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Coexistence of charge density waves and *d*-wave superconductivity in cuprates. Sharing of the Fermi surface

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Abstract. A self-consistent theory that describes charge density waves in a partially dielectrically gapped superconductor with $d_{x^2-y^2}$-pairing has been proposed. The dependences of dielectric, Σ, and superconducting, Δ, order parameters on the temperature and other problem parameters have been considered, and the phase diagram has been built. The corresponding angular diagrams for gap distribution over the Fermi surface have been plotted. The developed theory is used for the explanation of properties of high-temperature oxides. The influence of mismatch angle between the lobes of order parameters Σ and Δ on the gap distribution in the momentum space and the reentrance phenomenon for Σ with respect to temperature has been analyzed.

Pseudogapping, which coexists with genuine superconducting gapping in high-T_c cuprates, is an enigmatic phenomenon that divides the scholars into two camps. Namely, this phenomenon is considered as either an above-T_c precursor of Cooper pairing [1], which – below T_c – gives way to a coherent superconducting state with the long-range order (one-gap scenario), or a manifestation of a hostile phase [2], which can coexist with superconductivity only in certain situations (two-gap scenario). Several candidates may be responsible for pseudogapping, *e.g.*, charge density waves (CDWs), spin density waves (SDWs) or *d*-density waves, which may be of CDW or SDW nature [3].

Some time ago we worked out a self-consistent theory describing the coexistence between CDWs and *s*-wave superconductivity [4] with important implications to quasiparticle tunneling [5–7]. However, the majority of experiments testify that the superconducting order parameter is of the $d_{x^2-y^2}$ type for high-T_c oxides [8]. Therefore, leaving aside all deep controversies over the actual intrinsic order parameter symmetry [9], we are going to present a new self-consistent phenomenological theory of the phase, appropriate to cuprates, where two mutually perpendicular CDWs (a checkerboard pattern) and *d*-wave superconductivity coexist [10]. We suggest that CDW gaps should be identified with observed pseudogaps in various oxides. In the framework of our approach, CDWs are hostile to superconductivity and compete for the Fermi surface (FS).

As stems from various experiments, especially from angle-resolved photoemission spectroscopic (ARPES) ones, relatively undistorted *d*-wave superconducting energy gaps are observed in nodal directions of two-dimensional momentum plane, whereas pseudogaps appear in the anti-nodal sectors of the FS [2]. In the framework of our approach, we can consider a more generalized picture that could be inherent to cuprates. Specifically, our extended approach involves the mismatch angle β between the centers of the CDW order parameter sectors and the *d*-wave lobe maxima. The corresponding diagram is shown in Fig. 1. Here $\boldsymbol{Q}_1$ and $\boldsymbol{Q}_2$ are the CDW wave vectors, 2α is the opening of each CDW sector, the functions $\Delta(T,\theta) = \Delta(T)\cos 2\theta$ and $\Sigma(T)$ denote superconducting and CDW order parameters, respectively, T is temperature (the Boltzmann constant $k_B = 1$), and θ is reckoned from the direction of one of *d*-wave lobe maxima in the momentum space (the abscissa axis). The order parameters emerge due to the Cooper pairing and dielectric (Peierls or excitonic) instabilities. The latter appears because the cuprate parent quasiparticle spectrum has nested sections [11].

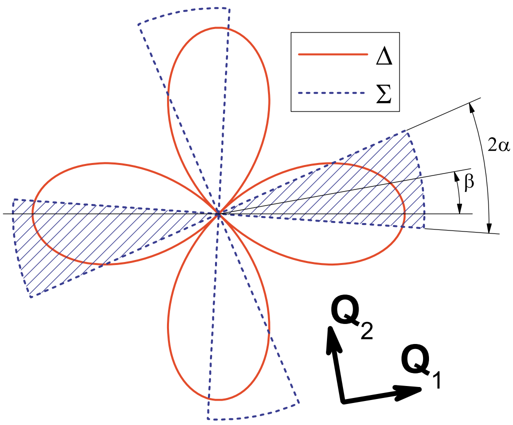

Fig. 1. Superconducting (Δ, solid curve) and dielectric (Σ, dashed curve) order parameter profiles in two-dimensional momentum space for the bare phases of $d_{x^2-y^2}$-superconductor and partially gapped metal with charge-density waves (CDW), respectively, *i.e.* when the competitive pairing channel is switched off.

