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Pair Fermi contour and repulsion-induced superconductivity in cuprates

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The pairing of charge carriers with a large pair momentum is considered in connection with high-temperature superconductivity of cuprate compounds. The possibility of pairing arises due to some essential features of quasi-two-dimensional electronic structure of cuprates: (i) *The Fermi contour with strong nesting features*. (ii) *The presence of an extended saddle point near the Fermi level*. (iii) *The existence of some ordered state (for example, antiferromagnetic) close to the superconducting one as a reason for the appearance of a "pair" Fermi contour resulting from carrier redistribution in momentum space*. In an extended vicinity of the saddle point, the momentum space has hyperbolic (pseudoeuclidean) metrics; therefore, the principal values of the two-dimensional reciprocal reduced effective mass tensor have unlike signs. At small momenta of the relative motion of a pair with a large pair momentum, the pairing is sensitive just to the sign and value of the effective mass and not to only the value of the Fermi velocity as in the case of Cooper pairing. The nesting of the Fermi contour results in an increase of the statistical weight of the pair with a large total momentum due to an extension of the momentum space domain which corresponds to permissible values of the relative motion momentum. The rearrangement of holes in momentum space results in the rise of a "pair" Fermi contour which may be defined as the zero-energy line for the relative motion of the pair. The superconducting gap arises just on this line. The pair Fermi contour formation inside the region of momentum space with hyperbolic metrics results in not only superconducting pairing but in a rise of a quasistationary state in the relative motion of the pair. Such a state has rather small decay, and may be related to the pseudogap regime of underdoped cuprates. It is concluded that pairing in cuprates may be due to screened Coulomb repulsion. The pairing mechanism and the pair Fermi contour conception may provide a qualitative interpretation for the key experimental facts relating to cuprates.

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I. INTRODUCTION

Recently, we proposed a mechanism for superconducting (SC) pairing in an anisotropic quasi-two-dimensional (2D) electron system typical of high-temperature superconducting (HTSC) cuprate compounds.[1–4] Pairs with large momentum $\boldsymbol{K}$ ($\boldsymbol{K}$ pairs) are considered; here $K \approx 2k_F$, and k_F is the value of the Fermi momentum directed along $\boldsymbol{K}$. It is well known[5] that the Cooper channel of pairing becomes inefficient when the pair momentum exceeds a value of the order of Δ/v_F; here Δ is the SC gap at $K=0$, and v_F is the Fermi velocity. The same relatively small value of the pair momentum corresponds to the wavelength of a spatially inhomogeneous SC phase arising in a weakly ferromagnetic electron system[6] as well. The Cooper channel at $K \neq 0$ is suppressed due to Pauli's exclusive principle, which restricts the phase volume accessible for the electron states contributing to the $\boldsymbol{K}$-pair state. This phase volume decreases with K, and SC pairing becomes impossible at $K \sim \Delta/v_F$ because of a decrease of a dimensionality of the locus in momentum space of zero-energy quasiparticle states. Therefore, pairing with a large pair momentum may be possible under the condition that some rearrangement in the electron system provides finite (and sufficiently large) phase volume for the states forming the $\boldsymbol{K}$ pair, and zero (or sufficiently small) excitation energy corresponds to a finite piece of the Fermi surface (FS). Any rearrangement of electrons in momentum space which transfers a part of them across the FS results in an increase of the energy. If the electron subsystem interacts with some other one, for example, an antiferromagnetic (AF) spin subsystem, and such an interaction results in a gain in total energy, a FS arises corresponding to the ground state of the system. We believe that there is more than one possibility to obtain such a gain besides the one particular case, relating to SC pairing with a large total pair momentum in cuprates with a stripe structure, that we considered in our previous papers.[4]

In this paper, we consider the problem of pairing with a large total pair momentum under essentially more general conditions following from some key features relating to electronic structure of cuprates. In this connection, we introduce the conception of the "pair Fermi contour" being, in a sense, a generalization of the conventional Fermi surface conception when one takes into account the relative motion of a pair. We obtain the solution of the SC gap equation and corresponding condensation energy in a rather general case which is, one can believe, typical of cuprates.

The electronic structure and physical properties of HTSC cuprates were studied in detail.[7,8] Angle-resolved photoemission spectroscopy (ARPES) measurements[9,10] result in the unambiguous conclusion that, in the normal (*N*) state, any HTSC cuprate has a large FS. In the case of hole-doped compounds, the Fermi contour (FC), that is the cross section of the FS which is parallel to conducting layers is a square with rounded corners. The FC of holes is centered at (π,π), and exhibits a strong nesting feature along [100]-type directions. At approximately half-filling, long parts of the FC are situated close to the saddle points of the hole dispersion.[7] Hole doping moves the Fermi level toward the saddle point, whereas electron doping acts in the reverse direction. Therefore, in a hole-doped compound, the nesting feature of the

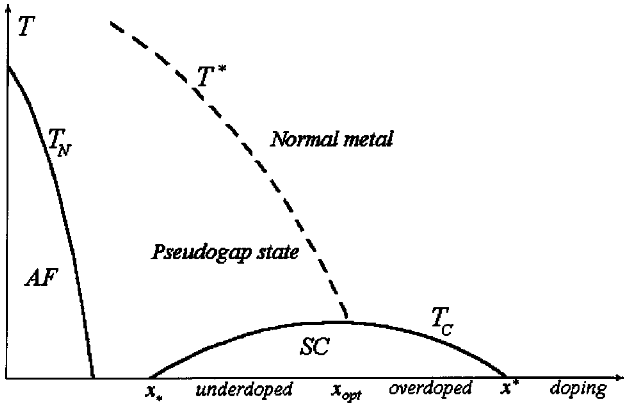

FIG. 1. Phase diagram (temperature vs doping level) typical of hole-doped HTSC cuprates.

