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Possible explanation of the pseudogap in high-temperature cuprates

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A concept describing the origin and some properties of the ''pseudogap phase'' of high-T_c superconducting cuprates is proposed based on the author's idea about resonant tunneling connection between the CuO_2 layers. The superconducting critical temperature in this picture is defined at low doping by establishment of a three-dimensional phase correlation between the layers, and at high doping by destruction of a d-wave superconductivity by disorder. The result is a nonmonotonic behavior of T_c with doping. The pseudogap phase is analyzed qualitatively on the basis of the recently discovered existence of vortices in this phase and one-dimensional fluctuations due to extended saddle points (''hot spots'').

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I. INTRODUCTION

One of the most mysterious phenomena in the physics of high-T_c superconducting cuprates is the so-called ''pseudogap.'' This notation refers to a large variety of phenomena which are manifested in angle-resolved photoemission spectroscopy (ARPES), tunneling conductance, NMR, thermodynamic, and kinetic properties. All of these phenomena present evidence that superconductivity in underdoped cuprates does not disappear entirely above T_c, and there is a temperature region where some of the superconducting properties persist, in spite of the absence of the principal features, described by the London equations: current without resistance and Meissner effect. The upper limit of this state, which we would like to call the ''pseudogap phase'' in correspondence with numerous papers on the subject, is at a temperature T^*, where some sort of crossover happens to the normal state. This temperature decreases with doping, and at optimal doping, corresponding to the highest T_c, or in the overdoped region it coincides with T_c. After that the metal behaves more or less conventionally. Contrary to that, the real T_c has a nonmonotonous dependence on doping, decreasing from optimal doping both to the underdoped and overdoped side.

Probably the first manifestation of the unusual properties was the ''spin gap'' observed in NMR.[1] Instead of a rather steep decrease of the Knight shift $K(T)$ below T_c a very slow decrease was observed starting rather high above T_c. The curve $K(T)$ passed T_c smoothly, as if there were no phase transition at this point. The first explanation was the idea of so-called ''preformed pairs.'' In the limit of very strong interaction between electrons the formation of pairs and their Bose condensation can start at different temperatures, contrary to the Bardeen-Cooper-Schrieffer model with weak interaction,[2] where both phenomena start at T_c. The pairs, being singlets, do not participate in the spin susceptibility, and therefore their formation leads to a decrease of $K(T)$, compared to the normal metal. On the other hand, since the Bose condensation happens in the gas of singlet pairs, it does not affect the total susceptibility, and hence nothing special can be seen for $K(T)$ at this point.

Numerical calculations performed for a simple ''attractive Hubbard model''[3] could be fitted easily to experimental data. The discovery of the pseudogap in the ARPES spectra[4,5] gave additional support to this conclusion. The ''preformed pairs'' idea dominated the explanations of the pseudogap for quite a while. Different, much more sophisticated models were proposed (see, e.g., Refs. 6–8), which looked very successful. Nevertheless, there was no complete satisfaction.

First of all, there was no understanding of why the pseudogap existed only from the underdoped side. If the reason for appearance of preformed pairs was an increase of relative interaction, i.e., of the ratio of the interaction energy to the Fermi energy, why did it happen? There existed no physical justification of an increase of the interaction, and the ARPES data on the Fermi surface[9] showed that it was displaced very little with underdoping. This, actually, could be expected. The most natural description of the antiferromagnetic insulating phase is a spin-density wave (SDW) formed due to ''nesting'' at half filling. Doping destroys this phase by introducing disorder and by changing the filling of the band. At the metal-insulator transition point a Fermi surface appears, corresponding approximately to half filling. Additional doping changes the Fermi surface only very slightly. This is rather clear evidence that there is no substantial change in the Fermi energy as well.

The second objection against preformed pairs came from the fact that the pseudogap, as a function of momentum, behaved very similar to the true gap in the superconducting state. How could a freely moving Bose particle remember anything about its constituents?

