Pis'ma v ZhETF, vol. 88, iss. 3, pp. 224 – 228

Reconstruction of the Fermi surface in the pseudogap state of cuprates

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Submitted 24 June 2008

Reconstruction of the Fermi surface of high-temperature superconducting cuprates in the pseudogap state is analyzed within nearly exactly solvable model of the pseudogap state, induced by short-range order fluctuations of antiferromagnetic (AFM), spin density wave (SDW), or similar charge density wave (CDW)) order parameter, competing with superconductivity. We explicitly demonstrate the evolution from "Fermi arcs" (on the "large" Fermi surface) observed in ARPES experiments at relatively high temperatures (when both the amplitude and phase of density waves fluctuate randomly) towards formation of typical "small" electron and hole "pockets", which are apparently observed in de Haas – van Alfen and Hall resistance oscillation experiments at low temperatures (when only the phase of density waves fluctuate, and correlation length of the short-range order is large enough). A qualitative criterion for quantum oscillations in high magnetic fields to be observable in the pseudogap state is formulated in terms of cyclotron frequency, correlation length of fluctuations and Fermi velocity.

PACS: 71.10.Hf, 74.72.–h

Pseudogap state of underdoped copper oxides [1 – 4] is probably the main anomaly of the normal state of high temperature superconductors. Especially striking is the observation of "Fermi arcs" in ARPES experiments, i.e. parts on the "large" Fermi surface around the diagonal of the Brillouin zone (BZ) with more or less well defined quasiparticles, while the parts of the Fermi surface close to BZ boundaries are almost completely "destroyed" [5 – 7].

However, the recent observation of quantum oscillation effects in Hall resistance [8], Shubnikov – de Haas [9] and de Haas – van Alfen (dHvA) oscillations [9, 10] in the underdoped YBCO cuprates, producing evidence for rather "small" hole or electron [11] pockets of the Fermi surface, seemed to contradict the well established ARPES data on the Fermi surface of cuprates.

Qualitatvive explanation of this apparent contradiction was given in Ref. [12] within very simplified model of hole-like Fermi surface evolution under the effect of short-range AFM fluctuations. Here we present an exactly solvable model of such an evolution, which is able to describe continuous transformation of "large" ARPES Fermi surface with typical "Fermi arcs" at high-enough temperatures into a collection of "small" hole-like and electron-like "pockets", which form due to electron interaction with fluctuations of SDW (CDW) short-range order at low temperatures (in the absence of any kind of AFM (or charge) long-range order). We also formulate a qualitative criterion for observability of quantum oscillation effects in high-magnetic field in this, rather unusual, situation.

We believe that the preferable "scenario" for pseudogap formation can be most likely based on the picture of strong scattering of the charge carriers by short–ranged antiferromagnetic (AFM, SDW) spin fluctuations [2, 3], i.e. fluctuations of the order parameter competing with superconductivity. In momentum representation this scattering transfers momenta of the order of $\mathbf{Q} = (\pi/a, \pi/a)$ (a – lattice constant of two dimensional lattice). This leads to the formation of structures in the one-particle spectrum, which are precursors of the changes in the spectra due to long–range AFM order (period doubling). As a result we obtain non–Fermi liquid like behavior of the spectral density in the vicinity of the so called "hot spots" on the Fermi surface, appearing at intersections of the Fermi surface with antiferromagnetic Brillouin zone boundary [2, 3], which in the low temperarure (large correlation length of the short-range order) can lead to a significant Fermi surface reconstruction, similar to that appearing in the case of AFM long-range order.

Within this approach we have already demonstrated [13, 14] the formation of "Fermi arcs" at high-enough temperatures, when AFM fluctuations can be effectively considered as static and Gaussian [15, 16]. Here we present an exactly solvable model, quite similar to that analyzed qualitatively in Ref. [12], which is capable to describe a crossover from "Fermi arc" picture at high temperatures (typical for most of ARPES experiments) to that of small "pockets" at low temperatures (typical for quantum oscillation experiments).