hole FC appears in a relatively wide concentration range. Weak dispersion along the nesting directions results in the fact that the longitudinal (along the nested straight-line parts of the FC) component of the Fermi velocity is sufficiently smaller than the transversal one.[11] This corresponds to an effective enhancement of the 2D density of states in the vicinity of the logarithmic van Hove singularity due to the saddle point.[12] Thus there is an extended vicinity of the saddle point in which the principal values of the 2D tensor of the reversed reduced effective mass have unlike signs. One can say that, in such a vicinity, the momentum space has *hyperbolic* (pseudoeuclidean) metrics. Due to nesting feature of the FC, the absolute values of the principal effective masses differ strongly from each other: the positive longitudinal mass is essentially more than the absolute value of negative transversal mass. In the case of any hole-doped cuprate compound, long straight-line parts of the FC are situated mainly just in such ''flat-band'' or ''extended van Hove singularity'' vicinities.[7]

In HTSC cuprates, the SC state appears in some doping interval $x_* < x < x^*$, bounded both above and below. Both the superconducting transition temperature T_C and the superfluid density (or phase stiffness) ρ_s may demonstrate a highly complicated dependence on doping in this interval.[8] The absolute maximum of T_C corresponds to the optimal doping, x_{opt}. The phase diagram typical of hole-doped HTSC cuprates is presented in Fig. 1.

In underdoped ($x < x_{opt}$) compounds, the one-particle density of states is suppressed essentially at $T_C < T < T^*$. Such a suppression may be interpreted as a rise of a so-called pseudogap in the excitation spectrum.[13] The temperature T^* corresponding to a crossover between the N state at $T > T^*$ and the ''pseudogap regime'' at $T_C < T < T^*$ decreases with the doping increase, and becomes approximately equal to T_C at $x \simeq x_{opt}$. The pseudogap Δ^*, just like the SC gap Δ, is strongly anisotropic, and the character of the anisotropy is the same[8] for both Δ^* and Δ. The maxima of their absolute values correspond to antinodal [100]-type directions. The minimal values (which, possibly, are equal to zero) of both Δ^* and Δ correspond to nodal [110]-type directions. Knight shift measurements indicate that there is singlet pairing of carriers when the electron system of HTSC cuprates is in the SC state.[14] Therefore, the observed momentum dependence of the SC gap may correspond to either anisotropic *s*- or *d*-type orbital symmetry.[15] The same orbital symmetry and the same energy scale of Δ and Δ^* enable one to suppose that the SC gap and the pseudogap are of the same origin.[16] However, there are two different points of view relating to the origin of the pseudogap (see, for example, Ref. 17) which can be interpreted either as a precursor of the superconductivity (the pseudogap regime as an incoherent state of paired charge carriers[18]) or a gap of nonsuperconducting nature.[19,20]

In the theory by Bardeen, Cooper, and Schrieffer (BCS),[21] attraction due to virtual phonon exchange is the driving force leading to pairing of carriers. In principle, the phonon mechanism of Cooper pairing should not be excluded as a mechanism of HTSC,[12] although it is difficult to explain some essential features of the HTSC state satisfactorily, for example, the symmetry of the SC gap. In view of the fact that the phase diagram of any HTSC cuprate has a region with long-range AF order, the AF fluctuation exchange as a mechanism of pairing[22] seems quite natural (neutron scattering experiments[23] exhibit broadened Bragg peaks up to the optimal doping). The other point of view is founded on the statement that the ground state energy gain at the SC transition in HTSC cuprates is due to a lowering of the kinetic energy arising when two like-charged carriers form a pair.[24] In such a case, generally speaking, one needs no attraction between carriers, and screened Coulomb repulsion remains a natural essential interaction in the electron system.

AF fluctuations (short-range AF order) may lead to a specific quasi-one-dimensional self-organization in 2D electron system of HTSC cuprates. An elastic neutron scattering study enables one to assume that holes doped into a crystal are situated in 1D antiphase boundaries (charge stripes) separating hole-depleted domains with AF order.[25] The rise of such a static stripe structure may be described as a transfer of excess holes from the AF part of a stripe into the antiphase boundary the (M part of a stripe). The dynamic stripe magnitude, just like the magnitude of AF fluctuations, decreases with doping and, at $x > x_{opt}$, the neutron scattering technique does not make possible a resolution of strongly broadened stripe peaks of rather low intensity. A stripe structure may exist independent of superconductivity, but such a structure (just like AF fluctuations) and superconductivity are closely, in a nontrivial way, connected with each other. As an indirect confirmation of this statement one may take into consideration the fact that at $x = 1/8$, when the static stripe magnitude is maximal, there is a local minimum on the doping dependence of the SC transition temperature.[26] Conversely, it is possible that dynamic stripes stimulate superconductivity.[8]

Available experimental data make it possible to determine the main features and details of the electronic structure which are essential to understand the character of the SC state of HTSC cuprates, and to interpret their physical properties qualitatively. First, all doped HTSC compounds have a 2D electronic structure with a strong nesting of the FC situated in an extended vicinity of the saddle point of the hole dispersion. Second, in all doped HTSC compounds, doping regions corresponding to AF and SC phases are close to each other and, in the SC region, there is a short-range AF order resulting in a stripe self-organization of spin and charge subsystems of the crystal. The theory developed here takes into account these principal features of the electronic structure, and can qualitatively explain the key experimental facts relating both to N and SC state of HTSC cuprates.

