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Breakdown of the Fermi arcs in underdoped cuprates by incommensurate charge density waves

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We studied interactions between the coherent excitations on disconnected arcs along a "bare" Fermi surface (the so-called Fermi arcs FAs) seen by angle-resolved photo emission spectroscopy (ARPES) in several underdoped (UD) cuprates and incommensurate charge density wave (IC CDW) ordering at lowering of the temperature. The carriers on FAs scatter strongly on the short-wavelength potential of CDW. The large momentum transfer relates FAs with the electronic states lying deeply under the chemical potential thus involving into consideration the Fermi liquid interactions. At low temperatures IC CDW may fully destroy low lying excitations on the Fermi arcs, leaving electrons on the pocket at the Γ-point as the only charged elementary excitations in the CDW phase in UD cuprates. The results infer competition between superconducting and CDW order parameters.

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1. Introduction. The high-temperature-superconductivity (HTS) remains one of the most fundamental outstanding problems of condensed matter physics since 1986. With no crucial breakthrough so far in understanding HTS mechanisms it is becoming more and clearer that any further progress in that direction hinges on better understanding properties of the so-call pseudogap (PG) phase from which transition into the superconducting state takes place at a temperature T_S.

The most striking peculiarity in the PG phase is the energy spectrum. Unlike in the ordinary metals, the angle resolved photoemission spectroscopy (ARPES) experiments see the coherent excitations only at parts of the "bare" Fermi surface (FS) known as the Fermi arcs (FAs) [1]. Observation of low frequency quantum oscillations (QOs) [2] revealed the second branch of the energy spectrum in the underdoped (UD) $YBa_2Cu_3O_{6.5+y}$ (YBCO) – that of a small electronic pocket. Although consensus is that these features are generic, direct access to the excitations' spectrum by ARPES is not available yet for every cuprate, with UD YBCO, among others, although the latter is most actively studied in experiments on QOs.

Another experimental fact is existence of the Fermi-liquid-like regime in UD cuprates in the PG phase below some temperature $T^{**}(x) < T^{*}(x)$ [3] ($T^{*}(x)$ is temperature of the PG phase as function of the holes concentration x). The theory [4] allows obtaining the microscopic characteristics of the FAs spectrum from the data on the resistivity and the Hall coefficient thereby compensating absence of the ARPES data. Experimentally, the small pocket is seen not only in QOs – it manifests itself indirectly in a non-monotonic temperature dependence of the Hall coefficient in YBCO [5] and $HgBa_2CuO_4$ (Hg1201) [6]. In both case, however, it refers to experiments at low temperatures where matters get complicated by the incommensurable (IC) charge density wave (CDW) ordering in cuprates [7–11].

Observed recently in diffraction and the resonant X-ray scattering experiments the tendency to charge order presents an additional and somewhat unexpected obstacle to our further understanding of processes in UD cuprates at low temperatures. In particular, IC CDW order seems to be detrimental for the superconducting state [12, 13].

The electronic pocket will be mentioned here only in passing (see [14] for the more detailed discussion). The view popular in the current literature is that the latter comes about owing to the FS reconstruction in the CDW transition [2, 5, 6, 15, 16]. The numerical calculations [17] specially undertaken to confirm possibility of such scenario find an electronic pocket bordering by one side with the Fermi arc [17]. Such pocket must inevitably be gapped below T_S by the superconducting order parameter. Meanwhile, the low temperature specific heat data [18] in the *superconducting* phase show that electrons on the pocket remain in the metallic state with the non-zero Sommerfeld coefficient down to $T \leq 5\,\mathrm{K}$.

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Thereby, not only is the pocket disconnected from FAs, but it must be at a high-symmetry point in the Billouin zone (BZ) [19].

With this last result in mind it becomes justified our concentration below only on the interactions between CDW and carriers at the Fermi arcs. The latter contribute most into the charge transport at higher temperatures [4], so that without resolving this question impossible compare the relative role of the arcs and of the pocket which, this way or another, assumed to be present below the CDW transition.

2. Interaction of FAs holes with CDW. In the model [4] for the Fermi-liquid-like regime the spectrum of carriers on FAs near each nodal point below $T^{**}(x) < < T^{*}(x)$ has the form:

$$\varepsilon(\mathbf{p}) = \pm\nu_{\rm F}(p_{\parallel} \mp p_{\rm F}) - \frac{p_{\perp}^2}{2m^*}. \qquad (1)$$

(The arc's length is $\Delta\varphi p_{\rm F}$; $p_{\rm F}$, $\nu_{\rm F}$ are the Fermi momentum and the Fermi velocity, respectively; $p^{\parallel}$, $p^{\perp}$ stand for the parallel and the perpendicular momentum projections on direction of one of the two diagonals; the Γ-point lies inside the area of the BZ occupied by electrons; the sign "$\pm$" varies depending on the chosen nodal point).

