Contents

ELECTRONIC SPECTRUM IN HIGH-TEMPERATURE CUPRATE SUPERCONDUCTORS

N.M.Plakida[1] **and V.S. Oudovenko**[1,2]

[1] BLTPh, JINR, Dubna, Russia
[2] Rutgers University, New Jersey, USA

Recent angle-resolved photoemission spectroscopy revealed an anomalous quasiparticle (QP) spectra in copper oxide superconductors in comparison with conventional metals. In particular, a pseudogap in the electronic spectrum and a “truncated” Fermi surface in the form of arcs at low doping were revealed, a substantial renormalization of the Fermi-velocity of QP (“kinks"in the dispersion) was observed (see, e.g., [1, 2]). These anomalous properties are believed to be caused by strong electron correlations in cuprates [3]. Below we report the results of electronic spectrum calculations within the Hubbard model where for the first time we go beyond the mean-field approximation [4] or perturbation approach [5]. We have solved the Dyson equation self-consistently for the thermodynamic Green functions (GFs) and the self-energy derived in the noncrossing approximation (NCA), as has been done by us for the *t*-*J* model [6]. (For details see [7]).

1. Model and Dyson equation

We consider an effective *p*-*d* Hubbard model for one-hole states with energy $\varepsilon_1 = \varepsilon_d - \mu$ and two-hole *p*-*d* singlet states with energy $\varepsilon_2 = 2\varepsilon_1 + U_{eff}$ where μ is the chemical potential and an effective Coulomb energy $U_{eff} = \Delta_{pd} = \epsilon_p - \epsilon_d$ (see, e.g., [4]):

$$H = \varepsilon_1 \sum_{i,\sigma} X_i^{\sigma\sigma} + \varepsilon_2 \sum_{i} X_i^{22} + \sum_{i\neq j,\sigma} t_{ij}\, \{X_i^{\sigma 0} X_j^{0\sigma} + X_i^{2\sigma} X_j^{\sigma 2} + 2\sigma (X_i^{2\bar\sigma} X_j^{0\sigma} + \text{H.c.})\}, \quad (1)$$

where $X_i^{nm} = |in\rangle\langle im|$ are the Hubbard operators (HOs) for 4 states $n, m = |0\rangle,\ |\sigma\rangle,\ |2\rangle = |\uparrow\downarrow\rangle$, $\sigma = \pm 1/2$, $\bar\sigma = -\sigma$. The dispersion of holes is determined by the hopping parameters: $t_{ij} = t\,\delta_{j,i\pm a_{x/y}} + t'\,\delta_{j,i\pm a_x \pm a_y}$ ($a_{x/y} = a$ - lattice constants). We take $\Delta_{pd} = 8t \simeq 3.2$ eV and $t' = -\,0.3\,t < 0$.

By applying the Mori-type projection technique for the matrix thermodynamic GFs $\mathsf{G}_{ij\sigma}(t-t') = \langle\langle \hat X_{i\sigma}(t)\,|\,\hat X^{\dagger}_{j\sigma}(t')\rangle\rangle$ in terms of the two-component HOs ($\hat X^{\dagger}_{i\sigma} = \{X_i^{2\sigma},\, X_i^{\bar\sigma 0}\}$) an exact Dyson equation was derived as described in [4] with a self-energy (SE) as a many-particle GF. By using NCA for the SE, a closed system of equations was obtained for the the GFs and the SE:

$$\tilde G_{1(2)}(\mathbf{q},\omega) = (\omega - \tilde\varepsilon_{1(2)}(\mathbf{q}) - \tilde\Sigma(\mathbf{q},\omega))^{-1}\,, \quad (2)$$

where $\tilde\varepsilon_{1(2)}(\mathbf{q})$ are spectra for two bands given by the matrix $\tilde\varepsilon_{ij} = \langle\{[\hat X_{i\sigma}, H], \hat X^{\dagger}_{j\sigma}\}\rangle \times \langle\{\hat X_{i\sigma}, \hat X^{\dagger}_{i\sigma}\}\rangle^{-1}$. The SE in (2) for the one- and two-hole Hubbard bands are equal:

$$\tilde\Sigma(\mathbf{k},\omega) = \frac{1}{\pi^2 N}\sum_{\mathbf{q}} |t(\mathbf{q})|^2 \iint_{-\infty}^{\infty} \frac{d\nu dz N(z,\nu)}{\omega - z - \nu} \mathrm{Im}\chi_{sc}(\mathbf{k}-\mathbf{q},\nu)\ \mathrm{Im}\{\tilde G_1(\mathbf{q},z) + \tilde G_2(\mathbf{q},z)\}, \quad (3)$$

where $N(z,\nu) = (1/2)(\tanh(z/2T) + \coth(\nu/2T))$. In our theory, the interaction is determined by the hopping parameter $t(\mathbf{q})$ and the charge-spin susceptibility $\chi_{sc}(\mathbf{q},\nu) = (1/4)\langle\langle N_{\mathbf{q}}|N_{-\mathbf{q}}\rangle\rangle_\nu + \langle\langle \mathbf{S}_{\mathbf{q}}|\mathbf{S}_{-\mathbf{q}}\rangle\rangle_\nu$ where $N_{\mathbf{q}}$ and $\mathbf{S}_{\mathbf{q}}$ are number and spin operators.

2. Results and discussions

The self-consistent system of equations (2), (3) was solved numerically for various hole concentrations $n = 1+\delta = 2\langle X_i^{\sigma\sigma} + X_i^{22}\rangle$ by using the Matsubara frequency representation at temperature $T \simeq 0.03t \simeq 140$ K. Neglecting charge fluctuations, the spin susceptibility was described by the model: $\operatorname{Im}\chi_s(\mathbf{q},\nu) = \chi_0/[1+\xi^2(1+\gamma(\mathbf{q}))]\,\tanh(\nu/2T)/[1+(\nu/\omega_s)^2]$ where ξ is an antiferromagnetic (AF) correlation length (in units of a), $\omega_s \simeq J = 0.4t$ is spin-fluctuation energy, and $\gamma(\mathbf{q}) = (1/2)(\cos q_x + \cos q_y)$. The constant $\chi_0 = [3(1-|\delta|)/2\omega_s]\{(1/N)\sum_{\mathbf{q}}[1+\xi^2[1+\gamma(\mathbf{q})]^{-1}\}^{-1}$ is defined by the equation $\langle \mathbf{S}_i\mathbf{S}_i\rangle = (3/4)(1-|\delta|)$.

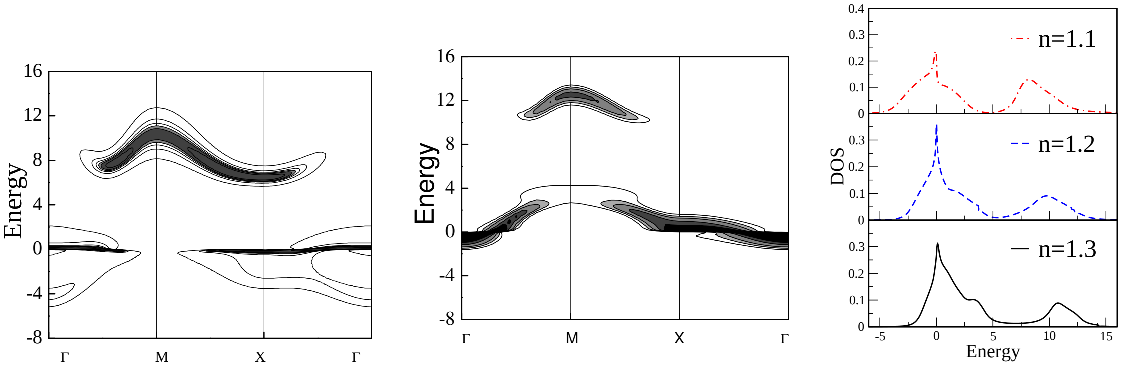

Рис. 1: Dispersion curves along the symmetry directions $\Gamma(0,0) \to M(\pi,\pi) \to X(\pi,0) \to \Gamma(0,0)$ for $\delta = 0.05$ (left panel) and $\delta = 0.3$ (central panel), and electronic density of states (right panel).