The paper is organized as follows: Section II is dedicated to a formulation of the conditions under which pairing with large pair momentum may be possible; in addition, we introduce the concept of the ''pair'' Fermi contour being a piece of the full Fermi contour on which the kinetic energy of the relative motion of the pair with a given total momentum turns out to be equal to zero. Thus, in the case of pairing with nonzero total momentum, the pair Fermi contour plays the same role that the full Fermi contour plays in the case of Cooper pairing of carriers with zero total momentum. In this connection, we discuss the peculiarities of the form of the domain in momentum space containing the momenta of the particles composing a pair. Also, we discuss the simple mechanism of an opening of the pair Fermi contour due to a rise of the stripe structure. In Sec. III we consider the problem of a single pair in momentum space with hyperbolic metrics, and discuss the symmetry properties of the pair wave function. It is shown that, due to crystal symmetry, the wave function of the pair may be related to either anisotropic *s*- or *d*-type orbital symmetry. In this section, we present an equation which determines two poles of the scattering amplitude corresponding to the relative motion of the pair. Section IV contains a discussion of the character of the two poles of the scattering amplitude corresponding to a quasistationary state (QSS) of the pair and superconducting instability. We consider both attractive and repulsive interactions between the components of the pair. It is stated that, in the case of repulsion, the pole having the larger energy corresponds to a QSS with infinitesimal positive decay, whereas the second pole with smaller energy has a finite negative decay so that this pole may be related to a SC instability. Such a disposition of the poles and the definite sign of their imaginary parts are in agreement with a phase diagram typical of cuprates. The approximate solutions of the equation which defines the SC order parameter are presented in Sec. V both in the case of attraction and repulsion between the components of the pair. In the latter case, the solution exists under the condition that the SC order parameter is not a function of a constant sign. Assuming that, crossing the pair Fermi contour, this parameter changes sign like a step function, we study the system of equations for two corresponding components of the order parameter. It is shown that the solution of such a system exists inside a doping interval bounded both above and below. In Sec. VI, we discuss the chemical potential shift due to SC condesation. This shift arises due to the essential asymmetry between the domains in momentum space corresponding to filled and vacant states and separated by the pair Fermi contour. Just such a shift mainly determines the value of the SC transition condensation energy which is studied in Sec. VII. Section VIII is dedicated to a brief discussion of some key experimental results related to both *N* and SC states of HTSC cuprates; also, we discuss some other possible reasons for an opening of the pair Fermi contour, and propose a qualitative interpretation of available experimental data in the scope of the theory developed here.

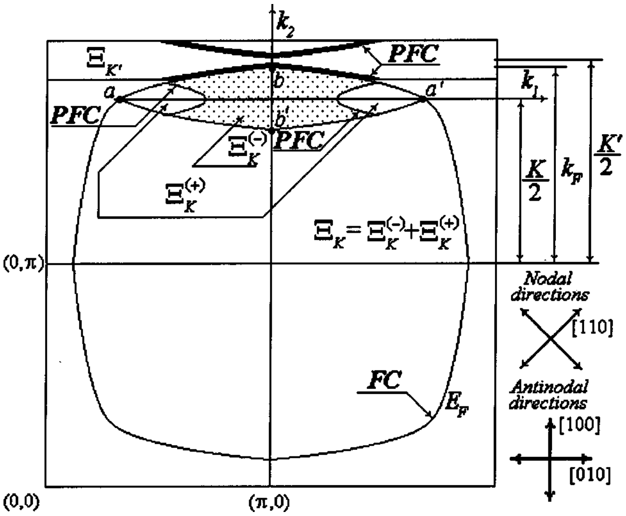

FIG. 2. Typical of hole-doped HTSC cuprates, the hole Fermi contour (FC) as a square with rounded corners (labeled the Fermi energy, E_F) centered at (π,π) . The domain of definition of momenta of the relative motion of **K** and **K**$'$ pairs are denoted as Ξ_K and $\Xi_{K'}$, respectively. Each such domain consists of two parts, $\Xi_K^{(-)},\Xi_K^{(+)}$ and $\Xi_{K'}^{(-)},\Xi_{K'}^{(+)}$, respectively. Inside the subdomains $\Xi_K^{(-)},\Xi_{K'}^{(-)}$ $(\Xi_K^{(+)},\Xi_{K'}^{(+)})$, the energy of the relative motion of corresponding pair measured from the pair chemical potential value 2μ is negative (positive). The total pair momentum is directed along an antinodal direction. The lines separating the subdomains of negative and positive relative motion energy form the pair Fermi contour (PFC). A doping decrease results in an opening of the PFC at two points, a and a', on the k_1 axis, corresponding to a doping level x_2. Then there is a rise and an extension of the subdomains $\Xi_K^{(+)}$ and $\Xi_{K'}^{(-)}$ accompanied by a corresponding decrease of the subdomains $\Xi_K^{(-)}$ and $\Xi_{K'}^{(+)}$. The PFC shrinks at two points b and b' on the k_2 axis, corresponding to a doping level $x_1 < x_2$.

II. ELECTRON AND HOLE PAIRS. PAIR FERMI CONTOUR

Let us consider two electrons or two holes with a total momentum $\boldsymbol{K} = \boldsymbol{k}_+ + \boldsymbol{k}_-$ where $\boldsymbol{k}_+$ and $\boldsymbol{k}_-$ are momenta of the particles composing a pair. This is a pair of noninteracting particles. Thus, now and below in this section, we do not fall outside the limits of the usual one-particle approximation, and the pair introduced here may be called as a *slave pair*. Further, taking account of the screened Coulomb interaction between particles, we use such pairs to construct a SC state. Filling the states inside the FC results in the fact that permissible values of a momentum of the relative motion of the $\boldsymbol{K}$ pair, $\boldsymbol{k} = (\boldsymbol{k}_+ - \boldsymbol{k}_-)/2$, belong to a certain domain of momentum space. Such a domain, which we denote as Ξ_K, has a form dependent on $\boldsymbol{K}$ and on a shape of the FC,[1] as in the case when the pair momentum is directed along [100] and $K < 2k_F$; this is represented schematically in Fig. 2. It is clear from Fig. 2 how one can define such a domain at any given $\boldsymbol{K}$. The area (labeled with the same symbol Ξ_K) of the domain Ξ_K tends to zero when $K \to 2k_F$. Thus the statistical weight of states which compose pairs with $K=2k_F$ is equal to zero even in a case of perfect nesting.[27] It should be noted that the model used in Ref. 27 did not take into account the existence of an extended saddle point and hyperbolic metrics of momentum space. For an arbitrary direction of $\boldsymbol{K}$, there are, generally speaking, eight domains corresponding to the pair momenta which are equivalent to given vector $\boldsymbol{K}$ (for special, antinodal, or nodal directions there are four equivalent vectors). However, at a preassigned deviation of $\boldsymbol{K}$ from $2k_F$, the statistical weight (the area Ξ_K) depends on the $\boldsymbol{K}$ direction, decreasing from a maximal value for antinodal directions to a minimal one for nodal directions. It is quite obvious that the binding energy of the $\boldsymbol{K}$ pair has to increase with Ξ_K; therefore, one may expect that a rise of the SC condensate should be due to pairs with momenta corresponding to antinodal directions.