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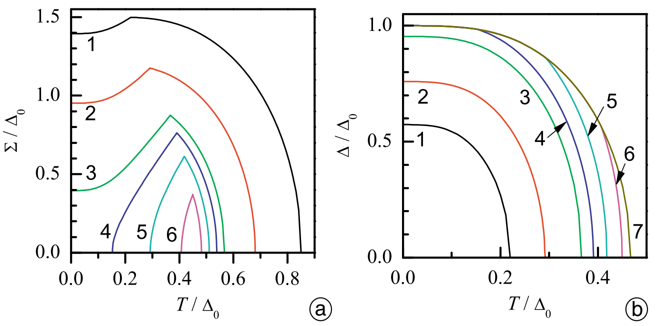

Fig. 2. Dependences of the normalized Σ (**a**) and Δ (**b**) order parameters on the normalized temperature $t = T/\Delta_0$. The values of $\sigma_0 = \Sigma_0/\Delta_0$, where $\Sigma_0 = \Sigma(T = 0)$in the absence of superconductivity and $\Delta_0 = \Delta(T = 0)$ in the absence of CDW, are 1.5 (1), 1.2 (2), 1 (3), 0.95 (4), 0.9 (5), 0.85 (6), and 0.8 (7); the portion of the Fermi surface (FS) gapped by CDWs $\mu = 0.3$.

Coupled equations connecting $\Delta(T)$ and $\Sigma(T)$ have the form

$$\int_{\beta-\alpha}^{\beta+\alpha} I_M(\sqrt{\Sigma^2 + \Delta^2 \cos^2 2\theta}, T, \Sigma_0)\, d\theta = 0\,, \tag{1}$$

$$\int_{\beta-\alpha}^{\beta+\alpha} I_M(\sqrt{\Sigma^2 + \Delta^2 \cos^2 2\theta}, T, \Delta_0 \cos 2\theta) \cos^2 2\theta\, d\theta + \int_{\beta+\alpha}^{\Omega+\beta-\alpha} I_M(\Delta \cos 2\theta, T, \Delta_0 \cos 2\theta) \cos^2 2\theta\, d\theta = 0\,, \tag{2}$$

and the quantity

$$I_M(\Delta, T, \Delta_0) = \int_0^\infty \left(\frac{1}{\sqrt{\xi^2 + \Delta^2}} \tan\text{h}\, \frac{\sqrt{\xi^2 + \Delta^2}}{2T} - \frac{1}{\sqrt{\xi^2 + \Delta_0^2}} \right) d\xi \tag{3}$$

may be called the Mühlschlegel integral. Hereafter, we use the dimensionless temperature $t = T/\Delta_0$ and the dimensionless order parameters $\sigma(t) = \Sigma(T)/\Delta_0$ $(\sigma_0 = \Sigma_0/\Delta_0)$ and $\delta(t) = \Delta(T)/\Delta_0$ $(\delta_0 \equiv 1)$. Σ_0 and Δ_0 are the zero-T values of the parent order parameters, existing in a bare CDW or a superconducting phase, respectively, in the absence of its competing counterpart. A fraction of the overall FS gapped by CDWs is determined by the control parameter $\mu = 4\alpha/\pi$ $(0 < \mu \le 1)$, whereas $\Omega = \pi$ for unidirectional CDWs and $\pi/2$ for a pattern with two mutually perpendicular CDWs (a checkerboard order).

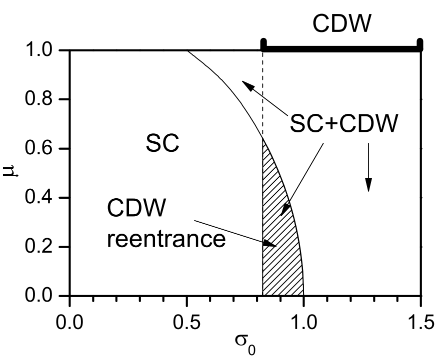

Fig. 3. Phase diagram of CDW $d_{x^2-y^2}$-superconductor on the $\mu - \sigma_0$ plane.

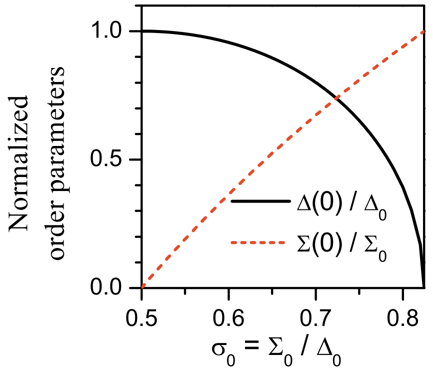

Fig. 4. Dependences of the ratios $\Delta(T = 0)/\Delta_0$ and $\Sigma(T = 0)/\Sigma_0$ on σ_0 at $\mu = 1$.