The dispersion curves given by maxima of spectral functions $A(\mathbf{k},\omega) = B_1(\mathbf{k})\,\tilde{A}_1(\mathbf{k},\omega) + B_2(\mathbf{k})\,\tilde{A}_2(\mathbf{k},\omega)$, where $\tilde{A}_{1(2)}(\mathbf{k},\omega) = -(1/\pi)\operatorname{Im}\tilde{G}_{1(2)}(\mathbf{k},\omega)$ and $B_{1,2}(\mathbf{k})$ are weights of the bands, were calculated for hole doping $\delta = 0.05 - 0.3$. The dispersion curves and the spectral function for $\delta = 0.05\,(\xi = 3.4)$ reveal a rather flat hole-doped band at the Fermi energy (FE) $(\omega = 0)$ (Fig. 1, 2, left panels). In the overdoped region, $\delta = 0.3\,(\xi = 1.4)$ (Fig. 1, 2, central panels) or at high temperature $T = 0.3t$ the dispersion becomes much larger which proves a strong influence of AF spin-fluctuations on the the electronic spectrum. With doping, the density of states (DOS) shows a weight transfer from the

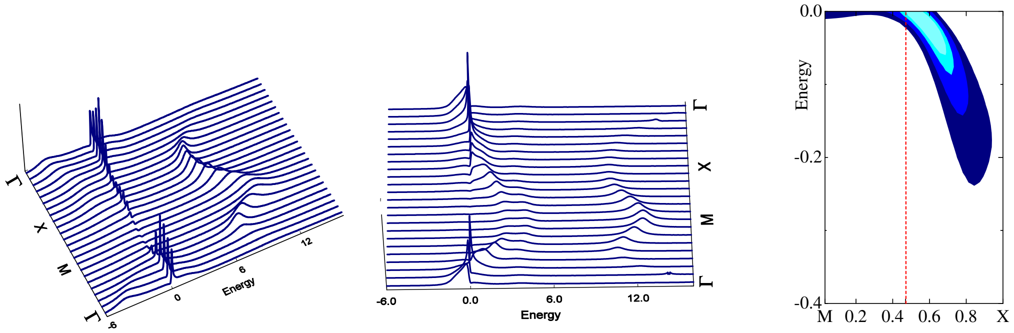

Рис. 2: Spectral functions along the symmetry directions $\Gamma(0,0) \to M(\pi,\pi) \to X(\pi,0) \to \Gamma(0,0)$ for $\delta = 0.05$ (left panel) and $\delta = 0.3$ (central panel), and $A(\mathbf{k},\omega)$ in the $M \to X$ direction at the Fermi level crossing (right panel).

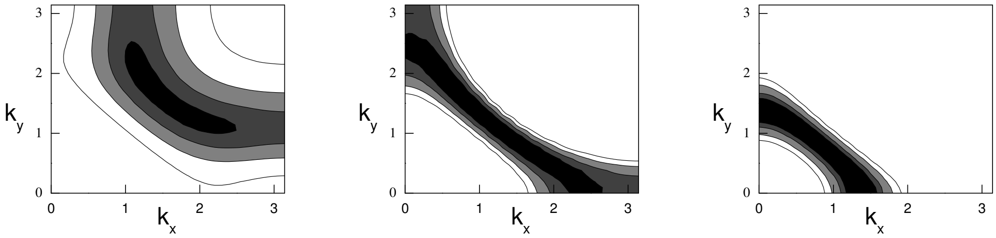

Рис. 3: $A(\mathbf{k}, \omega = 0)$ on the FS for $\delta = 0.1$, 0.2 and $\delta = 0.3$ (from left to right).