There is experimental evidence in behalf of the consideration of hole pairs with large total momentum. As an example, one may consider the so-called "commensurate" neutron resonance (41 meV) peak below T_C which is usually associated with a rise of the resonance collective triplet π mode[28] corresponding to the saddle point. Recently, "incommensurate" magnetic fluctuations in HTSC cuprates were observed.[29] The incommensurate mode transforms continuously into a commensurate one,[28] demonstrating a negative (downward away from the commensurate momentum) dispersion.[30] Such a tendency toward softening of this triplet π mode can be interpreted as indirect evidence of the phase transition possibility associated with a softening of a certain singlet mode corresponding to a large and "incommensurate" pair momentum.

Almost straight-line parts of the FC belong to the region of momentum space with hyperbolic metrics. Therefore, the energy of the relative motion of a pair inside Ξ_K,

$$\varepsilon_r(\boldsymbol{K},\boldsymbol{k})=\varepsilon\left(\frac{\boldsymbol{K}}{2}+\boldsymbol{k}\right)+\varepsilon\left(\frac{\boldsymbol{K}}{2}-\boldsymbol{k}\right)-2\varepsilon\left(\frac{\boldsymbol{K}}{2}\right), \tag{1}$$

at relatively small $\boldsymbol{k}$, may be approximately represented as

$$\varepsilon_r(\boldsymbol{K},\boldsymbol{k})\approx\frac{\hbar^2}{2m}(\nu k_1^2-k_2^2), \tag{2}$$

where $\varepsilon(\boldsymbol{k})$ is hole dispersion and, as follows from a symmetry consideration, the coordinate axes are directed parallel (the k_1 axis) and perpendicular (the k_2 axis) to the FC (Fig. 2). These coordinate axis directions correspond to the principal directions of the 2D tensor of the reciprocal reduced effective mass (ν/m and $-1/m$ are dependent on principal $\boldsymbol{K}$ values of this tensor). Due to the strong nesting of the FC, the absolute values of the effective masses differ considerably from each other, namely, a dimensionless parameter $\nu \ll 1$.

The domain Ξ_K consists of two parts, $\Xi_K^{(-)}$ and $\Xi_K^{(+)}$, in which the energy of the relative motion of the $\boldsymbol{K}$ pair is negative and positive, respectively. The domain $\Xi_{K'}$, also shown in Fig. 2, corresponds to a pair with total momentum $\boldsymbol{K}'$ ($\boldsymbol{K}'$ pair) outside of the FC; thus $K'>2k_F$. This domain consists of two parts, $\Xi_{K'}^{(-)}$ and $\Xi_{K'}^{(+)}$, corresponding to negative and positive energies of the relative motion of $\boldsymbol{K}'$ pair as well. Excitations composing the $\boldsymbol{K}$ pair inside the FC are electrons whereas the excitations which compose the $\boldsymbol{K}'$-pair outside of the FC are holes.

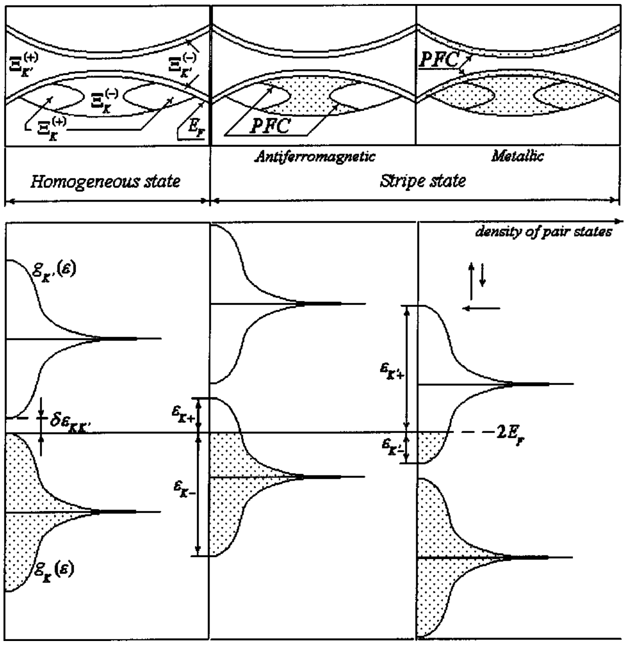

FIG. 3. Top panel: a sketch of the domains Ξ_K and $\Xi_{K'}$ and hole distribution in the cases corresponding to a homogeneous state of the electron system (left top panel) and a stripe state (the AF part of a stripe, middle top panel; the *M* part of a stripe, right top panel). Occupied and vacant pair states are separated by the PFC. Occupied states inside the domains are shadowed. Bottom panel: relative-motion band diagram for homogeneous state (left bottom panel), AF and *M* parts of a stripe (middle and right bottom panel, respectively).

In the case of hyperbolic metrics, the $\boldsymbol{K}$-pair density of states exhibits a logarithmic van Hove singularity corresponding to the zero energy of the relative motion, shown schematically in Fig. 3. Weak dispersion along one of the directions in 2D momentum space (the k_1 axis in Fig. 2) leads to the fact that $\boldsymbol{K}$-pair density of states has almost 1D character.[12]

By definition of the ground state of the electron system, all pair states inside Ξ_K are occupied, whereas the states inside $\Xi_{K'}$ are vacant. Such a filling of states in momentum space corresponds to a spatially homogeneous state of the electron system. At a given $\boldsymbol{K}$, states of the relative motion of the $\boldsymbol{K}$ pair are characterized by the relative motion density of states, $g_K(\varepsilon)$. The upper edge of pair density of states in the domain Ξ_K corresponds to the Fermi level (Fig. 3). There is a finite energy gap $\delta\varepsilon_{KK'}$ between the upper edge of $g_K(\varepsilon)$ and the lower one relating to pair density of states, $g_{K'}(\varepsilon)$, in the domain $\Xi_{K'}$. Therefore, any transfer of a pair from Ξ_K into $\Xi_{K'}$ is necessarily connected with an energy increase due to an increase of center-of-mass energy. However, it should be noted that the pairs having positive energy of the relative motion leave the domain Ξ_K whereas the pairs with negative energy arrive at the domain $\Xi_{K'}$.