The latest experiments[10,11] demonstrated that the pseudogap increased with underdoping, the same as the gap in the superconducting state, and roughly the BCS ratio $2\Delta(0)/T_c$ did not vary with doping, if the $\Delta(0)$ was taken from the tunneling measurements, and T_c was replaced by T^*. I would like to add that in the ARPES spectra above T_c a very broad maximum was observed, instead of a narrow quasiparticle peak, which, on one hand, compromised the applicability of the Fermi-liquid description, and, on the other hand, did not permit a unique definition of the pseudogap. In the superconducting state there exists a rather narrow maximum, which can justify a BCS-type description, although many questions still remain open.

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II. NERNST EFFECT AND ITS CONSEQUENCES

In a recent work by P. Ong's group[12] it was found that the Nernst effect in $La_{2-x}Sr_xCuO_4$ above T_c is far too large to be described by the usual electronic mechanism, and the most likely explanation is moving vortices. Of course LSCO differs in many respects from the ''true'' high-T_c superconductors, such as $YBa_2Cu_3O_{7-\delta}$(YBCO) and $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO), on which most of the experiments, described in the previous section, were performed. However, in the same paper[12] it was indicated that preliminary data suggest that YBCO behaves similarly. If this explanation is true, then we have to conclude that in the pseudogap phase there exist sufficiently large regions which can be considered as a real superconductor.

This assumption would explain the fact that the momentum dependence of the pseudogap resembles that of the true gap in the superconducting state, and the ''non-Fermi-liquid'' behavior is due to inhomogenity. Then what are T^* and T_c?

I would propose the following idea. The process of doping in the ''true'' high-T_c superconductors consists in adding oxygen atoms, mostly to the layers lying between the CuO_2 metallic layers. This procedure results not only in hole formation, but in disorder, particularly, if the additional oxygens fall into ''wrong'' positions compared to regular sites in the CuO chains, or BiO layers. Let us consider T^* as the self-consistent critical temperature of the disconnected CuO_2 layers. Since the order parameter has a *d*-wave symmetry, T^* will decrease rapidly with disorder. The latter will become very strong when all the regular oxygen sites in the intermediate layers will be taken, and hence one can expect even a stronger decrease of T^* on the overdoped side compared to the usual depairing formula.[13]

According to the idea proposed by the present author,[14] the CuO_2 layers are connected in the lattice by resonant tunneling of the electrons through localized states at the oxygen atoms in the intermediate layers. Contrary to the total number of carriers defined by the Fermi surface, the number of these atoms varies strongly with doping. In the paper[14] the true critical temperature was derived as the temperature where a new order parameter $\langle e^{i\varphi}\rangle$ is formed, which is a coherent phase factor averaged over all the layers. This critical temperature defines where true superconductivity or, in other words, the Meissner effect, appears. It depends strongly on the concentration of resonant centers and decreases rapidly with this concentration. The result is given by Eq. (41) of Ref. 14.

Here we will need a more quantitative definition. In order to have coherent resonant tunneling, necessary for *d*-wave superconductivity,[14] there must be a sufficient amount of centers per characteristic area, which for BSCCO is 120 Å^2. Let us assume that the minimal number is 4. Since the period in the plane is approximately 4 Å, and there are two BiO layers per period, the atomic concentration is $n/(\frac{2}{16}\,\text{Å}^2)$, where n is the concentration of oxygen atoms in the BiO layers per cm^2. Hence the critical atomic concentration $c^{(0)}$, defined in Ref. 14, is $(\frac{4}{120})/(\frac{2}{16})=\frac{4}{15}\approx 0.27$. Since the concentration becomes important only when it is small, we can assume that $c<c^{(0)}$ and use the formula

$$T_c=\varepsilon_0/(B+c^{(0)}/c)^2.$$

We will also assume that the most important pieces of the Fermi surface are the singular regions (or ''hot spots''), where the spectrum is ''flat,'' and the motion of quasiparticles is essentially one dimensional (see Ref. 15). For these regions the role of ε_O is taken over by μ_1-the Fermi energy calculated from the bottom of the band. According to our interpretation of the neutron data (see Ref. 16), μ_1 is not very large compared to Δ in the superconducting phase. On the basis of this reasoning we can write an interpolation formula for T_c:

$$T_c=\frac{1}{[T^{*-1/2}+(c^{(0)}/c)\mu_1^{-1/2}]^2}. \tag{1}$$

At $c\ll c^{(0)}$ the second term in the denominator dominates. Hence in this region $T_c\ll T^*$, and it decreases with the concentration. At large concentrations T^* decreases. At the highest concentrations (see Ref. 13)

$$T^*=\hbar(2\sqrt{6}/\pi)[w_c(w_c-w)]^{1/2}, \tag{2}$$

where $w=1/\tau$ is the scattering probability, proportional to the concentration of defects, and $w_c=\hbar^{-1}(\pi/4\gamma)T^*_{c=0}$ is its critical value. Hence the first term in the denominator dominates, and $T_c\approx T^*$. For illustration we can present the phase diagram based on a few simplifying assumptions. First of all, we will assume that the T^* is defined by the pair breaking formula (9) of Ref. 13. Then, introducing dimensionless variables $y=T^*/T_{co}$ and $x=w/T_{co}$ we get a formula

$$\ln(1/y)-\psi[\tfrac{1}{2}+x/(\pi y)]+\psi(\tfrac{1}{2})=0, \tag{3}$$

from which we define $y(x)$ (ψ is the digamma function).

For T_c we will use formula (1), where we will assume that the concentration of resonant centers is proportional to the concentration of scatterers, i.e., $c=aw$. Introducing $z=T_c/T_{co}$, we obtain

$$z=(1/\sqrt{y}+A/x)^{-2}, \tag{4}$$

where $A=(c^{(0)}/a)(T_{co}\mu_1)^{-1/2}$. Under these assumptions we have two fitting parameters: T_{co} and A, and for plots of dimensionless quantities $y(x)$ and $z(x)$, only the parameter A. Figure 1 presents the phase diagram for the choice $A=0.1$. Again, we would like to stress the crudeness of our assumptions.

It should be mentioned that the concentration of resonant centers can strongly fluctuate in the intermediate layer. Therefore at any given average concentration there would be regions with $c<c(T)$ and $c>c(T)$. Only the second ones are superconducting. The minimal size of such regions will be of the order of the superconducting coherence length. In such a medium the superconducting transition will have a percolative nature. For a two-dimensional model the percolation threshold is defined by the condition that the sum of areas of superconducting regions must be $\frac{1}{2}$ of the total area. At this point an infinite cluster is formed, and the Meissner

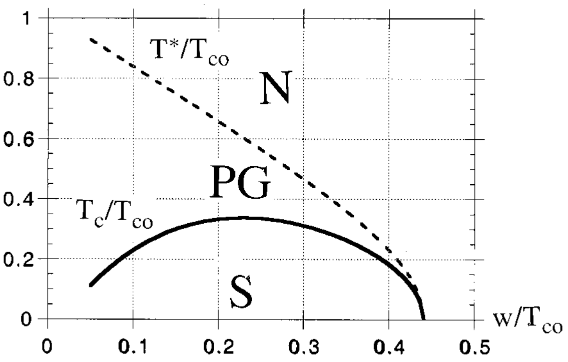

FIG. 1. The phase diagram of a high-temperature superconductor. The curves represent normalized temperatures T_c/T_{co} and T^*/T_{co} as functions of the normalized scattering probability, which is supposed to be proportional to the concentration of resonant centers. The normalization temperature T_{co} is a hypothetical self-consistent critical temperature of a clean sample.

effect appears. Since on both sides of the transition there exist superconducting and nonsuperconducting regions, the spin susceptibility will vary continuously through the critical temperature, in agreement with experiment. In reality, the $T_c(\overline{c})$ obtained for a percolative transition differs very little from formula (1).

III. PSEUDOGAP PHASE

It would be very tempting to use this idea for the explanation of the pseudogap. Unfortunately, it does not work. The reason is that in a percolative transition the width of the transition region decreases with the percolative critical temperature. It is possible to show that the spin susceptibility versus T at different concentrations can be scaled to a single curve, if, instead of T, the variable T/T_c is used. This contradicts the growth of T^* with decreasing concentration. Therefore we have to analyze the situation more carefully.