upper to the lower band as shown in Fig. 1, right panel. The self-energy $\tilde{\Sigma}(\mathbf{k}, \omega)$ reveals an appreciable variation with $\mathbf{k}$ and doping close to the Fermi level. Figure 2 (right panel) shows a change of the dispersion (kink) in the $M \rightarrow X$ direction at the Fermi level crossing for $\delta = 0.1$. For the coupling constant we get an estimation $\lambda = v_{\mathrm{F}}/v_0 - 1 \simeq 2.4$ ($\lambda \simeq 0.7$ for $\delta = 0.3$). The FS changes from a hole arc-type at $\delta = 0.1$ to an electron-like one at $\delta = 0.3$ (Fig. 3).

To conclude, the microscopic theory based on HO technique for the effective Hubbard *p-d* model (1) provides an explanation for doping and temperature dependence of electronic spectrum in cuprates which is controlled by the AF spin correlations. Therefore, the electron-phonon interaction may be not important in cuprates. Superconducting pairing in the model beyond the weak coupling approximation [8] will be considered elsewhere.

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CROSSOVER PHENOMENON
IN
SELF-ORGANIZING ACTIVE WALK.

Vl. V. Papoyan

The active walk is a paradigm for self-organization and pattern formation in simple and complex systems, investigated since 1992. In the active walk, a walker (an agent) changes the deformable landscape as it walks and is influenced by the changed landscape in choosing its next step. Active walk models have been applied successfully to various biological, chemical and physical systems from the natural sciences to economics and many other topics from the social sciences [1].

The recent studies of the special important issue, the non-equilibrium behavior of a medium with long memory have shown that the dynamics can be represented as a sort of random walk on an effective graph. The vivid examples are the so-called Eulerian Walk Model (EWM) [2] and the Relaxing Self-Avoiding Walk (RSAW) [3] which demonstrate this phenomenon: self-organization of the walker motion as well as the medium.

For finite lattices, during the evolution EWM and RSAW settle into the limit cycles, Eulerian and Hamiltonian, respectively. The underlying medium tends in both cases to the self-organized state which is characterized by long-range correlations.

Studding the mean square distance $R^2 \sim T^{2\nu}$ travelled by a walker for time T on the infinite lattice, an interesting fact emerged. Namely, the Eulerian walk on the square two-dimensional lattice calls up the diffusion law $\nu \simeq \frac{1}{3}$ [2] while on the chessboard lattice $\nu \simeq \frac{4}{7}$ [3] which coincides with the exponent for θ-polymers [4].

Our investigation shows that the exponent ν can be sensitive not only to dynamics of walker but also to the length of characteristic time interval where this exponent is determined.

In order to demonstrate different types of behavior of an active walker at different time scales, one can complicate the Eulerian walker rules in the following way. Visiting some lattice site i the walker reflects the arrow at i, and moves in the opposite direction. Visiting this site next time, it reflects the arrow again and moving this new direction. After the third return to this site it flips the arrow by 90^o and repeats the procedure it performed being at this site the first and second times. Denoting by N, E, S, W four possible directions of arrows, we can write the sequential orientations of arrows at site i after a series of visits as $...N, S, N, S, E, W, E, W, N, S, N, S...$ The resulting pattern at each site is the cross drawn by the arrow twice.

It is worth to note that the suggested “double cross” dynamics in a certain sense is intermediate between the clockwise Eulerian walk on a square lattice and the Eulerian walk model on the chessboard lattice. Indeed, each site allows all possible walk directions and in this respect it is similar to the clockwise Eulerian model on a square lattice. On the other hand the “double cross” model has common features with the Eulerian walk on chessboard lattice, since at local time intervals the motion is reflective.