Such transfers of pairs from the domain Ξ_K into a region of momentum space outside of the FC may bear a relation to well-known spatially inhomogeneous (stripe) structure in which there is an alternation of hole-enriched and -depleted 1D regions.[8] The region of momentum space into which $\boldsymbol{K}$ pairs may transfer is either that part, $\tilde{\Xi}_K$, of the domain Ξ_K which is situated outside of the FC or the domain $\Xi_{K'}$ corresponding to the total pair momentum $\boldsymbol{K}'$ (Fig. 2). As far as the relative motion of the density of states which corresponds to a $\boldsymbol{K}'$ pair belonging to the subdomain, $\Xi_{K'}^{(-)}$ is considerably greater than density of states corresponding to the subdomain $\tilde{\Xi}_K$ we may restrict ourselves to a consideration of the transfers $\Xi_K^{(+)} \Rightarrow \Xi_{K'}^{(-)}$ only. Suppose that a number of pairs, δN, passes from $\Xi_K^{(+)}$ into $\Xi_{K'}^{(-)}$, so that, in the subdomain $\Xi_K^{(+)}$, vacant pair states arise in a certain (small in comparison with $\delta\varepsilon_{KK'}$) energy interval near $2E_F$. The same number of pairs occupies a small energy interval (which may be determined using pair number conservation condition) near the lower edge of the band corresponding to the subdomain $\Xi_{K'}^{(-)}$. Thus the energy increase due to pair transfers from $\Xi_K^{(+)}$ into $\Xi_{K'}^{(-)}$ may be estimated as $\delta N \,\delta\varepsilon_{KK'}$.

Transfers of pairs, $\Xi_K^{(+)} \Rightarrow \Xi_{K'}^{(-)}$, in momentum space may be related to transfers of holes from AF parts of stripes into metallic (M) parts in real space. An enhancement of AF correlations due to such transfers results in some reducing of the energy which might compensate for the energy increase due to the excitation of hole pairs leading to transfers $\Xi_K^{(+)} \Rightarrow \Xi_{K'}^{(-)}$. An energy gain due to a removal of $\boldsymbol{K}$ pairs from $\Xi_K^{(+)}$, that is from AF parts of stripes, may be estimated phenomenologically if one introduces a parameter $I = I(x)$ which may be treated as a nearest-neighbor spin correlation function being a measure of AF short-range order. Let us assume that each hole pair transferring from the subdomain $\Xi_K^{(+)}$ into the subdomain $\Xi_{K'}^{(-)}$ gives an energy gain equal to I. Then total decrease in the energy of holes due to such transfers of δN hole pairs may be estimated as $-\delta N I$. Thus a rise of the stripe structure lowers the ground state energy provided that

$$I > \delta\varepsilon_{KK'} . \tag{3}$$

The existence in the domain Ξ_K of the hole filled part, $\Xi_K^{(-)}$, and the vacant part, $\Xi_K^{(+)}$, makes possible pairing of carriers in the vicinity of the lines separating filled and vacant subdomains. The energy of the relative motion of the $\boldsymbol{K}$ pair with respect to the value of the chemical potential is negative inside $\Xi_K^{(-)}$ and positive inside $\Xi_K^{(+)}$; therefore, the lines separating these subdomains play role of a peculiar "pair" Fermi contour (PFC) on which the SC gap may arise. Such a conclusion is related both to the domains Ξ_K and $\Xi_{K'}$, therefore, PFC is situated both inside and outside of the parent FC. If the value of the vector $\boldsymbol{K}-\boldsymbol{K}'$ which may be considered as a reciprocal spatial scale of the stripe structure appreciably exceeds a character scale, $\delta k_c \sim \Delta$, of nonzero SC order parameter in momentum space, one may consider the pairing problems in Ξ_K and $\Xi_{K'}$ independently from each other. In the following, we consider just the case when $|\boldsymbol{K}-\boldsymbol{K}'| \gg \delta k_c$.

III. PROBLEM OF A SINGLE PAIR

Now let us consider a $\boldsymbol{K}$ pair, taking into account two-particle potential interaction between the particles composing the pair. As stated above, the momenta of interacting particles are confined inside the domain Ξ_K. We suppose that this domain belongs to a region of momentum space with hyperbolic metrics. A wave function of the $\boldsymbol{K}$ pair can be written as

$$\Psi_K(\boldsymbol{r}_+ ,\boldsymbol{r}_-) = \frac{1}{\sqrt{S}} \varphi_K(\boldsymbol{r}) e^{i\boldsymbol{KR}}. \tag{4}$$

Here $\boldsymbol{r}_+$ and $\boldsymbol{r}_-$ are radius vectors of the particles, $\boldsymbol{R} = (\boldsymbol{r}_+ + \boldsymbol{r}_-)/2, \boldsymbol{r} = \boldsymbol{r}_+ - \boldsymbol{r}_-$, $\varphi_K(\boldsymbol{r})$ is a wave function of the relative motion, and S is a normalizing area.

On account of the crystal symmetry, all wave functions $\varphi_{\hat{g}K}$ corresponding to the momenta $\hat{g}\boldsymbol{K}$ turn out to be equivalent. Therefore, the $\boldsymbol{K}$-pair wave function should be represented as a linear combination of the form

$$\Psi_K^{(\Gamma)} = \sum_{[\hat{g}K]} c_{\hat{g}K}^{(\Gamma)} \Psi_{\hat{g}K} . \tag{5}$$

A choice of the coefficients $c_{\hat{g}K}^{(\Gamma)}$ is determined by the irreducible representation Γ of the crystal symmetry group according to which the wave function [Eq. (5)] transforms under the action of crystal symmetry operators $\hat{g}$. It should be noted especially that the wave function [Eq. (5)] corresponds to a currentless state in view of the fact that $\Sigma \hat{g}\boldsymbol{K} = 0$.