What really happens at T_c? As it was said before, at this temperature the coherent phase factor $\langle e^{i\varphi}\rangle$ vanishes (see Ref. 14). At the same time the absolute value of the order parameter remains finite. Hence different planes lose phase coherence but otherwise still keep some sort of superconductivity. The most natural idea would be about a Berezinsky-Kosterlitz-Thouless (BKT) transition but, as we will see below, the corresponding temperature actually equals T_c.

The following idea can be proposed. Let us assume that the most important are the singular regions of the Fermi surface (hot spots), where the motion of quasiparticles is one dimensional. Hence we can consider not two-dimensional but one-dimensional fluctuations. According to M. Rice,[17] in this case the correlation of the order parameter decreases exponentially with distance, namely $\|\Psi(0)\Psi^*(X)\| \propto \exp(-X/X_o)$, where $\|\cdot\cdot\|$ means averaging in the plane. If we compare the Ginsburg-Landau free energy for our model[18] with the one used in Ref. 17, we obtain

$$X_0 \sim \frac{\overline{h}\Delta^2 v}{T^{*2}T}, \tag{5}$$

where Δ is the self-consistent order parameter. Not too close to T^* we will have $X_o \sim \hbar v/T$, which at sufficiently low temperatures may be larger than the coherence length $\xi \sim \hbar v/T^*$.

In considering a one-dimensional problem, instead of a real two-dimensional one, we neglected in the free energy of Ref. 18 the cross term $\alpha\eta|\Psi_a+\Psi_b|^2$ compared to the terms $(1/4m)[|\partial\Psi_a/\partial x|^2+|\partial\Psi_b/\partial y|^2]$; here Ψ_a and Ψ_b are the values of the order parameter near (π, 0) and (0, π), respectively. Taking into account the definition of $\alpha\eta$ in Ref. 18 and the estimate $1/(mX_O^2)$ for the term with derivatives we conclude that our assumption is justified, if $\eta \ll (T/T^*)^2$. Since η is small, this requirement is fulfilled for most of the pseudogap phase. It fails at sufficiently low temperatures and then the BKT transition has to be considered. This can happen only close to T_c (according to Ref. 14, it actually defines T_c).

We do not have the apparatus to treat the pseudogap phase but according to experiment we know that it is inhomogeneous with some indications of superconductivity. One can imagine that it is slowly varying in time, and contains grains having a finite order parameter with different phases. The finite resistance and spin susceptibility show that part of the material will be normal. The size of the superconducting grains in X_O, and at temperatures sufficiently lower than T^* they may be large enough to carry vortices. On the other hand, local probes, such as ARPES, or tunneling will deliver a maximal gap corresponding to $|\Delta|$ connected in a more or less usual way to T^*. The inhomogenity will be reflected in a broad maximum in the ARPES spectrum, instead of a narrow Fermi-liquid quasiparticle peak. This state is different from all known phases and has to be considered, as a special state, which we call pseudogap phase, although it is not characterized by any long-range order and has no phase boundary with the normal state.

Recently a paper appeared[19] where the voltage dependent tunneling conductance $G(V)$ of tiny samples along the c axis was measured. The authors found a pseudogap which did not depend on magnetic field and temperature, contrary to the true superconducting gap. As it was explained in Ref. 14, despite the use of the same notation, the c-axis pseudogap, which I would prefer to call ‘‘c gap,’’ is very different from the one observed in usual tunneling, NMR, and ARPES experiments. The c gap is defined by the difference between the Fermi energy and the energy of localized resonant states at the oxygen atoms in the BiO layers. Naturally, this energy difference does not depend on field and temperature, and manifests itself both in the normal and superconducting state.

From the above reasoning it is clear that the theoretical problem is confined to the proper mathematical description of the nanostructured pseudogap phase. Of course, it would be very interesting to confirm the granular composition experimentally, better by scanning tunnel microscope than by decoration, since the structure may be too fine for the latter. Of course, this can be done only if the structure does not vary too fast with time.

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