This modification of the Eulerian walk dynamics leads to crossover phenomena at the different time scales (Fig.1). At the initial stage (up to 10^5 steps) the scaling behavior is consistent with $\nu \simeq \frac{1}{2}$, specific to the RSAW model. Then it passes through the intermediate regime and finally achieves the scaling law $\nu \simeq \frac{1}{3}$ at large number of steps ($t = 150 \times 10^6$). The last exponent corresponds to the Eulerian walk on a square lattice.

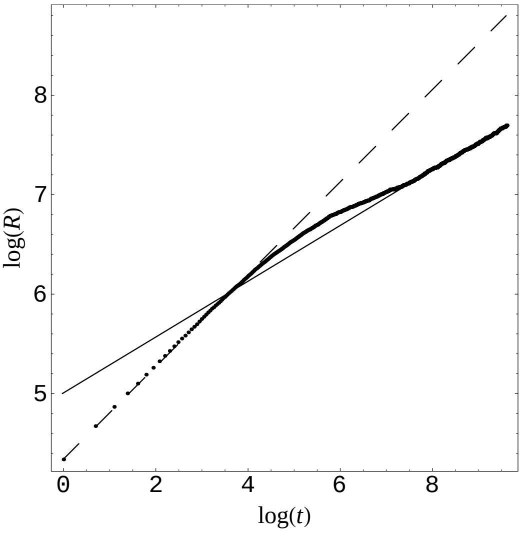

Рис. 1: Log-log plot of the diffusion law for the “double cross” dynamics. Simulations of 150×10^6 steps averaged over $2 \cdot 10^4$ runs (bold curve). The thin line correspond to the fit with incline $\nu \simeq \frac{1}{3}$ and dash one with $\nu \simeq \frac{1}{2}$ respectively.

Moreover understanding of the underlining phenomenon will shed light on the problem of universality for various classes of walks.

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SPHEROIDAL GEOMETRY APPROACH TO FULLERENE MOLECULES

R. Pincak

Graphite is an example of a layered material that can be bent to form fullerenes which promise important applications in electronic nanodevices. The spheroidal geometry of a slightly elliptically deformed sphere was used as a possible approach to fullerenes. We assumed that for a small deformation the eccentricity of the spheroid $e \ll 1$. We are interested in the elliptically deformed fullerenes C_{70} as well as in C_{60} and its spherical generalizations like big C_{240} and C_{540} molecules. The low-lying electronic levels are described by the Dirac equation in (2+1) dimensions. In the report [1] we show how a small deformation of spherical geometry evokes a shift of the electronic spectra compared to the sphere and both the electronic spectrum of spherical and the shift of spheroidal fullerenes were derived.

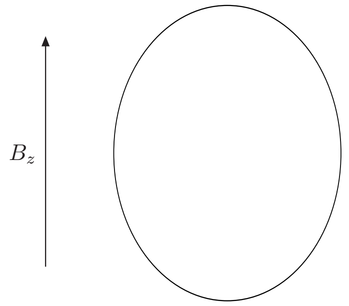

Рис. 1: The schematic picture of the spheroidal fullerene in a weak uniform magnetic field pointed in the z direction.

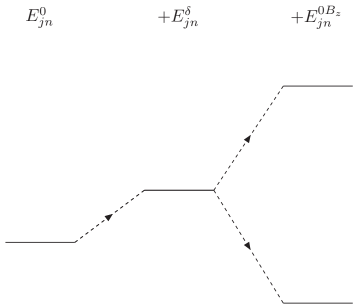

Рис. 2: The schematic picture of the first positive electronic level E^δ_{jn} for spheroidal fullerenes in a weak uniform magnetic field pointed in the z direction.