We shall consider a two – dimensional generalization of an exactly solvable model proposed in one – dimen-

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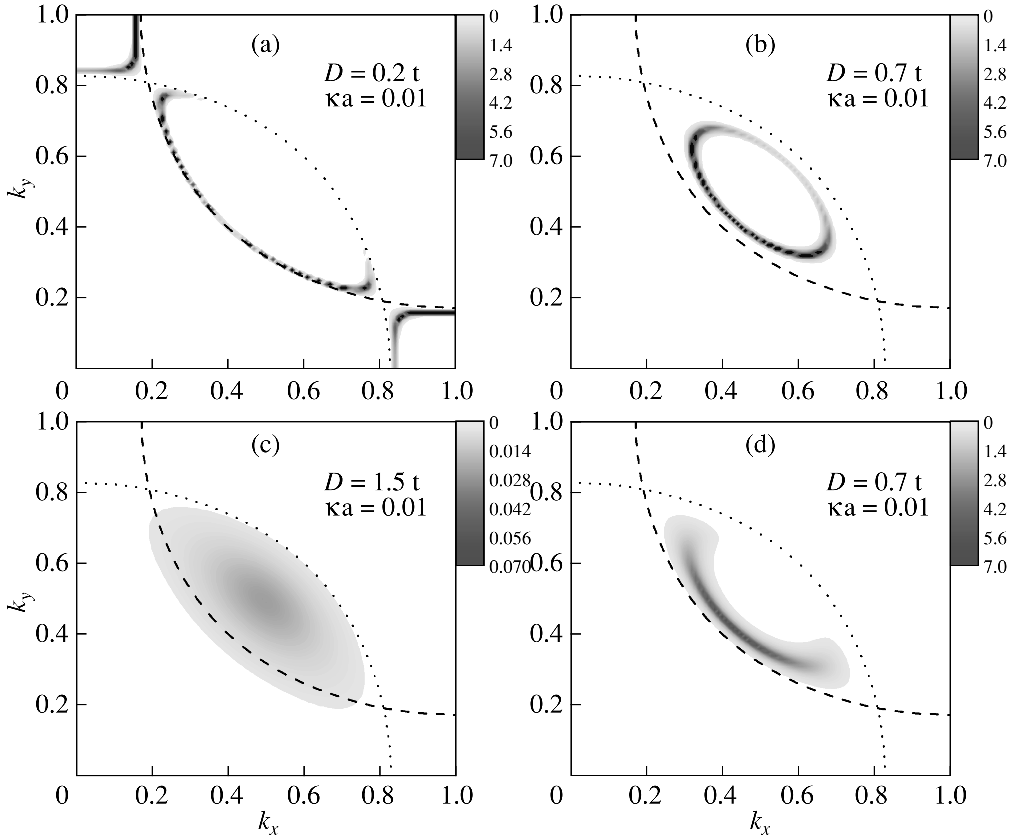

Fig.1. Reconstruction of the Fermi surface in the low temperature (large correlation length) regime of pseudogap fluctuations ($n = 0.9$, $t'/t = -0.4$. Shown are intensity plots of spectral density for $\varepsilon = 0$: (a) – $D = 0.2t$, $\kappa a = 0.01$; (b) – $D = 0.7t$, $\kappa a = 0.01$; (c) – $D = 1.5t$, $\kappa a = 0.01$; (d) – $D = 0.7t$, $\kappa a = 0.1$. Dashed line denotes "bare" Fermi surface, dotted line – shadow Fermi surface

sion in Ref. [17] (and also analyzed in a simplified two-dimensional approach in Ref. [18]), which is physically equivalent to the model of Ref. [12], but can produce a complete picture of Fermi surface reconstruction and formation of both hole and electron "pockets".