High energy features of the spectrum of the PG phase are assumed fixed; the antinodal gaps seem too large compared with $T_{\rm CO}$ ($T^{**}(x) > T_{\rm CO}$ [16]) and besides are material independent (at same doping level) [20, 21]. In $La_{2-x}Ba_xCuO_4$ (LBCO) at the "magic" concentration $x = 1/8$ the antinodal gap survives above temperature of the transition into the stripe phase [13]. In conjunction with the T^2 – dependence of resistivity, sizes of FAs below $T^{**}(x)$ are temperature independent [3, 4].

We trace evolution of the CDW from beginning of the fluctuations regime and down to onset of the thermodynamic CO phase; thereby the CDW potential is small *a priori*. Transparency of the analytical approach allows shedding new light on the controversy.

The experimental temperature interval for fluctuations is rather broad $|T_{\rm onset} - T_{\rm CO}| \geq T_{\rm CO}$ resembling the CDW transition, e.g., in $2H$-$TaSe_2$. This signifies a short coherence length [22] so, regretfully, the phase transition cannot be described by the Landau theory of the second order phase transitions. Fluctuations are quasistatic (see e.g. [10]), possibly being partially pinned by defects.

Without loss of generality it is enough to consider the unidirectional periodic potential with an IC vector $\mathbf{Q}_0$: $\mathbf{Q}_0 \to Q_{0x} \equiv Q_0$ (from now on the vector notation for $\mathbf{Q}_0$ and the sub-index x will be omitted).

For simplicity, we leave aside spins and the issue of possible antiferromagnetic (AFM) transition. The standard "density-density" Hamiltonian gives for the interaction of electrons with the charge density $n(r) \to N(r)$:

$$\hat{H}_{\rm CDW} = \iint \hat{\psi}^{+}(\mathbf{r})\hat{\psi}(\mathbf{r})U_0(\mathbf{r}-\mathbf{r}')n(\mathbf{r})d\mathbf{r}d\mathbf{r}'. \qquad (2)$$

In Eq. (2) $U_0(\mathbf{r}-\mathbf{r}')$ is a short-range Coulomb potential ($U_0(\mathbf{r}-\mathbf{r}') \sim 1\,$eV). Density may have the detailed structure, as e.g. in the so-called stripes, but for the sake of argument it is enough confine oneself below to first harmonics. Then in the ordered CO phase (below $T_{\rm CO}$):

$$N(\mathbf{r}) \equiv n(x) = \bar{n}_0(T)\exp[\pm iQ_0(x-x_0)]. \qquad (3)$$

Here $\bar{n}_0(T)$ is the CO order parameter. In the *fluctuation* regime $T_{\rm onset} > T > T_{\rm CO}$:

$$n(x) = \Sigma_{\pm}\int n_q dq \exp[\pm i(Q_0+q)(x-x_0)], \qquad (4)$$

or

$$n_{\pm}(x) = n(x)\exp[\pm iQ_0(x-x_0)] \qquad (5)$$

(x_0 stands for arbitrariness of the IC CDW position). Following [7], the fluctuations n_q were chosen in the Gaussian form:

$$n_q = (\bar{n}/\sqrt{2\pi})\xi\exp[-(q\xi)^2/2]. \qquad (6)$$

(At $\xi \to \infty$ the expression transforms into the δ-function $(1/\sqrt{2\pi})\xi\exp[-(q\xi)^2/2] \Rightarrow \delta(q)$. That would bring one back to the charge order parameter $\bar{n} \to \bar{n}_0(T)$ in Eq. (3)).

Rewrite the Hamiltonian (2) in the momentum representation as:

$$\hat{H}_{\rm CDW} = \sum_{\mathbf{p},\mathbf{p}\pm Q}\hat{M}(\mathbf{p};\mathbf{p}\pm Q). \qquad (7)$$

Here the operators $\hat{M}$ are:

$$\hat{M}(\mathbf{p};\mathbf{p}\pm Q) = \hat{a}_p^{+}\hat{a}_{\mathbf{p}\pm Q}U_0(\pm Q,0)n(Q)\exp(\mp iQx_0). \qquad (8)$$

In Eq. (8) $U_0(\pm Q,0)$ is the Fourier component of the potential $U_0(\mathbf{r}-\mathbf{r}')$; commonly, value $|Q| \approx Q_0$ is of the order of few tenths of $2\pi/a$, where a – the lattice period [7–11].

