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A joint scientific session of the Physical Sciences Division of the Russian Academy of Sciences (RAS) and the Joint Physical Society of the Russian Federation was held on 24 September, 2003, at the P N Lebedev Physics Institute, RAS. The following reports were presented at the session:

(1) **Belyavskiĭ V I, Kopaev Yu V** (P N Lebedev Physics Institute, RAS, Moscow) "Generalizing considerations about the nature of high-temperature superconductivity (based on the proceedings of M2S-HTSC-VII)";

(2) **Zvezdin A K** (General Physics Institute, RAS, Moscow), **Pyatakov A P** (Physics Department, M V Lomonosov Moscow State University, Moscow) "Phase transitions and the giant magnetoelectric effect in multiferroics".

A brief summary of the papers is given below.

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Generalizing considerations about the nature of high-temperature superconductivity (based on the proceedings of M2S-HTSC-VII)

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1. Problems of cuprate physics

Soon after the discovery of high-temperature superconductivity in cuprates, three points were noted by Anderson [1] which could potentially form the basis for understanding the unusual behavior of the cuprates in both the superconducting (SC) and normal (N) states. These points were (1) the crystal structure of the cuprates, the main element of which are weakly coupled copper – oxygen (CuO_2) planes, is quasi-two-dimensional (2D); (2) the SC state is due to the doping of CuO_2 planes, which are Mott insulators when undoped; and (3) the proximity of the SC to the insulating phase in a 2D system may be the reason why the electronic states of a doped insulator above the SC transition temperature T_c differ radically from those in a normal Fermi liquid.

The copper – oxygen planes of a cuprate form a correlated 2D electronic system dominated by a single nondegenerate electron band [2], with Coulomb repulsion between electrons on the same site as the dominant interaction. Since the characteristic repulsion energy (the Hubbard energy U_0) in a cuprate is comparable on the order of magnitude with the band width t_0, even the simplest models of strongly or weakly interacting electrons are of limited applicability to the undoped insulating phase. There is no fundamental difficulty here, because the antiferromagnetic (AF) insulating state arises both in the weak-interaction case, owing to the nesting of the Fermi contour (FC) into which the Fermi surface of a 2D system degenerates [3], and in the case of strong on-site repulsion, due to the constraint on the site occupation by two opposite-spin electrons. The SC state arises at finite doping, when the long-range AF order is already absent and insulating correlations show up in the short-range AF order.

The phase diagram of an HTSC cuprate [4] typically shows the SC state as lying in a finite doping range $x_* < x < x^*$ (x being the above-half-filling fraction of carriers in the CuO_2 plane). In the overdoped regime ($x_{opt} < x < x^*$, where x_{opt} is the doping level maximizing T_c), it is generally assumed that the transition from the SC phase with an unusual gap symmetry to the N state occurs in accordance with the Bardeen – Cooper – Schrieffer (BCS) theory, i.e., the nonsuperconducting phase has properties close to those of a normal Fermi liquid. In the underdoped ($x_* < x < x_{opt}$) regime, there exists a temperature range $T_c < T < T^*$ in which the density of one-particle excitations turns out to be suppressed, suggesting that a pseudogap has opened up. Here T^* is the gap-opening temperature, which increases with decreasing doping and appears to coincide with T_c for $x \approx x_{opt}$.

At a finite x, various phases of similar energy can coexist in the system, such as resonating valence bond (RVB) states, Wigner crystals of particles and of their pairs, charge density waves (CDWs), orbital antiferromagnetism (OAF), and superconducting states of various symmetry types. To establish the possible symmetry of ordered states, the phenomenology of such competing states based on very general symmetry considerations [5, 6] can be employed.

If three components of the AF order parameter are considered as generators of the SO(3) group and two (amplitude- and phase-related) components of the SC order parameter (for Cooper pairs of zero total momentum) as generators of the U(1) group, then a five-dimensional superspin vector composed of these generators can be introduced [5]. Extending the direct product $SO(3) \times U(1)$ to the minimal group SO(5) allowing the AF and SC order parameters to mutually transform into one another under superspin rotations, one is forced to introduce operators corresponding to the triplet pairs of particles with a large total (AF) momentum. In strong-coupling models with

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repulsion such excitations correspond to antibonding states outside the band of the continuous pair spectrum, according to Ref. [5].

The closed algebra containing generators discussed in Ref. [5] corresponds to symmetry SU(4) [6]. Among its generators, in addition to those already mentioned, are operators corresponding to singlet pairing with a large total momentum, as well as operators that describe OAF. The chains of subgroups of the SU(4) group (one of which contains SO(5) and hence links antiferromagnetism and superconductivity) produce a great diversity of ordered states which can prove to be energetically close to one another. Note that each of the chains contains SU(2) among its subgroups.

One of the key criteria for adequately choosing the microscopic model is that it must describe the pseudogap state observed in underdoped HTSC cuprates. There is currently unambiguous experimental evidence that the pseudogap regime in the cuprates at $T_c < T < T^*$ is due to the existence of incoherent SC pairs (so that T^* corresponds to bond breakdown in a pair and T_c to phase coherence appearing in the system of pairs [7]): (1) the symmetry of the pseudogap is identical to the d-wave symmetry of the SC gap [8]; (2) the Nernst effect in the pseudogap regime is anomalously large, presumably due to vortex motions [9]; (3) the real and imaginary parts of the high-frequency (to 660 GHz) conductivity in the pseudogap regime relate in a similar way to those of SC static conductivity [10]; and (4) the giant proximity effect is observed in systems with SC phases separated by an interlayer in the pseudogap state [11].

ARPES (angle resolution photoemission spectroscopy) data suggest that the pronounced quasiparticle peak observed close to the Fermi level at $T < T_c$ is absent in the pseudogap state [12]. This implies that one-particle excitations well-defined at $T < T_c$ rapidly damp out at $T > T_c$, making Landau's Fermi-liquid theory inadequate for describing the pseudogap state. Understanding the nature of this state is key to understanding both SC and other unusual properties of the HTSC cuprates [13].