We consider electrons in two-dimensional square lattice with nearest (t) and next nearest (t') neighbour hopping integrals, which leads to the usual "bare" dispersion:

$$\varepsilon(\mathbf{k}) = -2t(\cos k_x a + \cos k_y a) - 4t' \cos k_x a \cos k_y a - \mu, \quad (1)$$

where a is the lattice constant, μ – chemical potential, and assume that these electrons are scattered by the following (static) random field, imitating AFM(SDW) (or similar CDW) short-range order:

$$V(\mathbf{l}) = D \exp(i\mathbf{Q}\mathbf{l} - i\mathbf{q}\mathbf{l}) + D^* \exp(-i\mathbf{Q}\mathbf{l} + i\mathbf{q}\mathbf{l}), \quad (2)$$

where $\mathbf{l} = (n_x a, n_y a)$ numerates lattice sites and $D = |D|e^{i\phi}$ denotes the complex amplitude of fluctuating SDW (or CDW) order parameter, while $\mathbf{q} = (q_x, q_y)$ is a small deviation from the dominating scattering vector $\mathbf{Q} = (Q_x, Q_y) = (\frac{\pi}{a}, \frac{\pi}{a})$.

Generalizing the approach of Refs. [17, 18] (compare with Ref. [12]) we consider a specific model of disorder, where both q_x and q_y are random and distributed according to:

$$\mathcal{P}(q_x, q_y) = \frac{1}{\pi^2} \frac{\kappa}{q_x^2 + \kappa^2} \frac{\kappa}{q_y^2 + \kappa^2}, \quad (3)$$

where $\kappa = \xi^{-1}$ is determined by the inverse correlation length of short-range order. Phase ϕ is also considred to be random and distributed uniformly on the interval $[0, 2\pi]$.

Factorized form of (3) is not very important physically, but allows for an analytic solution for the Green' function which takes the form [18]:

$$G_D(\varepsilon, \mathbf{k}) = \frac{\varepsilon - \varepsilon(\mathbf{k}+\mathbf{Q}) + iv\kappa}{(\varepsilon - \varepsilon(\mathbf{k}))(\varepsilon - \varepsilon(\mathbf{k}+\mathbf{Q}) + iv\kappa) - |D|^2}, \quad (4)$$

$$v = |v_x(\mathbf{k}+\mathbf{Q})| + |v_y(\mathbf{k}+\mathbf{Q})|, \; v_{x,y}(\mathbf{k}) = \frac{\partial \varepsilon(\mathbf{k})}{\partial k_{x,y}}.$$

Spectral density $A(\varepsilon,\mathbf{k}) = -\frac{1}{\pi}\mathrm{Im}\,G_D(\varepsilon,\mathbf{k})$ at the Fermi level ($\varepsilon = 0$), is shown in Fig.1, and demonstrate the formation of small "pockets" instead of large "bare" Fermi surface. Here and in the following we have assumed rather typical (for cuprates) values of $t'/t = -0.4$ and doping $n = 0.9$ (10% hole doping), corresponding to $\mu = -1.08t$.

The poles of the Green's function (4), determining the quasiparticle dispersion and damping the limit of large enough correlation length ($v\kappa \ll t$, low temperature), are given by:

$$\tilde{E}^{(\pm)} = E_{\mathbf{k}}^{(\pm)} - i\frac{v\kappa}{2}\left(1 \mp \frac{\varepsilon_{\mathbf{k}}^{(-)}}{E_{\mathbf{k}}}\right), \qquad (5)$$

with $\varepsilon_{\mathbf{k}}^{(\pm)} = \frac{1}{2}[\varepsilon(\mathbf{k}) \pm \varepsilon(\mathbf{k}+\mathbf{Q})]$, $E_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}^{(-)2} + |D|^2}$, and

$$E_{\mathbf{k}}^{(\pm)} = \varepsilon_{\mathbf{k}}^{(+)} \pm \sqrt{\varepsilon_{\mathbf{k}}^{(-)2} + |D|^2} \qquad (6)$$

which is just the same as dispersion in the case of the presence of long-range AFM order. Equation $E_{\mathbf{k}}^{(-)} = 0$ determines the hole "pocket" of the Fermi surface, around the point $(\frac{\pi}{2a}, \frac{\pi}{2a})$ in the Brillouin zone, while $E_{\mathbf{k}}^{(+)} = 0$ defines the electronic "pockets", centered around $(\frac{\pi}{a}, 0)$ and $(0, \frac{\pi}{a})$, as shown in Fig.1a.