The solutions of Eqs. (1), (2) for the zero mismatch angle β and $\mu = 0.3$ are shown in Fig. 2. One can see that, for certain values of the system parameters σ_0 and μ, a reentrant behavior of CDW order parameter Σ is possible. The full ground-state phase diagram for $\beta = 0$ is shown in Fig. 3. It turns out that, for the chosen order parameter configuration appropriate to cuprates, $d_{x^2-y^2}$-wave superconductivity exists for all values of σ_0 and μ except the special case of full dielectric gapping $\mu = 1$. On the other hand, CDWs are suppressed by the competing Cooper pairing at small σ_0 or/and μ. The reentrance region (hatched) is confined by the vertical line $\sigma_0 = \sqrt{e}/2$, where e is the base of natural logarithms, and the curve $\sigma_0(\mu) = \exp\left[\frac{4}{\mu\pi}\int_0^{\mu\pi/4} \ln \cos 2\theta\, d\theta\right]$.

Isotropic s-wave superconductivity is known not to coexist with full $(\mu = 1)$ CDW-induced FS gapping [4]. On the contrary, in the $d_{x^2-y^2}$-wave case concerned here, the phase sub-diagram for $\mu = 1$ includes superconducting, CDW and coexistence (SC + CDW) line segments, as shown in Fig. 3. The mixed phase would emerge at $0.5 < \sigma_0 < \sqrt{e}/2$. The corresponding analytical dependences $\Delta(0)/\Delta_0 = 2\sigma_0\sqrt{1 - 2\ln(2\sigma_0)}$ and $\Sigma(0)/\Sigma_0 = 2\ln(2\sigma_0)$ taking place at $\mu = 1$ are depicted in Fig. 4.

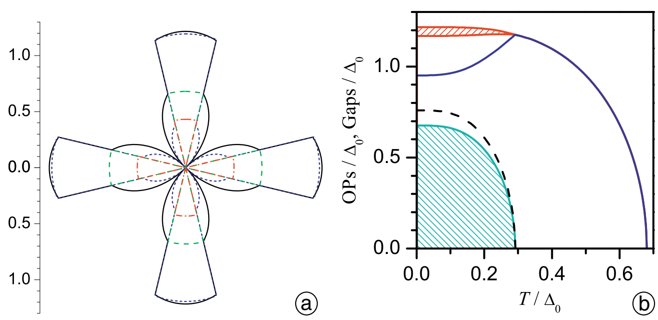

Fig. 5. (**a**) "Roses of gaps" in the momentum space for various $t = 0$ (solid), 0.25 (short dashed), 0.6 (dashed), and 0.65 (dash-dotted curve). (**b**) t-dependences of Σ (solid curve) and Δ (dashed curve) order parameters, and the gap bands (see explanation in the text) on CDW-gapped (right hatching) and non-gapped (left hatching) FS sections. For both panels, $\sigma_0 = 1.2$, $\mu = 0.3$, the mismatch angle $\beta = 0°$.

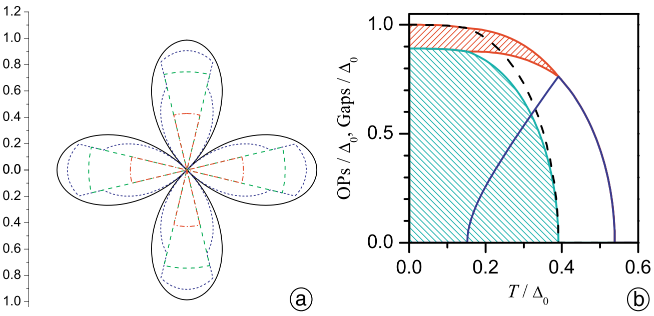

Fig. 6. The same as in Fig. 5, but for $\sigma_0 = 0.95$ and $t = 0.15$ (solid), 0.3 (short dashed), 0.4 (dashed), and 0.5 (dash-dotted curve).

One should bear in mind that both order parameters make contributions to FS gapping at nested sections, so that the angular dependence of the combined gap is rather involved. An example of such "roses of gaps" is shown in Fig. 5(a) for a non-reentrant pattern with $\beta = 0$ and $\sigma_0 = 1.2$. It is readily seen that the interplay between sectors and lobes makes the resulting curves very intricate. It might explain why it was so difficult to interpret ARPES or tunnel spectra in cuprate samples, especially in underdoped ones, where pseudogaps manifest themselves strongly [12]. The corresponding "bands" of gap values while scanning over the whole FS is shown in Fig. 5b. It comes about from Fig. 5(b) that, for any T below T_c, the observed combined gap on the dielectrically gapped FS sections is almost T- and θ-independent.

The dependences, similar to those in Fig. 5, but for the reentrant case occurring at $\beta = 0$ and $\sigma_0 = 0.95$, are demonstrated in Fig. 6. The T-evolution of the rose of gaps comprises a sequence of lobe-sector chimeras. The realization of such a scenario makes any interpretation of ARPES in terms of angle-resolved superconducting gaps versus pseudogaps ambiguous.