At present, two approaches are being developed to build the theory of the HTSC cuprates. One approach looks at how the SC phase emerges from one of the insulating phases as doping is increased. The second examines the way insulating correlations manifest themselves against the background of the SC state as doping is decreased.

2. Pseudogap. Algebraic Fermi liquid

The pseudogap can be considered as a 'footprint' the SC gap leaves when a transition to the N phase takes place. As the temperature is increased in the underdoped regime, this footprint becomes increasingly less visible, finally vanishing at temperatures $\sim T^*$. Thus, changing from the pseudogap state at $T < T^*$ to the normal Fermi liquid state at $T > T^*$ is some kind of crossover rather than phase transition [14]. The question is, what mechanism can preserve a gap in the fermion branch of the elementary excitation spectrum while destroying the phase coherence of the pairs?

The SC order parameter $\Delta(\mathbf{r}) = \Delta_0 \exp\left[i\Phi(\mathbf{r})\right]$ is characterized by an amplitude Δ_0, which determines the magnitude of the gap, and by a coordinate-dependent phase $\Phi(\mathbf{r})$. In the coherent state, the average value of the order parameter is nonzero $\left(\langle\Delta(\mathbf{r})\rangle \neq 0\right)$, whereas in the incoherent pseudogap regime clearly $\langle\Delta(\mathbf{r})\rangle = 0$ due to random fluctuations. According to the scenario of Ref. [7], phase slip occurs at a temperature T_{ph} which is determined by the superfluid stiffness $\rho_s \sim n_s(0)$, with $n_s(0)$ the density of SC electrons at $T = 0$. In conventional superconductors the superfluid stiffness is high, so $T_{ph} \gg T_c$, and phase fluctuations play only a minor role. T_c can then be determined in the mean-field approximation in accordance with the BCS theory. Cuprate superconductors viewed as doped Mott insulators are characterized by a low superfluid stiffness (proportional to the doping level x) and, as appears to be the case for the underdoped regime, $T_{ph} \sim T_c$, i.e., the phase transition is determined by precisely the temperature at which the order parameter undergoes a phase slip. This can qualitatively explain the so-called Uemura plot [15] for cuprates, according to which $T_c \sim n_s(0)$. The phase transition from the incoherent to the coherent state at T_c is considered in Ref. [7] as the *Bose condensation* of incoherent pairs that are already in existence (were created at $T \sim T^*$) in the system.

The low superfluid stiffness and the d-wave symmetry of the SC gap and pseudogap in a 2D electronic system are two features based on which those cuprate properties depending on low-energy excitations can be described within a unified phenomenological framework using a few parameters and *in a way independent of detailed microscopic behavior*. Unlike Ref. [7], in such a *quantum-protectorate* scheme [16] the phase transition from the SC to the pseudogap state is treated as a Berezinskiĭ – Kosterlitz – Thouless transition. Order-parameter-phase fluctuations are considered as either classical [17, 18] or quantum [19] and are due to elementary excitations arising from the breakup or weakening of a bond in a vortex – antivortex pair. This approach allows a qualitative tracing of a transition from the d-wave SC gap, whose nodal points, following the SC transition, transform into extended gapless arcs which form the Fermi contour in the pseudogap state.

The most consistent phenomenology — the one developed in Refs [20, 21] — includes quantum and thermal order-parameter fluctuations and assumes the d-wave SC state to arise from a strongly correlated insulating state as a result of doping. The unusual symmetry of the order parameter, which has nodal points at which the SC gap vanishes on the Fermi contour, leads to low-energy fermion excitations near these points. It is estimated that in the cuprates the dimensionless parameter $(\xi_0 k_F)^{-1}$ characterizing fluctuation effects (ξ_0 is the mean-field coherence length and k_F is the Fermi wave vector) exceeds 10^{-1} (compared to $(\xi_0 k_F)^{-1} \sim 10^{-4} - 10^{-3}$ in conventional superconductors), which provides a wide fluctuation temperature range $T_c < T < T^*$ where dephased pairs can exist.

The so-called '*inverted*' approach to cuprate superconductivity [21] aims at identifying a state at $T > T_c$ which is realized through a softer mode compared to one-particle excitations due to pair breakup. The fundamental point the theory makes is that the most significant thing electron correlations do at the microscopic level is creating a large d-wave-symmetric pseudogap which results from particle pairing. Just as Landau quasiparticles are produced from free-particle states by adiabatically turning on an interaction in the theory of a normal Fermi liquid, in the scheme of Ref. [21] the pseudogap regime arises from free d-wave symmetric Bogolyubov particles. The pseudogap-opening temperature T^* (proportional to the pseudogap amplitude) then plays the role of the theory's largest energy scale — similar to the Fermi energy in the Landau theory. This makes low-energy excitations rather well defined owing to a sort of *pairing protectorate* [21].

The elementary fermion excitations in this picture are Bogolyubov quasiparticles interacting with collective modes, which manifest themselves as the thermal and quantum fluctuations of the order-parameter phase, i.e., as excited vortex–antivortex pairs. According to Ref. [20], such an interaction can be described by two U(1) gage fields, one of which is massive in both the coherent and incoherent states and accounts for the Doppler shift in quasiparticle energies [17, 18, 22], whereas the other is massive in the coherent (SC) state and becomes massless on transition to the incoherent (pseudogap) state, implying that unbound vortex–antivortex states form. Such a soft (zero-mass) well-defined (weakly damped) collective mode plays, against the background of incoherent pairs, the same quantum-protectorate role as weakly damped one-particle states of a Fermi liquid play in the BCS theory. The small superfluid stiffness at low doping is explained by the small value of the vortex–antivortex binding energy.