Quasiparticle damping as given by the imaginary part of (5) is, in fact, changing rather drastically as particle moves around the "pocket" of the Fermi surface. Being practically zero in the nearest to point $\Gamma = (0,0)$ nodal (i.e. on the diagonal of the Brillouin zone) point of this trajectory on the hole "pocket", it becomes of the order of $\approx v_F^n\kappa$ in the far (from Γ) nodal point. Here we have introduced $v_F^n = |v_x(\mathbf{k}|) + |v_y(\mathbf{k})||_{\varepsilon(\mathbf{k})=0, k_x=k_y}$ – particle velocity at the nodal point of the "bare" Fermi surface. On the trajectory around the electronic "pocket" quasiparticle damping changes from nearly zero near the crossing points of the "bare" Fermi surface with Brillouin zone boundary up to $\approx v_F^a\kappa$ at points close to the similar crossing points of the "shadow" Fermi surface. Here $v_F^a = |v_x(\mathbf{k}|) + |v_y(\mathbf{k})||_{\varepsilon(\mathbf{k})=0, k_x=\frac{\pi}{a}}$ is the velocity in the antinodal point of "bare" Fermi surface.

Of course, the complete theory of quantum (Shubnikov – de Haas or de Haas – van Alfen) oscillations for such peculiar situation can be rather complicated. However, a rough qualitative criterion for the observability of quantum oscillations in our model can be easily formulated as follows. Effective width of spectral densities in our model, which determines smearing of the Fermi surfaces, can be roughly compared to impurity scattering contribution to Dingle temperature and estimated as $\tau^{-1} \sim < v_F > /\xi$, where $< v_F >$ is the velocity averaged over the Fermi surface. In fact it gives a kind of the upper boundary to pseudogap scattering rate in our model. Then our criterion takes the obvious form:

$$\omega_H \frac{\xi}{< v_F >} \sim \frac{\omega_H}{t}\frac{\xi}{a} \gg 1, \qquad (7)$$

where ω_H is the usual cyclotron frequency.

As the most unfavourable estimate (overestimating the effective damping) we take:

$$< v_F > = \begin{cases} v_F^n \text{ for hole "pocket"} \\ v_F^a \text{ for electronic "pocket"} \end{cases} . \qquad (8)$$

Experimentally oscillations become observable in magnetic fields larger than 50 T [8 – 11]. Taking the large correlation length $\xi = 100\,a$ and magnetic field H =50T we get $\omega_H\tau \approx 0.8$ for hole "pocket" and $\omega_H\tau \approx 1.3$ for electronic "pockets" in our model. Thus we need rather large values of correlation length $\xi \sim 50 - 100\,a$ for oscillations to be observable. However, this value may be smaller in the case of cyclotron mass larger than the mass of the free electron used in the above estimates.

From Luttinger theorem it follows that the number of electrons per cell is given by $n = 2a^2\frac{S_{fs}}{\pi^2}$, where S_{fs} is the area of the "bare" Fermi surface ($\varepsilon(\mathbf{k}) = 0$) in the quarter of the Brillouin zone. Similarly, we can determine this concentration as $n = 2a^2\frac{S_{sh}}{\pi^2}$ calculating the area S_{sh} of the "shadow" Fermi surface ($\varepsilon(\mathbf{k}+\mathbf{Q}) = 0$) around the point $M(\frac{\pi}{a}, \frac{\pi}{a})$. Obviously $S_{sh} = S_{fs}$. Then, in the limit of $|D| \to 0$, for hole doping we get [19, 20]:

$$p = 1 - n = a^2\frac{S_h - S'_e}{\pi^2} = a^2\frac{S_h - S_e/2}{\pi^2}, \qquad (9)$$

