should change at fixed k_y value. The first trajectory (line 1 in Fig.2(a)) reaches both the minimal kinetic energy surface $\varepsilon=E_1-U_0$ (this occurs in the layers with the maximal potential energy, point A) as well as the maximal kinetic energy surface $\varepsilon=E_1+U_0$ (in the layers with the minimal potential energy, point C). The second trajectory (line 2) reaches the former curve but does not reach the latter.

Hence, at $\varphi\geq\varphi_1$ there exist real roots of the system of equations (1,2) in each layer of the CO potential. Therefore, the states with the energy E_1 and $\varphi\geq\varphi_1$ are real QPs. It can be noted that 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. At $\varphi_0<\varphi_1$ and $E=E_1$ there are no real roots of the system (1,2) in some layers with negative carrier potential energy. Extinction of such states results in their absence among new QPs. Close situation takes place in the case of potential, depending on both x and y coordinates, as is illustrated by Fig.2(b).

Thus, the obtained momentum-space trajectories allow to demonstrate that in the case of hole-like dispersion QPs with average momentums near antinode cannot propagate [6]. One can obtain antinodal ARPES spectrum from the momentum space trajectories of real QPs, reaching the antinode (like that shown in Fig.2(b) with red). The result is presented in Fig.2(c) where intensities as functions of QP energy are inversely proportional to the area of the momentum-space trajectory (shown in inset of Fig.2(c)). It demonstrates shift of the spectral weight down in the binding energies, its value at k_F (PG width) is approximately the potential amplitude U_0, and giant broadening. Just the same displays are characteristic of PG in ARPES spectra of cupartes [3].

REFERENCES

[1] B. Keimer, S. A. Kivelson, M. N. Norman, S. Uchida and J. Zaanen, “From quantum matter to high-temperature superconductivity in copper oxides”, Nature, vol. 518, pp.179-186, 2015.

[2] P. A. Lee, “Amperean pairing and the pseudogap phase of cuprate superconductors” , Phys. Rev. X, vol.4, p. 031017, 2014

[3] M. Hashimoto et al., ”Particle–hole symmetry breaking in the pseudogap state of Bi2201”, Nat. Phys., vol. 6, pp. 414-418, 2010.

[4] A. E. Myasnikova et al., “Strong long-range electron–phonon interaction as possible driving force for charge ordering in cuprates”, J. Phys.: Condens. Matter, vol. 31, p. 235602, 2019.

[5] R. Comin et al, “The symmetry of charge order in cuprates”, Nat. Mater., vol.14, pp.796-802, 2015.

[6] S. V. Doronkina, A.E. Myasnikova, A. H. Dzhantemiov, A. V. Lutsenko, “Topological pseudogap in systems with strong electronphonon interaction and cuprates-like dispersion”, arXiv preprint, arXiv:2007.16064.