It turns out [21] that due to the d-wave order parameter having nodes, the corresponding theory is formally equivalent to anisotropic $(2+1)$-dimensional quantum electrodynamics (QED_{2+1}). According to this theory, the behavior of fermion excitations is essentially a non-Fermi-liquid one. The so-called '*algebraic*' Fermi liquid (AFL) that arises in this way replaces the ordinary Fermi liquid as the basis of the theory of the pseudogap state. The properties of AFLs put them closer to the Luttinger than to the Fermi liquid in that quasiparticle excitations have a large damping whereas the feature of being well-defined is, on the contrary, found in collective modes.

Analytical results obtained in the framework of QED_{2+1} are presented formally as a power series in $1/N$, where N is the number of pairs of nodes. For example, for a cuprate with a single CuO_2 plane in the unit cell, Ref. [21] assumes $N=2$ in accordance with the proposed d-wave gap symmetry. For more layers per unit cell, it is assumed [21] that $N=4$ (two CuO_2 planes) or $N=6$ (three CuO_2 planes). The larger N is, the better the estimate of the leading (proportional to $1/N$) term in the power series in $1/N$.

As noted in Ref. [21], for $N<N_c$, where $N_c=32/\pi^2$, a gap is spontaneously developed in the fermion excitation spectrum at $T=0$ due to the violation of chiral symmetry in QED_{2+1}, which signals, in accordance with the cuprate phase diagram, a phase transition from the AFL to the AF state. The formation of the gap leads to the AF state, which can be considered as a precursor of the Mott AF half-filling state. For $N>N_c$, the nonsuperconducting state preserves its chiral symmetry even for $T\to 0$, and the only way this state can give rise to AF order is by decreasing doping. This conclusion, as noted in Ref. [21], is in principle not inconsistent with a number of theories linking the pseudogap behavior to the competition of ordered states that arise in the particle–hole pairing channel. In particular, OAF with a d-wave symmetric gap and the associated d-density wave (DDW) can be considered as such chiral-symmetry-violating ordering.

QED_{2+1} phenomenology is not concerned with what is the microscopic mechanism that produces BCS type states with d-wave pairing, nor does it include the effect of Coulomb interaction, i.e., the dielectrization of the system at half filling and the appearance of a state other than BCS (possibly with d-symmetry preserved). Therefore, the predictions of the theory of Ref. [21] preserve their validity upon inclusion of the Coulomb interaction (to be discussed below).

3. Resonating valence bonds. Separation of charge and spin degrees of freedom

Whatever microscopic approach is taken to cuprate superconductivity as a perturbationally inaccessible problem of many strongly interacting particles, a certain guess must be made in some way or another, as in the BCS theory, as to what ground-state wave function describes the key properties of the system best.

The function proposed by Anderson [1] relies on the concept of *resonating valence bonds* and is represented as a linear combination of configurations of singlet bonds (opposite spin electron pairs localized on copper atoms in the CuO_2 plane) and vacancies (doping-induced holes), under the absolute prohibition on one and the same site being occupied doubly by opposite spin electrons. The bonds are treated as already-formed electron pairs, so that their wave function (assuming a d-wave symmetric gap) could be written in the usual BCS form

$$|\mathrm{BCS}\rangle = \prod_k (u_k + v_k \hat{c}^\dagger_{k\uparrow}\hat{c}^\dagger_{-k\downarrow})|\mathrm{vac}\rangle\,, \tag{1}$$

where $|\mathrm{vac}\rangle$ is the vacuum state, u_k and v_k are the Bogolyubov transformation amplitudes, and $\hat{c}^\dagger_{k\uparrow}(\hat{c}_{-k\downarrow})$ are the creation (annihilation) operators for electrons with momenta $\pm k$ and spins $\sigma=\uparrow,\downarrow$, respectively. The double occupation prohibition can be included using the Gutzwiller projection operator [24]

$$\hat{P} = \prod_i (1-\hat{n}_{i\uparrow}\hat{n}_{i\downarrow})\,, \tag{2}$$

where $\hat{n}_{i\sigma}$ is the occupation number operator for an electron of spin σ on site i. Thus, Anderson's RVB wave function is written as

$$|\mathrm{RVB}\rangle = \hat{P}|\mathrm{BCS}\rangle\,. \tag{3}$$

This is considered as a trial wave function in which the order parameter Δ in $|\mathrm{BCS}\rangle$ is a variational parameter interpreted as the pseudogap magnitude. As doping decreases, the value of Δ increases, in qualitative agreement with the observed $T^*(x)$ dependence. The superfluid stiffness turns out to be proportional to doping x rather than to total electron concentration $1-x$. Thus, the Gutzwiller projection corresponds to the dielectrization of the system for $x\to 0$ in a natural way.

The implications of choosing the wave function of the form (3) have been examined numerically by many authors using the Hubbard model (see, for example, Refs [25, 26]). It has been found that a theory involving RVBs predicts a wide diversity of behaviors the system exhibits depending on the ratio of the Hubbard energy to the energy band width U_0/t_0, which is the parameter of the theory. Some of the predictions of the RVB model (in particular, those concerning the magnetic properties of the cuprates) are in qualitative agreement with the experimental data available.

A widely used framework for describing the insulating (Mott) half-filling state is the $t-J$ model, in which electron hopping integrals between neighboring sites are suppressed compared to the initial value (t_0) due to the prohibited occupation of a site by two opposite-spin electrons and turn out to be proportional to the doping level x. The exchange interaction between electrons on neighboring sites is proportional to t^2/U_0. Although this is currently a widespread approach to the theoretical study of the cuprates, it has been noted (Laughlin [27]) that the Hubbard-model or $t-J$-model results obtained by different authors turn out to be highly

sensitive to calculation details and often are hardly consistent with one another. There is apparently no convincing evidence to support the possibility of the SC state within the 2D Hubbard model [27].