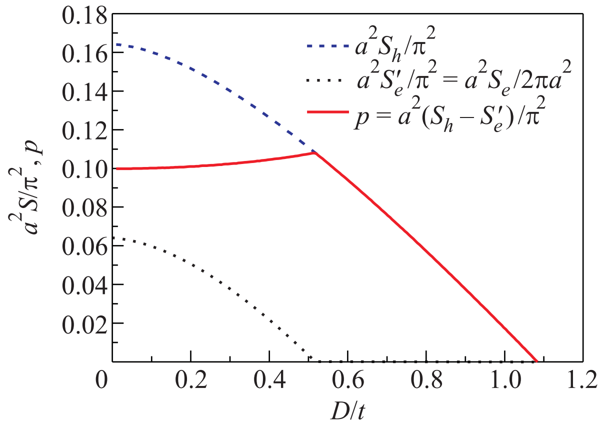

Fig.2. The area of hole ($a^2\frac{S_h}{\pi^2}$) and electronic ($a^2\frac{S'_e}{\pi^2}$) "pockets" in the quarter of Brillouin zone and "doping" $p = a^2\frac{(S_h - S'_e)}{\pi^2}$ as fuctions of the pseudogap amplitude D/t ($n = 0.9$ ($\mu = -1.08t$), $t'/t = -0.4$)

