Formation of extended coherent states in cuprates up to $T = 1200$ K

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Abstract

The proposed microscopic model purports to reveal the genesis of pseudogap anomalies in underdoped cuprates. An analysis is based on a concept of "polymerization" of pseudo-atoms with quantized hole "orbitals" of the same rank η into spin-charge stripes by means of strong electron correlations and self-organization effects. At rather low doping level $\bar{n}_p \approx 1/18$, this "reaction" is accompanied by the hole pairing at $T''_\eta \leq 1450$ K on such orbitals and the subsequent formation of *extended coherent states* below $T^*_\eta \leq 1200$ K under a spatially modulated Coulomb extra-potential relief. The evolution of modeled electronic spectra under increasing $\bar{n}_p$ is consistent with experimental findings "suggesting that the pseudogap has the same origin as the superconducting gap".

Key words: cuprates; pseudogap; stripes; superconductivity

In recent years, the study of unusual doping dependences of electronic properties in cuprates has attracted increasing attention [1]. The main challenge is to understand the puzzling properties of the *pseudogap region* [2] in the generic $T^* - \bar{n}_p$ diagram [3], where $\bar{n}_p$ is the average quantity of holes in oxygen shells per CuO_2 unit and $T^* \leq 800$ K is the temperature of a pseudogap development.

A simplified version of the proposed microscopic model is based mainly on a consideration of upper electronic (hole) states [4] in the sublattice of overlapped O $2p$ shells [5]. In accord with the tight-binding approximation, the upper band $E_{n,\mathbf{k}}$ of undoped CuO_2 layers can be represented by the antisymmetric combination of Wannier functions which involve antibonding $2p(\sigma^*)$ molecular orbitals predominantly, neglecting their hybridization with Cu $3d$ states [4]. In the first approximation, the analysis of a variety of states at $T \to 0$ can be reduced to the diagonal *collective* [1] modes with $\mathbf{k} \leq (\pi, \pi)$ which are arising in the 1D orthogonal oxygen chains due to strong electron correlations (the string approach). These Bloch-like solutions constitute a band of $\mathcal{W}_B = \hbar^2/4m_e\bar{r}_o^2$ in width centered around a binding energy $\bar{E}_0 = \hbar^2/2m_e\bar{r}_o^2 \approx 2.05$ eV [4], where $\bar{r}_o = 0.136$ nm is half the typical O–O separation in CuO_2 layers and m_e is the electron mass.

At $\bar{n}_p \approx 1/18$, a given hole from CuO_2 layer is bounded with the ion-dopant from an adjacent layer. A mean radius of hole states in such "pseudo-atoms" does not exceed $d \approx 0.8$ nm [5] and each hole has to hop within a "cage" composed of eight O ions [4] (d is the double Cu–Cu separation). A raise in $\bar{n}_p$ brings about smoothing the extra-potential relief from dopants and hence increasing the average number $\bar{N}_\eta = 4\eta$ of oxygen sites involved in centrosymmetric quantized hole "orbital" $\mathcal{R}_{\eta\uparrow}$, where η is its rank. Following to the Feynman path-integral representation, one can derive both the average binding energy $\bar{E}_\eta = \bar{E}_0/2\eta$ for excitation $\mathcal{R}_{\eta\uparrow}$ with a single hole and the maximum pairing strength $|\Delta_\eta| = \bar{E}_0/8\eta$ for $\mathcal{R}_{\eta\uparrow\uparrow}$ with a hole pair in the *triplet* state [4]. Though it contradicts prevalent speculations about the symmetry of the superconducting order parameter but experiments argue that the stripes in UD cuprates should have local *ferromagnetic* moment [6]. The excitations $\mathcal{R}_{\eta\uparrow}$ and $\mathcal{R}_{\eta\uparrow\uparrow}$ are termed rhombons [4] and birhombons respectively since their ordering into stripes is associated with the local rhombic distortion of the undoped lattice.

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An ordering of $\mathcal{R}_{\eta\uparrow\uparrow}$ with the same η into stripes (the concept of polymerization of "pseudo-atoms") results in a formation of *extended coherent states* (ECS) below the critical temperature $T^*_{c\eta} = \mathcal{C}_\eta \bar{E}_0 [2k_B(2\eta^2 + \eta)]^{-1}$, where k_B denotes the Boltzmann constant and $\mathcal{C}_\eta \leq 1$ is the factor of compatibility of self-organized longitudinal potential wells to the optimal realization [4]. Thus, the values $\bar{E}_\eta$, $|\Delta_\eta|$ (or $T''_\eta = k_B|\Delta_\eta|$), and $T^*_{c\eta}$ can be treated as the basic discrete coordinates on the energy scale, reflecting the inherent spatial inhomogeneity of cuprates with the same *basis* generative (vacuum) mode $\bar{E}_0 \approx 2$ eV.

It should be noticed that there is little probability of a creation of ECS from $\mathcal{R}_{1\uparrow\uparrow}$. Rather one can expect the formation of an impurity band composed of $\mathcal{R}_{1\uparrow}$ with $E_B = E_0/2\eta \approx 1$ eV. Indeed, the dispersive peak at $E_B = 0.8 \div 1.2$ eV has been found in the ARPES spectra of the nearly insulating $Sr_2CuO_2Cl_2$ [7]. Besides, the ARPES spectra of $YBa_2Cu_3O_{6.9}$ also demonstrate the striking peak at $E_B \approx 1$ eV [8], but its origin has to be related to $(CuO_3)_n$ chains.