Taking account of the fact that the domains $\Xi_{\hat{g}K}$, corresponding to equivalent momenta $\hat{g}\boldsymbol{K}$, either do not overlap at all or overlap in a small way (Fig. 2) and, also, that a scattering of a $\boldsymbol{K}$ pair from any such domain into an equivalent one corresponds to a rather large change in the total momentum of the pair, one can, in a first approximation, neglect any inter-domain scattering. Then, the equivalent Hamiltonian of the relative motion of the $\boldsymbol{K}$ pair may be presented in the form[1]

$$\hat{H}_K = -\frac{\hbar^2}{2m} \left(\nu \frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} \right) + U_K^*(r), \tag{6}$$

where $r = \sqrt{x_1^2 + x_2^2}$, $U_K^*(r)$ is an effective potential energy of the particles composing the $\boldsymbol{K}$ pair. This energy depends on the domain Ξ_K in which scattering due to interaction is permitted. When the area Ξ_K is large enough, one can suppose that[1] $U_K^*(r) \sim \Xi_K$.

Generally speaking, all of the eigenfunctions of the operator [Eq. (6)] belong to a continuous spectrum. Therefore, it is quite natural to represent such a function in the form of a sum of an incident wave with the momentum $\boldsymbol{q}$ and scattered (expanding) wave:

$$\varphi_K(\boldsymbol{r}) \Rightarrow \varphi_{Kq}(\boldsymbol{r}) = e^{i\boldsymbol{qr}} + \chi_{Kq}(\boldsymbol{r}). \tag{7}$$

The Fourier transform of the scattered wave, $\tilde{\chi}_{Kq}(\boldsymbol{k})$, is a solution of the integral equation[31]

$$[\omega - \omega(\boldsymbol{k})]\tilde{\chi}_{Kq}(\boldsymbol{k}) = u(\boldsymbol{k}-\boldsymbol{q}) + \int u(\boldsymbol{k}-\boldsymbol{k}')\tilde{\chi}_{Kq}(\boldsymbol{k}')\frac{d^2k'}{(2\pi)^2}. \tag{8}$$

Here $\omega(\boldsymbol{k}) = \nu k_1^2 - k_2^2$, $\hbar^2\omega/2m$ is an energy of the incident wave, and $u(\boldsymbol{k}) = 2m\tilde{U}_K^*(\boldsymbol{k})/\hbar^2$, $\tilde{U}_K^*(\boldsymbol{k})$ is the Fourier transform of the effective interaction energy. In Eq. (8) one has to integrate over the domain Ξ_K, which is the domain of definition of momenta $\boldsymbol{k}$ and $\boldsymbol{k}'$. As far as this domain is small in comparison with the 2D Brillouin zone, one can approximately take $u(\boldsymbol{k}-\boldsymbol{k}') \approx u_0$. This approximation leads to the solution of the Eq. (8) in the form[1]

$$\tilde{\chi}_{Kq}(\boldsymbol{k}) = -\frac{u_0}{1+u_0B_K(\omega)}\frac{1}{\omega(\boldsymbol{k}) - \omega - i0 \operatorname{sgn}\omega}, \tag{9}$$

where the signum function provides a necessary condition in order that Eq. (9) is an expanding wave. The function $B_K(\omega)$ is defined as

$$B_K(\omega) = \int_{(\Xi_K)} \frac{1}{\omega(\boldsymbol{k}) - \omega - i0 \operatorname{sgn}\omega}\frac{d^2k}{(2\pi)^2} \equiv B_{K1}(\omega) + iB_{K2}(\omega). \tag{10}$$

At a real argument, the functions $B_{K1}(\omega)$ and $B_{K2}(\omega)$ can be written in the forms

$$B_{K1}(\omega) = \int_{(\Xi_K)} \frac{1}{\omega(\boldsymbol{k}) - \omega}\frac{d^2k}{(2\pi)^2},$$

$$B_{K2}(\omega) = \pi \operatorname{sgn}\omega \int_{(\Xi_K)} \delta[\omega(\boldsymbol{k}) - \omega]\frac{d^2k}{(2\pi)^2}, \tag{11}$$

where the integral defining $B_{K1}(\omega)$ has the meaning of the Cauchy principal value.

A denominator, $1 + u_0B_K(\omega)$, of the scattering amplitude, generally speaking, is not equal to zero at any real value of the argument ω. In the special case, when the function $B_{K2}(\omega)$ is equal to zero identically inside some interval of ω, scattering amplitude poles, which are solutions of the equation

$$1 + u_0B_{K1}(\omega) = 0, \tag{12}$$

correspond to bounded states.

When some complex value $\omega = \omega_K^{(0)} - i\Gamma_K$ is a solution of Eq. (12) and, in addition, $B_{K2}(\omega_K^{(0)}) \neq 0$, where $\omega_K^{(0)}$ makes sense of the energy of QSS provided that $0 < \Gamma_K \ll \omega_K^{(0)}$. At $|\omega - \omega_K^{(0)}| \ll \omega_K^{(0)}$, the QSS decay can be written as

$$\Gamma_K \approx B_{K2}(\omega_K^{(0)})/B'_{K1}(\omega_K^{(0)}). \tag{13}$$

Here the prime denotes differentiation with respect to ω.