A more consistent approach to the problem is one that underlies the RVB model [1] and assumes charge and spin variables to be separable (which is strictly justified for one dimension only). The reason for such separation is a strong electron – electron interaction, whose elimination allows new quasiparticles — a spinless *holon* carrying the hole charge and an uncharged *spinon* carrying spin $\sigma = \pm 1/2$ — to be defined. The holons and spinons can be considered as weakly interacting quasiparticles; and for their description, the mean-field approximation can be used.

The simplest U(1)-symmetry separation form $\hat{c}^{\dagger}_{n\sigma} = \hat{f}^{\dagger}_{n\sigma}\hat{b}_n$ [28] ($\hat{c}^{\dagger}_{n\sigma}$ is the creation operator for a particle of spin σ on site n; $\hat{f}^{\dagger}_{n\sigma}$ is the same for a spinon of zero charge and spin σ on site n; and $\hat{b}_n$ is the annihilation operator for a zero spin holon on site n) leads to a number of difficulties, for the overcoming of which an SU(2)-symmetry-based transformation which introduces a doublet of Fermi operators instead of $\hat{f}^{\dagger}_{n\sigma}$ [29] has been proposed. Since the deviation from half-filling violates the SU(2) symmetry, in order to restore it at $x \neq 0$, the boson singlet $\hat{b}_n$ was replaced by a doublet of Bose operators $\hat{b}_{n1}, \hat{b}_{n2}$ [30, 31]. The diversity of phase transitions is accounted for by sets, of different symmetry, of anomalous averages which are defined on operators $\hat{f}$ and $\hat{b}$ and violate SU(2) symmetry. Going beyond the mean-field approximation — which corresponds to projecting the thus found wave functions of various ordered states onto SU(2) space — restores the SU(2) symmetry and can correspond to strongly developed fluctuations of such ordered states.

The materials with large values of U_0 clearly are insulators under all conditions and show no signs of superconductivity. In the cuprates, U_0 are moderate in value, so the complete prohibition — realized by the Gutzwiller operator — on the occupation of a site by two opposite-spin electrons appears to be an excessively stringent constraint. Reference [26] offers a trial wave function of the form

$$|\mathrm{PRT}\rangle = e^{i\hat{S}}|\mathrm{RVB}\rangle\,, \tag{4}$$

where the operator $e^{i\hat{S}}$ partially restores the possibility of a site being occupied by two electrons. As before, the variational parameter Δ in $|\mathrm{BCS}\rangle$ plays the role of a pseudogap, and the off-diagonal long-range order (ODLRO) parameter calculated in Ref. [26] — and hence T_c — vanishes at $x = 0$ and has a maximum at a certain optimum doping. The jump in the distribution function at the Fermi momentum in the directions of SC gap zeros tends to zero for $x \to 0$, which corresponds to the dielectrization of the system and to a low superfluid stiffness, $\rho_s \sim x$. According to experimental data, ρ_s and T_c in the strongly underdoped regime are proportional to $x - x_*$, and their domain of definition, as is seen from the phase diagram of the cuprates, is the doping interval $x_* < x < x^*$.

We note also that there is apparently no reason in principle why QED_{2+1} phenomenology based on the $|\mathrm{BCS}\rangle$ function with a d-wave gap cannot be extended to the corresponding $|\mathrm{RVB}\rangle$ and $|\mathrm{PRT}\rangle$ functions.

4. Laughlin Hamiltonian

Experimental data are by and large consistent with the understanding that, as the temperature is increased, superconductivity persists at $T > T_c$ in the pseudogap regime of underdoped cuprates and that it coexists with antiferromagnetism [27]. Since the SC state (which is dominated by the insulating state in the pseudogap regime) manifests its properties extremely weakly, an electron system that makes the SC transition has a low superfluid stiffness and exhibits strong fluctuation effects. 'Hidden' deep in the insulating state, this kind of superconductivity has come to be known as *gossamer superconductivity* [27], a very difficult term to translate into Russian.

Laughlin [27], allowing for site occupation by two opposite spin electrons — the possibility completely ruled out only in the limit of very large U_0 — proposed the following wave function to describe a *gossamer superconductor* (GS):

$$|\mathrm{GS}\rangle = \hat{\Pi}(\alpha)|\mathrm{BCS}\rangle\,, \tag{5}$$

where $0 \leqslant \alpha_0 \leqslant 1$ is a measure of how effective the operator

$$\hat{\Pi}(\alpha) = \prod_j^N z_0^{(\hat{n}_{j\uparrow}+\hat{n}_{j\downarrow})/2}(1 - \alpha_0 \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}) \tag{6}$$

is in preventing double site occupation. In a real material, α_0 is determined by the Coulomb repulsion U_0. Although called the partial projection operator, $\hat{\Pi}(\alpha)$ is not actually a projection operator and, unlike the Gutzwiller operator $\hat{P}$, it has the inverse operator $\hat{\Pi}^{-1}(\alpha)$. The point of introducing the parameter z_0 in Eqn (6) is to keep the total number of particles $1 - x$ unchanged as the parameter α_0 is varied. The parameter $\alpha = 1 - (1 - \alpha_0)^2$, so that for $\alpha = 0$ function (5) is identical to $|\mathrm{BCS}\rangle$ and for $\alpha = 1$, to $|\mathrm{RVB}\rangle$, because $\hat{\Pi}(1) \equiv \hat{P}$.

Using the partial projection operator (6) to transform the Bogolyubov quasiparticle operators $\hat{b}_{k\sigma}$, i.e., introducing new operators

$$\hat{B}_{k\sigma} = \hat{\Pi}(\alpha)\hat{b}_{k\sigma}\hat{\Pi}^{-1}(\alpha)\,, \tag{7}$$

the Hamiltonian of the system becomes

$$\hat{H} = \sum_{k\sigma} E_k \hat{B}^{\dagger}_{k\sigma}\hat{B}_{k\sigma}\,, \tag{8}$$

where the quasiparticle energy is $E_k = (\xi_k^2 + \Delta_k^2)^{1/2}$, ξ_k is the electron kinetic energy measured from the chemical potential, and $\Delta_k = \Delta_0(\cos k_x a - \cos k_y a)$ is the d-wave gap. By definition,

$$\hat{B}_{k\sigma}|\mathrm{GS}\rangle = 0\,, \tag{9}$$

i.e., $|\mathrm{GS}\rangle$ is the exact wave function of Hamiltonian (8). Because this latter in a non-negative operator, $|\mathrm{GS}\rangle$ turns out to be the exact zero-energy ground state.