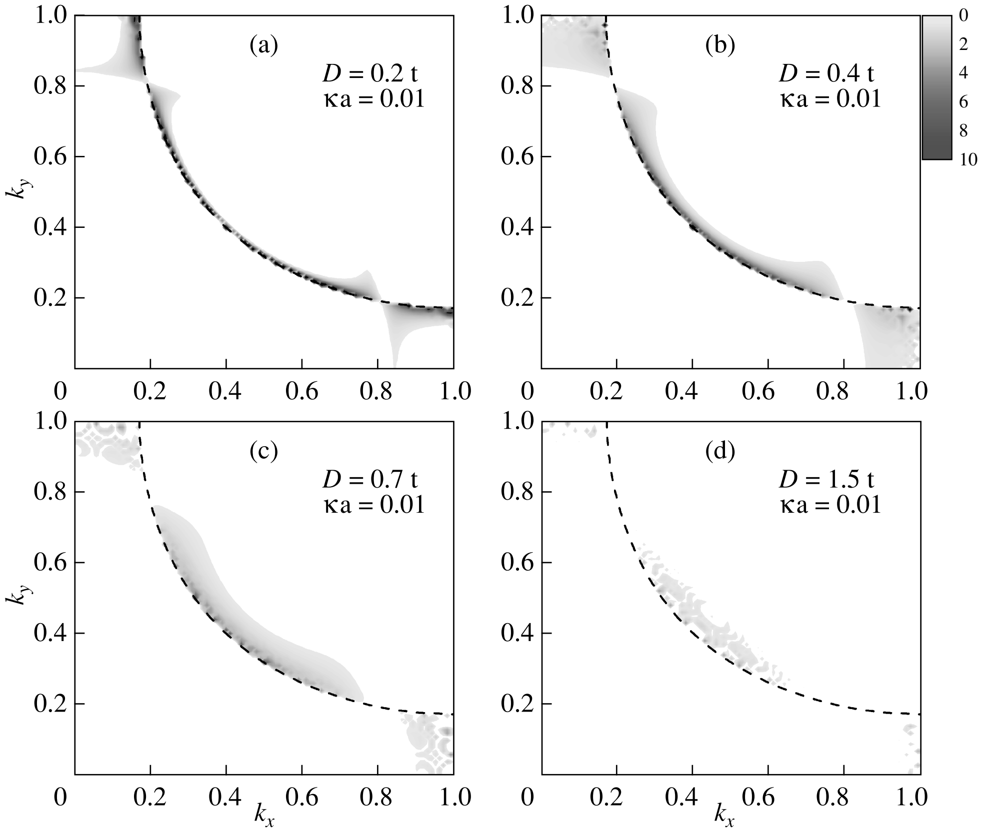

Fig.3. Formation of the Fermi "arcs" in the high-temperature regime of pseudogap fluctuations ($n = 0.9$, $t'/t = -0.4$, $\kappa a = 0.01$). Shown are intensity plots of spectral density for $\varepsilon = 0$. (a) – $\Delta = 0.2t$; (b) – $\Delta = 0.4t$; (c) – $\Delta = 0.7t$; (d) – $\Delta = 1.5t$; Dashed line denotes "bare" Fermi surface

where S_h is the area of hole "pocket" and S_e' is the area of the parts of electronic pocket inside the quarter of the Brillouin zone (which is a half of the total area of electronic "pocket" S_e).

However, these expressions are valid only for $|D| \to 0$. With the growth of the pseudogap amplitude $|D|$ the area of both hole and electronic "pockets" diminish (as can be seen from Fig.1 and Fig.2). In the presence of electronic "pocket" this suppression of the area of both "pockets" compensate each other, leaving the doping given by Eq. (9) almost unchanged (Fig.2). After the disappearance of electronic "pocket", taking place at $|D| = \mu - 4t' = 0.52t$ (i.e. when $E^{(+)}_{\mathbf{k}=(\pi/a,0)} = 0$), there is no way to compensate the suppression of the area the hole "pockets" with the growth of $|D|$ and the number of carriers, determined by (9), will also be suppressed, going to zero with the disappearance of the hole "pocket", taking place at $|D| = -\mu = 1.08t$ (which is defined by $E^{(-)}_{\mathbf{k}=(\pi/2a,\pi/2a)} = 0$) and dielectric (AFM) gap "closes" the whole Fermi surface (Fig.1c). Thus, the doping calculated according to Eq. (9) in the case of large enough pseudogap amplitude (in the absence of electronic "pocket") will be significantly underestimated.

Experimentally, only one frequency of quantum oscillations $F \approx 540T$ was observed in YBCO [9]. Assuming it corresponds to the presence of only the hole "pocket", we obtain for the area of this "pocket" $a^2 S_h/\pi^2 = 0.078$, which, according to Fig.2 corresponds to $|D| \approx 0.7t$.

Green's function (4) describes the "low temperature" regime of pseudogap fluctuations, when the amplitude fluctuations of the random field (2) are "frozen out". In the "high temperature" regime both the phase and the amplitude $|D|$ of (2) are fluctuating. Assuming these fluctuations Gaussian we take the probability distribution of amplitude fluctuations given by Rayleigh distribution [18]:

$$\mathcal{P}_D(|D|) = \frac{2|D|}{\Delta^2} exp\left(-\frac{|D|^2}{\Delta^2}\right). \qquad (10)$$

Then the averaged Green's function takes the form:

$$G_\Delta(\varepsilon, \mathbf{k}) = \int_0^\infty d|D|\mathcal{P}_D(|D|)G_D(\varepsilon, \mathbf{k}). \qquad (11)$$

Profiles of the spectral density at the Fermi level ($\varepsilon = 0$), corresponding to (11) and different values of the pseudogap width Δ are shown in Fig.3. The growth of the pseudogap width leads to the "destruction" of the Fermi surface close to Brillouin zone boundaries and formation of typical Fermi "arcs", qualitatively (and quantitatively) similar to that obtained in our previous work [13, 14] and in accordance with the results of ARPES experiments, which are typically done at much higher temperatures, than experiments on quantum fluctuations.

This work is supported by RFBR grant # 08-02-00021 and RAS programs "Quantum macrophysics" and "Strongly correlated electrons in semiconductors, metals, superconductors and magnetic materials". MVS is gratefully acknowledges a discussion with L. Taillefer at GRC'07 Conference on Superconductivity, which stimulated his interest in this problem.

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