Interactions (7), (8) cannot affect carriers on the Fermi arc directly. The matrix elements for transitions between two states with the two momentums $\mathbf{p}$, $\mathbf{p}'$ *inside the arc* appear in the second order.

Introducing for shortness $W(p_x, p_x'; p_y) = \langle\Sigma_{\pm,l}\hat{M}(\mathbf{p};\mathbf{l}\pm Q)\hat{M}(\mathbf{l}\mp Q;\mathbf{p}')\rangle$ for the latter obtain:

$$W(p_x,p_x';p_y) = |U_0|^2 e^{i(p_x'-p_x)x_0}\int\frac{dl}{2\pi}\times$$

$$\times \Sigma_{\pm}\left[\frac{\tilde{n}(p_x-l)\tilde{n}(l-p'_x)}{\varepsilon(p_x;p_y)+\mu-E(p_x+l_x\pm Q_0;p_y)}\right]. \quad (9)$$

(Notice that with the new notations $U_0(\pm Q,0)\equiv U_0a^2$ the "density" $\tilde{n}=na^2$ in Eq. (9) is dimensionless.) If the coherence length $\xi(T)$ is large $\xi\gg a$ one can omit in $E(p_s+l_x\pm Q_0;p_y)$ the dependence on l_x. In (9) p_x, p_y are in a vicinity of the arc; so that the energy $\varepsilon(p_x;p_y)\equiv\varepsilon(\mathbf{p})$ from Eq. (1) is small; large is the value of $|\mu-E(p_x+l_x\pm Q_0;p_y)|$ ($\varepsilon_{\rm F}\equiv\mu$ is the chemical potential). Substituting $\tilde{n}$ from (6) and integrating over l_x one finds:

$$W(p_x,p'_x;p_y)=\frac{|U_0|^2}{\bar{E}(\pm Q;p_y)}\left(\frac{\tilde{\tilde{n}}}{4\pi^{3/2}\xi}\right)\times$$

$$\times\, e^{i(p'_x-p_x)x_0}\exp\left[-\frac{(p_x-p'_x)^2\xi^2}{4}\right]. \quad (10)$$

(Notice the dependence on the position p_y along the arc.) One could proceed further and calculate the inverse scattering time for the arc's carriers on fluctuation in IC CDW:

$$\frac{1}{\tau_{\rm FA,CDW}}=\sqrt{\pi^3/2}\,\tilde{\tilde{n}}(T)^4\frac{\xi(T)p_{\rm F}}{\Delta\varphi}\times$$

$$\times\,\frac{1}{2}\Sigma_{\pm}\left[\frac{|U_0|^4}{\varepsilon_{\rm F}\bar{E}(p_x\pm Q;p_y)^2}\right]. \quad (11)$$

(Here and below in notations: $p_x+l_x\pm Q_0\to p_x\pm Q$.)

3. The Fermi liquid interactions. Substitution of Eq. (3) into (9) below $T_{\rm CO}$ ($p_x=p'_x$) would *formally* give correction to the energy spectrum in the CO phase:

$$\Delta\bar{\varepsilon}(p_x;p_y)=|U_0|^2\tilde{\tilde{n}}(T)^3\times$$

$$\times\,\Sigma_{\pm}\left[\frac{1}{\varepsilon(p_x;p_y)+\mu-E(p_x\pm Q;p_y)}\right]. \quad (12)$$

Such procedure suffers, however, from the significant oversimplification. Remind once again that the "bare" FS encircles states in the momentum space in the BZ *filled* by electrons. Electron-electron correlations are known to be strong in cuprates and below the chemical potential (i. e. under the "bare" FS) electrons form the Fermi liquid (FL). Among fundamentals of the FL concept is that *no individual* elementary excitations exist far below the Fermi level. Experimentally, excitations are identified by ARPES as peaks in the spectral function $A(\mathbf{p},\omega)$ [1]:

$$A(\mathbf{p},\omega)=-\frac{1}{\pi}\frac{\Sigma''(\mathbf{p};\omega)}{[\omega-\varepsilon(\mathbf{p})-\Sigma'(\mathbf{p},\omega)]^2+[\Sigma''(\mathbf{p},\omega)]^2}. \quad (13)$$

Away from the Fermi surface, large in the latter are both the real and the imaginary self-energy parts $\Sigma(\mathbf{p},\omega)=\Sigma'(\mathbf{p},\omega)+i\Sigma''(\mathbf{p}\omega)$, in the Green function $G(\mathbf{p},\omega)=\{\omega-\varepsilon(\mathbf{p})-\Sigma(\mathbf{p},\omega)\}^{-1}$.