Since transformation (7) is noncanonical, it fails to preserve the anticommutation relations between the Fermi operators $\hat{b}^{\dagger}_{k\sigma}, \hat{b}_{k\sigma}$ on changing to the new operators $\hat{B}^{\dagger}_{k\sigma}, \hat{B}_{k\sigma}$, preventing these latter from being considered as creation and annihilation operators for new Fermi quasiparticles. The physical content of this result is associated with the interaction of quasiparticles, whose definition is obtained by introducing variational functions

$$|k\sigma\rangle = \hat{\Pi}(\alpha)\,\hat{b}^{\dagger}_{k\sigma}|\mathrm{BCS}\rangle\,, \tag{10}$$

allowing the energy of a quasiparticle to be determined. It turns out [27] that partial projection has virtually no effect on the quasiparticle dispersion law.

A continuous adiabatic transition $\alpha_0 \to 0$ causes the ground state $|\mathrm{GS}\rangle$ to continuously transform to the ground state $|\mathrm{BCS}\rangle$. Since the ground states and low-energy excitations of GS and BCS superconductors are in one-to-one-correspondence, GS describes the same state of the material that BCS does, according to Ref. [32].

The partial prohibition of the double occupation of a site leads to the pseudogap-state-inherent renormalization of the BCS coherence factors, as well as suppression of the photoemission intensity and superfluid stiffness: as α_0 varies from 0 to 1, the stiffness ρ_s decreases from 1 to $2|x|/(1+|x|)$, vanishing at $x = 0$. When ρ_s decreases, the 'partial projection' at the same time leads to increased AF insulating correlations.

Hamiltonian (8) contains a Hubbard term U, resulting from 'partial projection' (5). As the half-filled state is approached, U increases indefinitely. But so does the renormalized kinetic energy ($t_0 \to t$), and this in such a way that the physically meaningful dimensionless parameter keeps a finite value $U/t \sim 1$. In this sense Hamiltonian (8) provides a reasonable description of AF correlations and dielectrization at half-filling [33]. That part of Hamiltonian (8) that accounts for superconductivity is also renormalized, with the consequence that as $x \to 0$, the amplitude of the SC order parameter increases — with the superfluid stiffness simultaneously decreasing, as already mentioned. Near half-filling, provided the 'partial projection' is sufficiently strong, Hamiltonian (8) corresponds to the Hubbard Hamiltonian complemented with an interaction that produces d-wave pairing in the system [32].

Although the ground state of a GS has much in common with $|\mathrm{RVB}\rangle$ as the ground state of a doped Mott insulator, the chemical potential in the GS scheme turns out to lie about midway between the edges of the lower and upper Hubbard bands (which is exactly what is found experimentally) — unlike the RVB scheme, where the chemical potential is shifted toward the edge of the lower band as a result of doping [34].

In Ref. [34], an 'effective' Hubbard Hamiltonian supplemented by a term accounting for the AF spin–spin interaction (term that arises in a natural way in the t–J model) is used to find (as a function of the probability $d \equiv \langle \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\rangle$ of the double site occupation) the renormalization factors g_t and g_s for the order parameter components corresponding to the charge and spin degrees of freedom. Near half-filling and for $d \ll 1$, it turns out that $g_t \sim 8d$ and $g_s \approx 4$. An important point to note here is that in the RVB scheme $g_t \sim 2x$ [34].

Knowing what the variational parameter α_0 in Eqn (7) and the corresponding renormalizations mean makes somewhat clearer the way d-wave superconductivity in the presence of DDW is treated in Ref. [35]. Let $\Delta_1(k) = \Delta_1 f(k)$ and $\Delta_2(k) = \Delta_2 g(k)$ be the SC and DDW order parameters, respectively, where Δ_1 and Δ_2 are the amplitudes and the functions $f(k)$ and $g(k)$ give the angular dependences of the order parameters. Then, if these dependences are identical, i.e., $f(k) = g(k) = \cos 2\varphi$ (which is most probably the case in the cuprates), the superconducting stiffness has the form [35]

$$\rho_s = \frac{\Delta_1^2}{\Delta_1^2 + \Delta_2^2}\,, \tag{11}$$

which corresponds to ρ_s being significantly suppressed at small x, when the dominant correlations are AF ones, and $\Delta_1 \ll \Delta_2$. Note that for the case $f(k) = \cos 2\varphi$, $g(k) = \sin 2\varphi$, it is found [35] that $\rho_s = \Delta_1/(\Delta_1 + \Delta_2)$.

5. Hidden order and current circulations

In Ref. [23] it is assumed that the pseudogap observed in the cuprates is a true gap in the spectrum of one-particle excitations with momenta $(\pi, 0)$ and that it arises due to the appearance of a certain ordered state related to OAF (DDW order, leading to a staggered distribution of the signs of orbital current circulations over units cells, or the so-called staggered-flux state [36]). Earlier studies of ordered current states both used the Fermi-surface-nesting version of the band theory (toroidal magnetic ordering) [37] and relied on the Hubbard model [38, 39]. Since the OAF-related order is hard to observe experimentally, the term 'hidden' was introduced [23] for the order assumed to compete with superconductivity. There is evidence that such 'hidden' order is observed in underdoped cuprates [40].

This model explains many properties of the cuprates, e.g., the fact that the symmetry of the pseudogap (DDW gap Δ_2) is identical to that of the d-wave SC gap [23]. One objection to the pseudogap state model of Ref. [23] is the absence at $T = T^*$ of thermodynamic singularities inherent in second-order phase transitions (in heat capacity, for example).