The proposed model predicts that the most favorable segments in $T - \bar{n}_p$ diagram for realization of ECS composed of given $\mathcal{R}_{\eta\uparrow\uparrow}$ have to be centred around $\bar{n}_{p\eta} = \eta/\eta_m^2$, where $\eta_m = 6$ determines a location of "golden mean" ($0.125 \leq \bar{n}_p \leq 0.21$) on the bottom of $T - \bar{n}_p$ diagram which is usually limited by $2\bar{n}_{p6} = 1/3$. An analysis shows also a possibility of the percolation superconductivity with suppressed T_c at $1/18 \leq \bar{n}_p \leq 5/18$, i.e., beyond the "golden" segment. Since (bi)rhombons can be considered as microvortices, their participation in a charge-spin transport at $T \to 0$ supposes the deciding contribution from tunneling and resembles the phenomenon of quantum creep in superconductors with the short coherence length $\xi_s \leq 5$ nm [9].

The dynamical ordering of stripes (directed along Cu-O-Cu bonds) has to be most spatially uniform at $\bar{n}_{pm} \approx 1/6$ because ones have to dot the whole CuO_2 layer bearing in mind that the rhombon periodicity along stripes equals to d. However the phase coherence size along stripes are restricted by a topological length $\xi_m = 4\eta d$ at $T \to 0$ which results from minimization of the infrared divergence of angular field fluctuations. Taking into account the absence of holes on borders of this texture, the optimal doping level must be located near $\bar{n}_{po} = 4/(4\eta_m + 1) = 0.16$ [4]. For this case, the mentioned relations yield $\bar{E}_6 = \bar{E}_0/2\eta_m \approx 170$ meV, $|\Delta_6| = \bar{E}_0/8\eta_m \approx 42$ meV and $T^*_{c6} \approx 153$ K at $\mathcal{C}_6 = 1$. The value T^*_{c6} is consistent with our earlier (1990) extrapolation of $T_c(\bar{\varepsilon})$ dependences to $T_{c,max} \approx 150$ K with reducing the normalized interlayer distance $\bar{\varepsilon} \to 0.95$ [10] and subsequent studies of Hg-based cuprates under pressure. In addition, the analysis of hole distribution in $YBa_2Cu_3O_{6.94}$ permits to derive $\mathcal{C}_6 = 0.6$ [4] that corresponds to $T^*_{c6} \approx 92$ K.

The modeled value of $|\Delta_6|$ is in accord with the amplitude of the anisotropic superconducting gap $|\Delta_{sc}|$ at $\bar{n}_p \approx 0.16$, generally determined from the location of the peak in the ARPES [1] or tunneling spectra [11]. Along with the peak, the spectra demonstrate also a hump (so called the peak-deep-hump structure) [1] which can be related to $\mathcal{R}_{\eta\uparrow}$ with unpaired holes. Both the peak and the hump move to higher energy with lowering $\bar{n}_p$ (or η). Moreover, the experiments show the nearly unchanged ratio "hump/peak" (≈ 4) for the whole investigated doping range $\bar{n}_p = 0.08 \div 0.21$ [1] as it follows from the relation $\bar{E}_\eta = 4|\Delta_\eta|$.

Numerous experimental signatures (> 20) in favour of superconducting ingredient of the (pseudo)gap conundrum in UD cuprates and some other oxides can be supplemented by recent observations of resistance drops and other concomitant phenomena indicative of possible localized superconductivity with "heatproof" values of $T^*_{c\eta}$ up to 1200 K in composite samples Cu/CuO [12].

In summary, the present model permits to simulate the evolution of electron spectra in the UD cuprates with doping without application of any adjustable parameters. Obtained results are consistent with experimental findings "suggesting that the pseudogap has the same origin as the superconducting gap" [11].

References

[1] J. C. Campuzano, H. Ding, M. R. Norman et al., Phys. Rev. Lett. **83** (1999) 3709.

[2] B. Batlogg, C. M. Varma, http://physicsweb.org/article/world/13/2/8 (2000).

[3] B. Batlogg, H. Y. Hwang, H. Takagi et al., Physica C **235-240** (1994) 130.

[4] A. V. Mitin, Proceedings of the XIV Ural International Winter School on the Physics of Semiconductors, Ekaterinburg, 18 - 22 Febr. 2002, L10.

[5] A. V. Mitin, G. M. Kuz'micheva, V. V. Murashov et al., Zh. Eksp. Teor. Fiz. **107** (1995) 1943 [JETP **80** (1995) 1075].

[6] Y. Ando, A. N. Lavrov, K. Segawa, Phys. Rev. Lett. **83** (1999) 2813.

[7] B. O. Wells, Z.-X. Shen, A. Matsuura et al., Phys. Rev. Lett. **74** (1995) 964.

[8] J. G. Tobin, C. G. Olson, C. Gu et al., Phys. Rev. B **45** (1992) 5563.

[9] A. V. Mitin, Phys. Rev. Lett. **73** (1994) 2275 and references therein.

[10] N. E. Alekseevskii, A. V. Mitin, V. I. Nizhankovskii et al., Physica B **163** (1990) 659.

[11] Ch. Renner, B. Revaz, J.-Y. Genoud et al., Phys. Rev. Lett. **80** (1998) 149.

[12] V. V. Osipov, I. V. Kochev, S. V. Naumov, Zh. Eksp. Teor. Fiz. **120** (2001) 1246 [JETP **93** (2001) 1082].