In the case of a tetragonal crystal, one can separate all of the equivalent vectors $\hat{g}\boldsymbol{K}$ into two subsets. One of them, which contains the vector $\boldsymbol{K}$ itself, also contains all of the vectors $\hat{g}\boldsymbol{K}$ related to each other by reflections with respect to the coordinate axes. The other subset is generated in a similar way by the vector resulting from the reflection of $\boldsymbol{K}$ with respect to a diagonal of the square Brillouin zone. The coefficients $c_{\hat{g}K}^{(A_{1g})}$, corresponding to the trivial irreducible representation A_{1g}, are equal to each other. In the case of the irreducible representation B_{1g}, the coefficients $c_{\hat{g}K}^{(B_{1g})}$ have one and the same absolute value, and differ in sign for the two above-introduced subsets. Taking into account the explicit form of the functions $\tilde{\chi}_{\hat{g}Kq}(\boldsymbol{k})$ one can easily conclude that, in the case of an appropriate choice of coordinate axis directions, $\omega(\boldsymbol{k}) = \nu k_1^2 - k_2^2$ for any $\hat{g}\boldsymbol{K}$ belonging to the first subset, whereas $\omega(\boldsymbol{k}) = \nu k_2^2 - k_1^2$ when $\hat{g}\boldsymbol{K}$ belong to the second one. Thus the wave function corresponding to the irreducible representation A_{1g} has the form

$$\Psi_{Kq}^{(A_{1g})} \sim \frac{2\omega}{(\omega + k_1^2)(\omega + k_2^2)}, \tag{14}$$

provided that $\nu \ll 1$. The full symmetry of this function with respect to the crystal group enables one to relate it to an *s*-type orbital symmetry. Under the same condition, $\nu \ll 1$, the wave function corresponding to the irreducible representation B_{1g} may be written as

$$\Psi_{Kq}^{(B_{1g})} \sim \frac{k_1^2 - k_2^2}{(\omega + k_1^2)(\omega + k_2^2)}. \tag{15}$$

This function may be conditionally related to d-type orbital symmetry.

IV. QUASISTATIONARY STATES

One can calculate the functions [Eq. (11)] which define the scattering amplitude. For the sake of simplicity, we suppose that the domain Ξ_K is a long and narrow rectangular strip which is roughly similar to a real domain Ξ_K in the case of the antinodal direction. We denote the length and width of the strip as Δk_1 and Δk_2, respectively. The coordinate k_1 axis is directed along one of the principal directions of the 2D reciprocal effective mass tensor which corresponds to the positive effective mass $m_1 = m/\nu$. Another axis, k_2, is directed along the principal direction corresponding to the negative effective mass $m_2 = -m$. Taking into account that $\nu \ll 1$ and $\Delta k_1 \gg \Delta k_2$ one may assume, for the sake of simplicity, that $\omega_{-1} \equiv (\Delta k_2)^2 = \omega_{+1} \equiv \nu(\Delta k_1)^2 \equiv \omega_1$. This assumption, used later on, is sufficient to study the main features of the scattering amplitude. Using such an approximation, one can represent the function $B_{K2}(\omega)$ in an explicit form at any ω:

$$B_{K2}(\omega) = \frac{\operatorname{sgn}\omega}{2\pi\sqrt{\nu}}\ln\left|\frac{\sqrt{\omega_1 - |\omega|} + \sqrt{\omega_1}}{\sqrt{|\omega|}}\right|. \tag{16}$$

Here $0\leqslant|\omega|\leqslant\omega_1$. It should be noted that, at $|\omega|>\omega_1$, we have $B_{K2}(\omega)=0$.

The function $B_{K2}(\omega)$ is connected with the density of states of the relative motion of $\boldsymbol{K}$ pair inside the domain Ξ_K,

$$B_{K2}(\varepsilon)=\pi\varepsilon_0 g_K(\varepsilon)\operatorname{sgn}\varepsilon, \tag{17}$$

where $\varepsilon_0=(\hbar^2\omega_1/m)$ is the energy width of the domain Ξ_K, $a^2=S/N$, N is the number of unit cells in conducting plane, and $\varepsilon=(\hbar^2\omega/m)$. The average (inside the domain Ξ_K) density of states per unit cell can be written in the form

$$g_K=\frac{1}{\varepsilon_0}\frac{\Xi_K a^2}{(2\pi)^2}=\frac{ma^2}{\pi^2\hbar^2}\frac{1}{\sqrt{\nu}}. \tag{18}$$

Due to the condition that $\nu\ll 1$, the average density of pair states inside the domain Ξ_K may be considerably more in comparison with the total average (inside 2D Brillouin zone) density of states, which is equal to $ma^2/\pi^2\hbar^2$. This is a consequence of peculiar features of saddle point vicinity in HTSC cuprates associated with hyperbolic metrics and strong effective mass anisotropy.

The function defined by Eq. (16) has a logarithmic singularity at $|\omega|\to 0$,

$$B_{K2}(\omega)\sim\frac{\operatorname{sgn}\omega}{4\pi\sqrt{\nu}}\ln\left|\frac{4\omega_1}{\omega}\right|, \tag{19}$$

corresponding to a logarithmic van Hove singularity in the density of states due to saddle points. Near the edges of the energy band, $-\omega_1\leqslant\omega\leqslant\omega_1$; this function behaves as follows: $B_{K2}(\omega)\sim\operatorname{sgn}\omega\sqrt{\omega_1-|\omega|}$ at $|\omega_1-|\omega||\ll\omega_1$.

Now, let us consider the function $B_{K1}(\omega)$ defined in Eq. (11). Taking into account Eq. (17), we have

$$B_{K1}(\omega)=\frac{1}{\pi}\int_{-\omega_1}^{\omega_1}\frac{B_{K2}(\omega')\operatorname{sgn}\omega'}{\omega'-\omega}d\omega'. \tag{20}$$

First of all, let us estimate $B_{K1}(\omega)$ using the average value [Eq. (18)], of the pair density of states. We obtain

$$B_{K1}(\omega)\approx\frac{1}{2\pi^2\sqrt{\nu}}\ln\left|\frac{\omega_1-\omega}{\omega_1+\omega}\right|. \tag{21}$$

Function (21) is presented in Fig. 4 (dashed line). It should be noted that just the function of the form Eq. (21) was used[32] to analyze the ARPES experiment. Such a self-energy structure was studied in detail using the analysis of energy and momentum distribution curves.[33] The explicit expression of $B_{K1}(\omega)$,

$$B_{K1}(\omega)=\frac{\omega}{\pi^2\sqrt{\nu}}\int_0^\infty\ln\left|\frac{\sqrt{\omega_1-\omega'}+\sqrt{\omega}_1}{\sqrt{\omega'}}\right|\frac{d\omega'}{\omega'^2-\omega^2}, \tag{22}$$

in the form of a combination of elementary or special functions, is unknown. It is obvious that, at $|\omega|\to\infty$,