In Ref. [41] it is shown that a phase transition from the insulating DDW state occurs not due to the breakdown of the electron–hole pairs but rather due to fluctuations which translate d-symmetric current contours into p-symmetric ones (this corresponds to the $\mathrm{div}\,\mathbf{j} = 0$ constraint on fluctuating currents $\mathbf{j}$, equivalent to prohibiting a site from being occupied by two electrons in the Hubbard model). Fluctuations with symmetry change d $\to$ p are analogous to the appearance of a vortex–antivortex pair in QED_{2+1} phenomenology. In Ref. [41] it is shown that such a phase transition is an infinite-order transition, which does not lead to a heat capacity singularity.

The DDW order splits the Brillouin zone into two magnetic subzones, so that an FC should consist of isolated hole pockets if doping is low. ARPES shows, however [42], that in hole-doped cuprates the FC appears in arc rather than pocket form. According to Ref. [43], the spectral density corresponding to the first magnetic Brillouin subzone greatly exceeds the contribution from the second. The difference in the intensity and structure of ARPES spectra between the superconducting and pseudogap states is explained in Ref. [43] by two facts: first, the coherent factors of these states are different in nature; and second, the d-wave SC gap has only zero points — as opposed to the zero lines of the DDW order parameter in the pseudogap state (antinodal quasiparticles, which are relatively high-energy excitations, are assumed to damp out due to the creation of electron–hole pairs along the FC arcs in the DDW state).

Within the framework of the generalized t–J model, which preserves SU(2) symmetry even away from half-filling [30], the pseudogap state is described as fluctuations between SC and OAF (staggered-flux phase) d-wave states. Ivanov et al. [44] employed this model to study current–current correlations in the $|\mathrm{RVB}\rangle$ state with a d-wave order parameter. The study established the existence of slowly falling (with distance) correlations of currents that have opposite signs of circulation in neighboring unit cells [44, 45]. This suggests that in the pseudogap region $T_c < T < T^*$ it is precisely these correlations that manifest themselves as broken vortices and antivortices (which are current circulations of opposite sign). In accordance with the QED_{2+1} scheme, it is their existence that causes the violation of phase coherence. In this way, it is possible to describe the evolution

of the insulating SC state into the SC state as doping increases.

In Ref. [44] it is assumed that the state of a d-density wave manifests itself in the form of well-developed fluctuations obtained from an ordered $|\mathrm{DDW}\rangle$ state by projecting it by means of $\hat{P}_{\mathrm{SU}(2)}$ onto a subspace of group SU(2) such that one of the following three states on each site is allowed: (1) one of two fermions of the doublet $\hat{\mathrm{f}}_\uparrow$, $\hat{\mathrm{f}}_\downarrow$; (2) boson $\hat{\mathrm{b}}_1$ with no fermions; and (3) boson $\hat{\mathrm{b}}_2$ together with both fermions $\hat{\mathrm{f}}_\uparrow$, $\hat{\mathrm{f}}_\downarrow$. As a result of this projection, the translational and time reversal symmetry violated by the DDW state are restored. The pseudogap state arises due to the Bose condensation of bosons $\hat{\mathrm{b}}_1$ and $\hat{\mathrm{b}}_2$ into the minima $(0,0)$ and (π,π) of their corresponding bands.

In Ref. [44] it is shown that there is attraction between bosons $\hat{\mathrm{b}}_1$ and $\hat{\mathrm{b}}_2$, which ensures the formation of a large-momentum pair (π,π). For each component $\hat{\mathrm{b}}_1$ or $\hat{\mathrm{b}}_2$ of this pair there is a vortex or antivortex which can be put into correspondence with it. The state obtained in this way is equivalent to the $|\mathrm{RVB}\rangle$ state: $\hat{P}_{\mathrm{SU}(2)}|\mathrm{DDW}\rangle \equiv |\mathrm{RVB}\rangle$. Thus, when moving from small x values we can gain deeper insight into the structure of both the SC and pseudogap states. Qualitatively, the conclusion of Ref. [44] on replacing $|\mathrm{RVB}\rangle$ with $|\mathrm{PRT}\rangle$ or $|\mathrm{GS}\rangle$ remains valid. Note also that the QED_{2+1} scheme, which is based on the $|\mathrm{BCS}\rangle$ state, can be realized in any of the above states.

6. Large-momentum pairing for Coulomb repulsion

It should be noted that many results on cuprate properties obtained in models with strong electron – electron interaction (when $U_0/t_0 \gg 1$) are often recovered in the band ($U_0/t_0 \ll 1$) scheme. Since in cuprates, most likely, $U_0/t_0 \sim 1$, the situation here seems to be one is which the same problem — the description of the insulating and SC properties of these compounds — is approached from two different angles.

There is reason to believe that in addition to the usual Cooper channel for zero-momentum superconducting pairing, SC pairing with large total momentum can play a major role in 2D systems like cuprates [5, 6, 44, 46, 47]. Such pairing [48] differs considerably from the usual Cooper pairing, primarily due to the existence of a *kinematic* constraint [49] on the domain where the momentum of the relative motion of a pair, $\mathbf{k}$, is defined, the domain being strongly dependent on the magnitude and direction of the pair momentum $\mathbf{K}$ and on the FC shape. For zero-momentum pairing, there are no kinematic constraints, since $\mathbf{k}$ coincides with the momentum of a particle in a pair, and in the BCS model the domain of definition of $\mathbf{k}$ is limited *dynamically* by that band in momentum space where the pair-forming interaction is nonzero.

