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Percolation theory of the pseudogap state

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A concept of the pseudogap state in high-T_c layered cuprates on the basis of percolation theory is proposed. Contrary to the self-consistent BCS critical temperature, which defines T^*, the upper boundary of the pseudogap state, the real critical temperature T_c is defined as the percolation threshold, where the infinite cluster appears. This permits the exact formula for T_c to be obtained as a function of doping and its "domelike" shape to be understood.

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The physics of the so-called "pseudogap state" remains the last big problem of the theory of high-T_c layered cuprates. The main difficulty is its inhomogeneity, which does not permit the application of regular theoretical approaches. This inhomogeneity is well established experimentally, and recently it proved to be independent of temperature.[1] This strengthens the concept that the pseudogap state is an irregular "patchwork" of finite superconducting and normal regions, and the phase of the order parameter differs in different superconducting "patches" (see Refs. 2 and 3). The independence of the density of states on temperature shows that the origin of the "patchwork" is inhomogeneous doping.

Let us for definiteness consider $Bi_2Sr_2CaCu_2O_{8+\delta}$. The doping is associated with increasing the oxygen concentration in the BiO layers located between the CuO_2 planes. In the previous works (see Ref. 4) we stressed the role of these oxygen atoms not only for introducing holes in the CuO_2 planes, but also for connecting the planes due to resonant tunneling of holes.

The subsequent consideration will be based on the ideas of percolation theory (see Ref. 5). The simplest presentation of that theory is the idea of clusters. In the problem under consideration it is natural to assume that the "elementary cluster" consists of two superconducting regions in two adjacent CuO_2 planes around one oxygen atom in the BiO plane (we consider the complex of two close CuO_2 planes as one plane). We will assume that the relevant oxygen atoms are located randomly. This assumption can be violated by ordering of these atoms, which can happen in the "chains" of $YBa_2Cu_3O_{7-\delta}$ (see Ref. 6). If our assumption is true, the applicable version is the "random site" problem (Ref. 5, Sec. 18). The increasing doping leads to the merger of elementary clusters and formation of larger clusters, and eventually the infinite cluster appears, which has a coherent phase of the order parameter. The corresponding temperature is the real T_c, and thus we get the phase diagram. This will be the topic of the present paper. For this problem the phase fluctuations in finite clusters are of no importance (their influence on physical properties of the pseudogap state, including the "Fermi arcs", was analyzed in Ref. 3).

In the previous work,[2] we defined the phase diagram by an interpolation between a "coherent state" and T^*. The percolation approach permits an exact formula to be obtained.

The appearance of an infinite cluster is described by a formula [5]

$$(NV)_c = B, \tag{1}$$

where V is the volume of an "elementary cluster," N its density, equal to the density of oxygen atoms in the BiO planes, and B some dimensionless constant of order of unity. Although B can in principle depend on the shape of the elementary cluster, it actually varies very little for different shapes and depends only on the dimensionality (see Ref. 5). For a three-dimensional (3D) case it is around 2.8. According to the preceding arguments, we can write

$$V = q\xi^2 d, \tag{2}$$

where ξ is the planar coherence length, d the interplane distance, and $q \sim 1$.

As it was described earlier (see Ref. 7), the most important regions in momentum space are the vicinities of the extended saddle point singularities at the Fermi surface. There the motion of holes is virtually one-dimensional and therefore, the following formula for ξ, derived by Rice for that case,[8] may be applied:

$$\xi = \frac{|\Psi_0|^2}{mT} = \frac{2v}{\pi}\frac{T^* - T}{T^* T}. \tag{3}$$

In the work[8] the Ginzburg–Landau free energy was used. We inserted the coefficients from our work[9] about the extended saddle point model and used the idea (see Ref. 2) that the self-consistent BCS theory, as well as its limiting case, the GL theory, define not the real superconducting transition but the crossover temperature T^* from the pseudogap state to the normal state. Strictly speaking, Eq. (3) applies only in the vicinity of T^*. However, it gives the correct order of magnitude also at low temperatures, since at the boundary, $T \sim T^*$, it must be correct by order of magnitude and at $T \ll T^* |\Psi_0|^2$ does not depend on temperature.

From Eqs. (1)–(3) we can get the real critical temperature (v is the Fermi velocity),

$$\frac{1}{T_c} - \frac{1}{T^*} = \frac{\pi}{2v}\left(\frac{B}{qNd}\right)^{1/2}, \tag{4}$$

The limiting cases are

$$T_c = \alpha_1 v\sqrt{Nd}, \quad T_c \ll T^* \tag{5}$$

$$T^* - T_c \approx \alpha_2 \frac{T^{*2}}{v(Nd)^{1/2}}, \quad T^* - T_c \ll T^*, \tag{6}$$

where α_1 and α_2 are constants of the order of 1.

From Eq. (5) it follows that at low doping T_c decreases with decreasing doping. The Fermi velocity is equal to $v = \sqrt{2\mu/m}$, where μ is the chemical potential calculated from the bottom of the band in the vicinity of the extended saddle point singularity. According to Ref. 10, μ is proportional to the density of holes and the latter is proportional to N. Hence, at small N T_c decreases proportionally to N.

In the opposite limit T_c approaches T^*. This is due not only to $N^{1/2}$ in the denominator of Eq. (6) but mostly to the rapid decrease of T^* due to disorder (see Ref. 2). According to Ref. 11,

$$\ln\left(\frac{T_0^*}{T^*}\right) = \psi\left(\frac{1}{2} + \frac{1}{\pi T^* \tau}\right) - \psi\left(\frac{1}{2}\right), \tag{7}$$

where ψ is the di-gamma function, T_0^* the value of T^* for a clean sample, and τ is the scattering time. The limiting values of T^* are

$$T^* \approx \begin{cases} T_0^*[1 - \pi/(2T_0^*\tau)], & (\pi T_0^* \tau)^{-1} \ll 1 \\ (2\sqrt{6}/\pi)[\tau_c^{-1}(\tau_c^{-1} - \tau^{-1})]^{1/2}, & (\tau_c^{-1} - \tau^{-1}) \ll \tau_c^{-1} \end{cases}, \tag{8}$$

where the critical value of the scattering probability is

$$\tau_c^{-1} = (\pi/4\gamma)T_0^*, \tag{9}$$

(γ=1.78). The approach of T_c to T^* happens much faster than the decrease of T^* and therefore may give the impression that these curves merge before T^*=0, the more so, that T^* is not precisely defined.

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