Still, measuring actual energy gaps by ARPES on non-nested FS sections in the nodal region, one can extract the true amplitude $\Delta(T)$ of the $d_{x^2-y^2}$-wave superconducting order parameter [10, 12]. The same quantity can be found from tunnel experiments as well, if one gets rid of the concomitant pseudogaps (CDW gaps) [13, 14]. It turns out that the measured ratio $2\Delta(0)/T_c$ is much larger [15] than its s- (≈ 3.53) and d-wave (≈ 4.28) theoretical values [16]. In our approach, the influence of Σ on superconductivity is also significant, which can be seen from Fig. 7, where $\mu = 0.3$ and the mismatch angle β varies. For $\beta = 0$, which corresponds to the cuprate configuration case, the ratio $2\Delta(0)/T_c$ is large indeed, substantially exceeding the conventional values. On the other hand, with growing β, the ratio is reduced becoming, for large σ_0, even less than the indicated "bare" values. It should be noted that anomalously large values of $2\Delta(0)/T_c$ can be inferred from a totally different microscopic theory based on the spin-fluctuation mechanism [17].

To summarize, our model allows a wide range of problems concerning cuprates and other CDW superconductors to be considered properly.

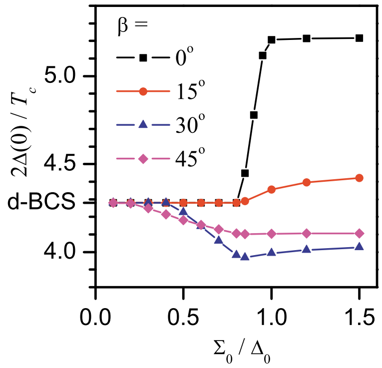

Fig. 7. Dependences of the ratio $2\Delta(T=0)/T_c$ on σ_0 for various β.

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References

[1] Valla, T.; Lee, A. V. J.; Davis, J. C.; Gu, G. D.: Science **314** (2006) 1914.
[2] Gabovich, A. M.; Voitenko, A. I.; Ekino, T.; Li, M. S.; Szymczak, H.; Pękała, M.: Adv. Condens. Matter Phys. **2010** (2010) 681070.
[3] Ghosh, A.: In: Progress in Superconductivity Research (Ed. O. A. Chang), p. 123–162. Nova Science, (New York) (2008).
[4] Gabovich, A. M.; Li, M. S.; Szymczak, H.; Voitenko, A. I.: J. Phys.: Condens. Matter **15** (2003) 2745.
[5] Gabovich, A. M.; Voitenko, A. I.: Phys. Rev. B **75** (2007) 064516.
[6] Ekino, T.; Gabovich, A. M.; Li, M. S.; Pękała, M.; Szymczak, H.; Voitenko, A. I.: Phys. Rev. B **76** (2007) 180503.
[7] Ekino, T.; Gabovich, A. M.; Li, M. S.; Pękała, M.; Szymczak, H.; Voitenko, A. I.: J. Phys.: Condens. Matter **20** (2008) 425218.
[8] Tsuei, C. C.; Kirtley, J. R.: In: Superconductivity. Vol. 2: Novel Superconductors (Eds. K. H. Bennemann, J. B. Ketterson), p. 869–921. Springer Verlag, (Berlin) (2008).
[9] Klemm, R. A.: Phil. Mag. **85** (2005) 801.
[10] Lee, W. S.; Vishik, I. M.; Tanaka, K.; Lu, D. H.; Sasagawa, T.; Nagaosa, N.; Devereaux, T. P.; Hussain, Z.; Shen, Z.-X.: Nature **450** (2007) 81.
[11] Wise, W. D.; Boyer, M. C.; Chatterjee, K.; Kondo, T.; Takeuchi, T.; Ikuta, H.; Wang, Y.; Hudson, E. W.: Nature Phys. **4** (2008) 696.
[12] Kurosawa, T.; Yoneyama, T.; Takano, Y.; Hagiwara, M.; Inoue, R.; Hagiwara, N.; Kurusu, K.; Takeyama, K.; Momono, N.; Oda, M.; Ido, M.: Phys. Rev. B **81** (2010) 094519.
[13] Ekino, T.; Sezaki, Y.; Fujii, H.: Phys. Rev. B **60** (1999) 6916.
[14] Boyer, M. C.; Wise, W. D.; Chatterjee, K.; Yi, M.; Kondo, T.; Takeuchi, T.; Ikuta, H.; Hudson, E. W.: Nature Phys. **3** (2007) 802.
[15] Damascelli, A.; Hussain, Z.; Shen, Z.-X.: Rev. Mod. Phys. **75** (2003) 473.
[16] Gabovich, A. M.; Voitenko, A. I.: Phys. Rev. B **80** (2009) 224501.
[17] Manske, D.: Theory of Unconventional Superconductors. Cooper-Pairing Mediated by Spin Excitations. Springer Verlag, New York (2004).