In the general case, the kinematic constraint has the consequence that the pair excitation energy vanishes only at two points within the domain of definition of $\mathbf{k}$ rather than on a line. In addition, the density of states of the relative motion vanishes at these points, eliminating the logarithmic singularity in the self-consistency equation and ruling out SC pairing no matter how small the coupling constant is. However, for a special shape of the FC — provided it is compatible with the FC being located in an extended vicinity of the saddle point of the electron dispersion law [50] and provided, further, that a stripe structure can arise in the system [13] — it turns out that for certain specific $\mathbf{K}$s the domain of definition of the relative-motion momentum can include not separate points on the FC, but rather its finite portions where the excitation energy becomes zero. This *mirror nesting* of the FC already ensures SC pairing for an arbitrarily small coupling constant (provided the mirror nesting 'quality' is high enough [51]).

The internal structure of a pair with a large $\mathbf{K}$ is determined by the way its component particles interact while in relative motion, and the wave function of the pair is represented as a linear combination accounting for all crystallographically equivalent $\mathbf{K}$s. Coefficients in this combination (and hence the symmetry of the resulting state) are determined by the interaction between the component particles with different (but equivalent) $\mathbf{K}$s. The ground state of the system is constructed — exactly as in the BCS theory — from the wave functions of pairs, i.e., can be designated $|\mathrm{BCS}\rangle$. Clearly, no prohibition on the occupation of a site by two electrons is introduced formally.

Views differ as to what interaction leads to superconductivity in the HTSC cuprates, the noteworthy ones including both the electron – phonon mechanism characteristic of the BCS theory [52, 53] and mechanisms involving direct electron correlations, considered in the Hubbard model and in its variations of the types discussed above. References [48, 54] use the band scheme to consider large-momentum SC pairing that arises for Coulomb repulsion. In this case, simply replacing the interaction matrix element $U(\varkappa)$ ($\boldsymbol{\varkappa} = \mathbf{k} - \mathbf{k}'$ being the momentum transfer upon scattering) by a single constant $U(\varkappa) \to U(0) > 0$ clearly can lead only to a trivial solution for the self-consistency equation (such a replacement proves sufficient in the BCS model with attraction, when $U(0) < 0$). Therefore, noting that the region kinematically allowed for relative-motion momenta of a large-$\mathbf{K}$ pair is limited in size, the matrix element within this region can be approximated by

$$U(\varkappa) = U_0 r_0^2 \left(1 - \frac{\varkappa^2 r_0^2}{2}\right), \tag{12}$$

where r_0 is the effective Coulomb screening length, and U_0, as can be seen in the site representation, is identical to the one-site Hubbard energy. It should be noted that the second term in Eqn (12) can be interpreted as a certain effective attraction which, as shown in Ref. [32], should be added to the Hubbard repulsion to obtain the SC solution. Note that in order for the Hubbard model (which allows for pairing with momenta 0 and π [46]) to produce the SC solution, interaction corresponding to pair exchange between neighboring sites should be added to it (giving the so-called Penson – Kolb – Hubbard model [47]).

Expression (12), viewed as the degenerate kernel of a linear integral operator, has four eigenfunctions (two even and two odd) [54], and the SC solution of the self-consistency equation with kernel (12) is determined only by the two even eigenfunctions, one with a positive and the other with a negative eigenvalue. The necessary condition for the existence of an SC solution is that the kernel $U(\varkappa)$ have at least one negative eigenvalue. Since a screened Coulomb potential in a Fermi system clearly has this property, it follows that to describe the SC state there is, in principle, no need for any other boson-field-mediated electron – electron interaction (for example, BCS electron – phonon interaction) to be considered.

In addition to the bound state, there is one more possible solution to the Cooper problem of two attracting particles with Fermi occupation — a strongly damped one in the continuous spectrum of the relative motion of a zero-

momentum pair. A similar problem concerning a large-momentum pair with repulsion (12) also leads to a bound state, in addition to which a weakly damped quasistationary state (QSS) can develop near the edge of the continuous spectrum of the relative motion of the pair [55]. Such QQSs correspond to special elementary excitations that are formed by pairs of one-particle states and show up as a sharply increased density of states in a narrow (on the order of QSS damping) energy range. Thus, to the formation of a QSS there corresponds the suppression of the density of one-particle states over the entire range of relative-motion energies. In this case, the pseudogap appearing in the spectrum of one-particle excitations in a limited temperature range $T_c < T < T^*$, with T^* increasing with decreasing doping [55], can be directly related to the appearance of a QSS. The point to make here is that both the QSS and the stationary state of the pair arise as the solutions of *one and the same* equation for the wave function of the relative motion of the pair.

There are analogies to be drawn between the QSS and phase slip inducing excitations in QED_{2+1} phenomenology (broken vortex–antivortex pairs) as well as between the QSS and excitations in the form of fluctuations of countercirculating orbital currents [41, 44].

Whether a (large-momentum) pair is in a bound or quasistationary state, the wave function of its relative motion, for repulsion of the form (12), is sign alternating in the domain of definition of the relative-motion momentum, changing its sign on a certain line that crosses FC twice within the domain. The same property is possessed by the SC order parameter, which hence has as many pairs of nodal points, N, as there are crystallographically equivalent **K**s contained in the $|\mathrm{BCS}\rangle$ state. For example, for the CuO_2 plane of tetragonal symmetry, this number is $N = 4$, which exceeds the critical value $N_c \approx 3$ in the QED_{2+1} scheme and thus justifies its application to the pseudogap state even for cuprates with one copper–oxygen plane in a unit cell. Importantly, the analysis of experimental data shows [56] that the SC gap (as well as the pseudogap) in the cuprates may possess symmetry other than d-wave. The SC order parameter and QSS studied in Refs [48, 54, 55] have eight nodal points (whose same-**K** points are close to one another) and can be ascribed $s + g$ symmetry [56].

Evidence that the SC gap depends significantly on the momentum of the relative motion of a pair came from an analysis of $I-V$ curves of HTSC cuprates carried out in Ref. [57] under the assumption that the asymmetry of an SC gap can be described by a simple linear dependence on the excitation energy of a pair. The dependence of the SC gap on **k** has a strong effect on coherence factors, supporting the conclusion about their renormalization which was reached in Ref. [32].