In the next study the expanded field-theory model was proposed to study the electronic states near the Fermi energy in spheroidal fullerenes. The low energy electronic wave functions obey a two-dimensional Dirac equation on a spheroid with two kinds of gauge fluxes taken into account. The first one is so-called K spin flux which describes the exchange of two different Dirac spinors in the presence of a conical singularity. The second flux (included in a form of the Dirac monopole field) is a variant of the effective field

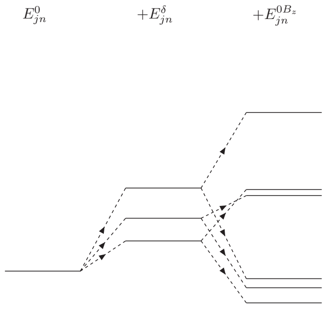

Рис. 3: The schematic picture of the second positive electronic level E^{δ}_{jn} for spheroidal fullerenes in a weak uniform magnetic field pointed in the z direction.

approximation for elastic flow due to twelve disclination defects through the surface of a spheroid. We consider the case of a slightly elliptically deformed sphere which allows us to apply the perturbation scheme. We shown exactly how a small deformation of spherical fullerenes provokes an appearance of fine structure in the electronic energy spectrum E^{δ}_{jn} as compared to the spherical case E^0_{jn}. In particular, two quasi-zero modes in addition to the true zero mode are predicted to emerge in spheroidal fullerenes. An additional 'hyperfine' splitting of the levels (except the quasi-zero-mode states) was found [2].

The effect of a weak uniform magnetic field on the electronic structure of slightly deformed fullerene molecules was also studied. In the report [3] was shown how the existing due to spheroidal deformation fine structure of the electronic energy spectrum splitted in the presence of the magnetic field. Exact analytical solutions for zero-energy modes was also found and compare with HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) gap calculated in density-functional methods approaches of fullerenes. As an illustration, Figs. 1,2,3 schematically show with accuracy at about one percent of E^0_{jn}, how the electronic spectra of spheroidal fullerenes are splitted $E^{0B_z}_{jn}$ in the presence of weak magnetic field pointed in the z directions.

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BREAKPOINT PHENOMENON
IN INTRINSIC JOSEPHSON JUNCTIONS

Yu.M.Shukrinov[1] **and F.Mahfouzi**[2]
[1] BLTP, JINR, Dubna, Russia
[2] IASBS, Zanjan, Iran

Creating new materials with given properties is an actual problem of physics, chemistry, and material science. This is related to the system of Josephson junctions, too, which is a perspective object for superconducting electronics and is being investigated intensively now. A simulation of the current-voltage characteristics (IVC) of a stacks of intrinsic Josephson junctions (IJJ) at different values of the model parameters such as the coupling α and dissipation β parameters is a way to predict the properties of the IJJ. McCumber and Steward have investigated the return current as a function of dissipation parameter in a single Josephson junction a long time ago.[1] In the case of the system of junctions, the situation is cardinally different. The IVC of IJJ is characterized by a multiple branch structure and branches have a breakpoint region with its breakpoint current (BPC) and transition current to another branch. [2, 3] The BPC is determined by the creation of the longitudinal plasma waves (LPW) with a definite wave number k, which depends on the parameters α and β, the number of junctions in the stack, and boundary conditions. [4]

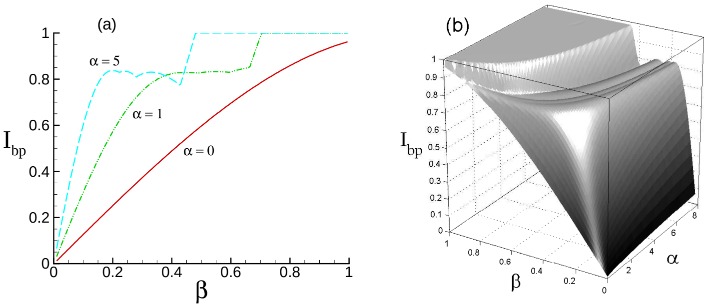

Рис. 1: (Color online) (a) - The β-dependence of the BPC I_{bp} of the outermost branch in the IVC at different values of coupling parameter α; (b) - The $\alpha\beta$-dependence of the I_{bp} for a stack of 10 IJJ. From Ref.[5].