Therefore, for Eq. (12) to be the self-energy part of the Green functionfor $G_{\rm FA}(p_x,p_y;\omega)$ the Fermi arcs carriers $G^{-1}_{\rm FA}(p_x,p_y;\omega)=\omega-\varepsilon(p_x,p_y)-\Sigma_{\rm FA}(p_x,p_y;\omega)$ the Fermi liquid interactions must be accounted more attentively:

$$\Sigma_{\rm FA}(p_x,p_y;\omega)=|U_0|^2\tilde{\tilde{n}}_0(T)^2[G(\mathbf{p}-Q,\omega)+G(\mathbf{p}+Q,\omega)]. \quad (14)$$

Consider, for example, the Fermi arc in the upper right quadrant of the BZ near the $(\pi/2,\pi/2)$ nodal point. In this particular case it is the vector(p_x-Q,p_y) in (14) that falls into the area filled by electrons. (Vector (p_x+Q,p_y) lies in the unoccupied area.) $\Sigma'(\mathbf{p}-Q,\omega\simeq\simeq 0)\sim\Sigma''(\mathbf{p}-Q,\omega\simeq 0)$ in Eqs. (13), (14) are of the same magnitude. Defining in $G^{-1}_{\rm FA}(p_x,p_y;\omega)=\omega-\varepsilon(p_x,p_y)-\Sigma_{\rm FA}(p_x,p_y;\omega)$ the pole $\omega=\bar{\varepsilon}(p_x,p_y)$, one ends up with

$$\bar{\varepsilon}(p_x,p_y)=\varepsilon(p_x,p_y)+$$

$$+\,|U_0^2/\varepsilon_{\rm F}|\tilde{\tilde{n}}_0(T)^2[f(p_x,p_y)-i\tilde{\Gamma}(p_x,p_y)], \quad (15)$$

where dimensionless $f(p_x,p_y)$ and $\tilde{\Gamma}(p_x,p_y)$ are known only by the order (of the order of unity).

Below temperature of the CDW transition $T_{\rm CO}$ $\tilde{\tilde{n}}(T)$ is non-zero and increases. Excitations at FAs for which $\varepsilon(p_x,p_y)<|U_0^2/\varepsilon_{\rm F}|\tilde{\tilde{n}}(T)^2$ have the real and imaginary parts of the same magnitude and, hence, cannot be considered anymore as elementary excitations.

Formally, same FL effects should be accounted for in Eq. (11), but that would leave the qualitative conclusions basically unchanged as the parameters U_0, $\varepsilon_{\rm F}$, $\bar{E}(\pm Q;p_y)$ are not known (intuitively, U_0 in $U_0(\pm Q,0)\equiv U_0a^2$ proportional to the coupling energy with CDW parameter seems to be the smallest of the three).

4. Conclusion. Expressions (11) and (15) are the main results of this presentation: FAs excitations scatter strongly on IC CDW with short wavelengths. The Fermi liquid interactions may even fully *destroy* coherence on FAs. The only elementary excitations intact by the CDW transition and remaining in the CO phase down to the lowest temperatures are electrons on the pocket located at the Γ-point of the BZ [19]. The results have obvious implications at the Cooper pairing between carriers on the opposite Fermi arcs.

Above $T_{\rm CO}$ the inverse scattering time for holes (Eq. (11)) is proportional to $\tilde{\tilde{n}}(T)^4[\xi(T)p_{\rm F}/\Delta\varphi]$ and increases with lowering of the temperature ($\xi(T)p_{\rm F}\to\infty$ in the ordered phase). The imaginary part in Eq. (15) increases proportional to $\tilde{\tilde{n}}_0(T)^2$ below $T_{\rm CO}$. To the extent that U_0 can be rather large (one may expect $U_0\sim 1\,$eV in Eq. (15)), FAs excitations cease contributing into the charge transport. (Mobility of electrons at low temper-

atures, fortunately, is known *experimentally* from the value of the Dingle temperature $T_D \simeq 6\,K$ [18]).

In summary, we have shown that IC CDW tend to destroy low lying excitations on the Fermi arcs, leaving electrons on the pocket at the Γ-point as the only charged elementary excitations in the CO phase in UD cuprates. The decrease of the Hall coefficient and its change of the sign at lowering the temperature in experiments [2, 5, 6, 12] are caused by destruction of FAs carriers by IC CDW order.

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