Ideas about large-momentum pairing in the case of repulsive interaction lead to the conclusion that the SC state exists in a limited doping range $x_* < x < x^*$, and that for weak doping the transition temperature T_c scales with $x - x_*$, as does the superfluid stiffness.

The fact that the SC order parameter is determined only (in the general case, at least) by two eigenfunctions of the kernel $U(\varkappa)$ has to do with its choice in the form of (12) — a choice which reflects the maximum dynamic symmetry possible for the interaction which leads to superconductivity in the case of repulsion (in the attraction case this symmetry is higher, which, as already mentioned, makes it possible to consider the interaction as point one). The eigenfunctions of the kernel are a natural basis in terms of which to expand the order parameter. Thus, the SC parameter is two-component, and it is the invariant combinations of its components that must enter into the free energy, thus leading to the Ginzburg–Landau system of equations. In a similar manner to Ref. [58], where two coexisting charged condensates interact via an electromagnetic field, one would expect that the topological defects of the order-parameter phase have a more complex structure compared to the vortex–antivortex excitations in the QED_{2+1} scheme.

In Ref. [54] it is assumed that the ground state is described by a function of the $|\mathrm{BCS}\rangle$ form. One would think that the presence in Eqn (12) of the Hubbard term $U_0 r_0^2$ determining the efficiency of 'partial projection' in the Laughlin ground state already takes this projection into account in some sense — and to the extent allowed by band theory.

7. Conclusion

To what extent the current knowledge of the cuprate superconductors can form the basis for their theory and what this theory might look like are moot questions. What is clear is that the theory of the cuprates cannot be presented in as simple a form as the BCS theory, in which an SC transition from the state of a normal Fermi liquid is not complicated by the presence of energetically close phases competing with superconductivity. In principle, the BCS theory in its simplest form is concerned with the instability of a weakly nonideal Fermi gas toward the formation of singlet pairs due to weak attraction between the particles. For a real (not weak) interaction, Eliashberg's equations are taken to replace the BCS equation in the electron–phonon model.

Given the strong anisotropy of the cuprates, the important role of electron correlations which lead to dielectrization and AF order upon decreasing doping, and, finally, the strong fluctuation effects in these materials, there seems to be little or no hope for constructing a theory as simple and easy-to-follow as BCS.

One would think, however, that the basic results we have summarized here — obtained as they are from a variety of approaches and methods and often similar in their implications — already provide a general and by and large adequate picture of the unusual properties of the cuprates.

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Phase transitions and the giant magnetoelectric effect in multiferroics

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1. Introduction

It has long been noted that despite the different nature of structural phase transitions in them, the three classes of crystalline solid bodies — ferromagnets, ferroelectrics, and ferroelastics — have a whole series of similarities such as the existence of specific domains, anomalous physical properties in the neighborhood of a transition, hysteresis, etc. In 1969, K Aizu unified them into a single class of materials collectively named ferroics, due to the prefix 'ferro' they share [1]. Multiferroics are a class of crystalline solids in which at least two of the three order parameters — magnetic, electrical, or mechanical — coexist.

The subject matter of this work is ferromagnetoelectrics, i.e., materials with magnetic and electric order simultaneously present [2, 3]. The relationship between magnetic and electric subsystems in ferromagnetoelectrics manifests itself as *magnetoelectric* (*ME*) *effects* and opens up the possibility of using an electric field to control the magnetic properties of a material or, vice versa, to use a magnetic field to modulate the electrical properties. All this makes ferromagnetoelectrics likely candidate materials for magnetic field sensors and writing/reading devices.

Although this theme is not new (the first ferromagnetoelectric was synthesized back in 1961 [4]), it has long been of purely academic interest because of the relatively small values of the observed magnetoelectric effects and because these effects have usually only been seen at low temperatures. For example, for the classical magnetoelectric material Cr_2O_3 (chromite) the magnitude of the magnetoelectric effect is $\alpha = P/H = 3\times10^{-10}$ C (m^2 Oe)$^{-1}$ (3.7×10^{-12} s m^{-1} or 10^{-4} in the CGS system). ME effects two orders of magnitude stronger were observed in $TbPO_4$ [5]: 10^{-2} (in the CGS system) or 3×10^{-10} s m^{-1}. In current terminology such effects are referred to as *giant*. However, in this particular compound the magnetoelectric effect only exists at temperatures below 2 K. It is only recently that materials showing giant magnetoelectric effects at room temperature have been obtained [6].

The discovery of giant ME effects is of particular interest in the light of the rapid development of *spin electronics*, a new branch of microelectronics which makes use of the transport properties of spin-polarized electrons. The main concern of spin electronics is converting information in the form of magnetization into an electrical voltage. Currently, this problem is being solved by using the phenomenon of *giant magnetic resistance* (GMR) [7]. With the alternative offered by the giant magnetoelectric effect, devices working on the giant magnetoelectric effect can possibly present competition to GMR devices in the future.

Also of interest are prospects for using magnetoelectric materials in magnetic memory devices. The major limiting factor in increasing the data-recording density is the magnetic dipole interaction, and this gives promise to the use of magnetoelectrics, most of which are antiferromagnets in which magnetoelectric domains can act as information bits.

Thus, for a ferromagnetoelectric to be used for practical purposes, the following are simultaneously required: (1) high (above room) electric and magnetic transition temperatures, (2) a large ME effect, and (3) low electrical conductivity at room temperature.

2. The ferromagnetoelectric bismuth ferrite $BiFeO_3$

Among various ferromagnetoelectric materials, one of the most attractive is bismuth ferrite $BiFeO_3$. There are both fundamental science and applied aspects of interest in this material. The relatively simple chemical and crystal structure of bismuth ferrite makes it interesting as a model object for first-principles studies. Moreover, bismuth ferrite is of practical interest as the basis for creating magnetoelectric materials — to a large measure due to its record high temperatures for electric ($T_c = 1083$ K) and magnetic ($T_N = 643$ K) ordering.