We generalized the McCumber-Steward dependence of the return current for the case of IJJ in the HTSC.[5] We investigate the BPC I_{bp} on the outermost branch as a function of the coupling α and dissipation β parameters for the stacks with a different number of IJJ and demonstrate a plateau with BPC oscillation, which is shown in Fig. 1 Based on the idea of the parametric resonance in the stack of IJJ, a modeling of the $\alpha\beta$-dependence of the BPC has been done, and good qualitative agreement with the results of simulation has been obtained. We show that the $\alpha\beta$-dependence of the BPC is an instrument to determine the mode of LPW created at the breakpoint in the stacks with a different number of junctions.

Fig. 2(left) shows the result of simulation of the outermost branch in the IVC near the breakpoint for a stack with $\alpha = 3$, $\beta = 0.3$ and N from $N = 3$ to $N = 15$. We can see that

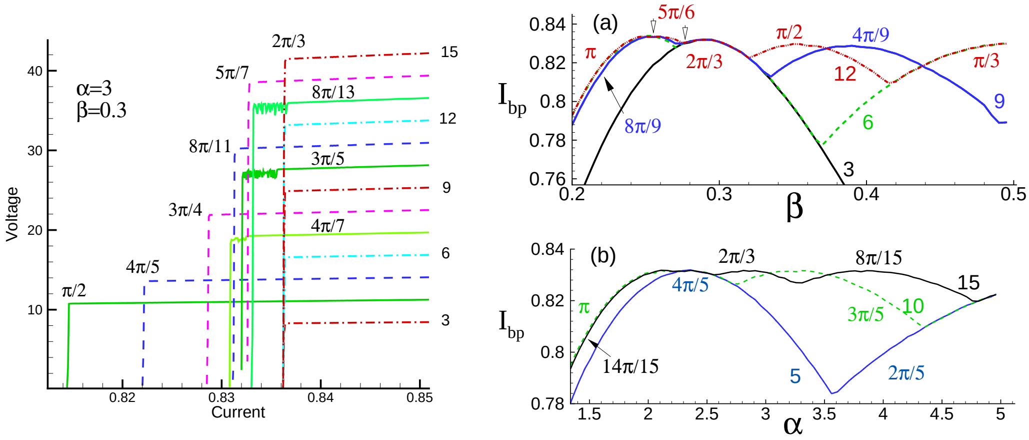

Рис. 2: (Color online) Left: The simulated IVC of the outermost branch in the stacks with a different number of junctions at $\alpha = 3$, $\beta = 0.3$; Right: a) - The simulated β-dependence of the I_{bp} for the stacks with 3, 6, 9 and 12 IJJ at $\alpha = 3$. The region corresponding to the creation of the LPW mode with wave number $k = 5\pi/6$ is shown by arrows . b) - The simulated α-dependence of the I_{bp} for the stacks with 5, 10 and 15 IJJ at $\beta = 0.3$. From Ref.[5].

the value of I_{bp} depends on the number N of IJJ in the stack, excluding the stack with $N = 3n$, where n is an integer number. We explain these results using the idea of LPW creation at the breakpoint. We predict also a different commensurability manifestation in the IVC of stacks with a different number of IJJ.[4, 5]

Comparison of the α- or β-dependence of the I_{bp} for stacks with a different number of IJJ give us a simple method to determine the wave numbers k of the LPW. Fig. 2(right) shows the β- and α-dependence of the I_{bp}. It demonstrates that, in some intervals of β and α, the stacks with different N have the equal value of the I_{bp}. Using these data, we can determine all modes of LPW, which might be created in stacks with different parameters α and β and a different number of IJJ.

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