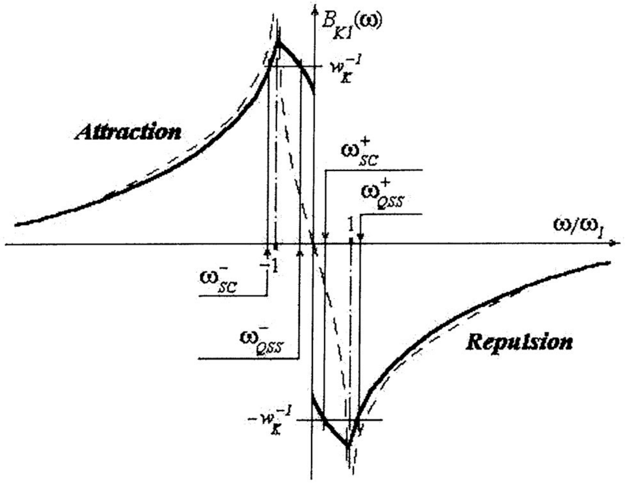

FIG. 4. Plots of the function $B_{K1}(\omega)$: solid line [Eq. (22)] and dashed line [Eq. (21)]. An illustration of the graphic solution of Eq. (12), schematically.

$$B_{K1}(\omega)\sim-\frac{\Xi_K}{(2\pi)^2}\frac{1}{\omega},\quad|\omega|\to\infty. \tag{23}$$

At $\omega\to\pm 0$, we have from definition (20),

$$B_{K1}(\pm 0)=\pm\frac{1}{2\pi^2\sqrt{\nu}}\int_0^1\ln\left|\frac{1-x}{1+x}\right|\frac{dx}{x}=\pm\frac{1}{8\sqrt{\nu}}. \tag{24}$$

Thus a logarithmic singularity of density of states appears in $B_{K1}(\omega)$ as a finite discontinuity at $\omega\to\pm 0$. At $\omega=\pm\omega_1$, the function $B_{K1}(\omega)$ has the finite values

$$B_{K1}(\pm\omega_1)\approx\mp\frac{0.164}{\sqrt{\nu}}, \tag{25}$$

with $|B_{K1}(\pm\omega_1)|>|B_{K1}(\pm 0)|$. The function $B_{K1}(\omega)$ [Eq. (22)], is plotted in Fig. 4 (solid line).

The obtained function, $B_{K1}(\omega)$, allows us to analyze qualitatively the solutions of Eq. (12) which determines the poles of the scattering amplitude. In the case of repulsion between particles composing the $\boldsymbol{K}$ pair ($u_0>0$), solutions corresponding to a positive energy ($\omega>0$) exist provided that $-u_0B_{K1}(\omega_1)<1$. One of the solutions, ω_{QSS}^+, corresponding to greater energy, exists as the desired value of the coupling constant u_0. The second solution ω_{SC}^+ exists in a bounded interval of coupling constant values: $|B_{K1}^{-1}(+0)|<u_0<|B_{K1}^{-1}(\omega_1)|$. The first solution takes place when $\omega_1<\omega_{QSS}^+<\infty$ and the second one exists in an energy interval bounded both above and below, $0<\omega_{SC}^+<\omega_1$. At $\omega>0$, we have $B_{K2}(\omega)>0$; therefore, the sign of decay which corresponds to both poles of the scattering amplitude is determined by the behavior of the function $B_{K1}(\omega)$. In the interval $\omega_1 < \omega < \infty$, this function increases with ω; therefore, a positive decay, $\Gamma^+_{QSS} > 0$, corresponds to the pole ω^+_{QSS}. Hence this pole may be associated with a QSS. But, in fact, as it follows from the definition [Eq. (11)], $\Gamma^+_{QSS} = +0$; therefore, the approximation used here leads to the pole ω^+_{QSS} being a real stationary state. Indeed, one can see that, due to hyperbolic metrics of momentum space, at $\omega > \omega_1$, any decomposition of a $\boldsymbol{K}$ pair becomes impossible because of the restrictions connected with momentum and energy conservation.

At $0 < \omega < \omega_1$ the function $B_{K1}(\omega)$, on the contrary, decreases with ω; therefore, the finite and negative decay $\Gamma^+_{SC} < 0$ corresponds to the pole. This fact may be considered as evidence of an instability with respect to a rise of $\boldsymbol{K}$ pairs, and the imaginary part of the pole, Γ^+_{SC}, may be directly connected with a SC gap. However, the presence of a positive real part of the pole, $\omega^+_{SC} > 0$, indicates that a rise of the SC state becomes possible only if an energy increase connected with the finite value of ω^+_{SC} is compensated for by a sufficient energy decrease produced by a corresponding rearrangement of the electron system which does not bear a direct relation to $\boldsymbol{K}$-pair formation. As an example of such a rearrangement in HTSC cuprates, one may consider the above-mentioned rise of a spatially inhomogeneous spin and charge structure because of a partial restoration of AF order. Thus, because of the positive sign of the real part of the scattering amplitude, the SC pole without any renormalization of the ground state may be considered to correspond to a metastable state. The QSS state has to be related not to a minimum but a maximum of total energy.

In the case when the attraction between particles composing a $\boldsymbol{K}$ pair dominates $(u_0 < 0)$, at $0 < |u_0| < B_{K1}(-\omega)$, as seen in Fig. 4, there is a solution ω^-_{SC} of Eq. (12) which exists in an infinite energy region, $-\infty < \omega^-_{SC} < -\omega_1$, and, in the approximation used here, has an infinitesimal decay, $\Gamma^-_{SC} = -0$. Another pole ω^-_{QSS}, existing inside the energy interval $-\omega_1 < \omega^-_{QSS} < 0$, corresponds to a real QSS with finite and rather large decay. Therefore, in spite of the fact that, due to the assumption that $\omega_{-1} = \omega_{+1}$, there is a symmetry of the function $B_{K1}(\omega)$ with respect to a change of the sign of the argument, namely, $B_{K1}(-\omega) = -B_{K1}(\omega)$, there is an essential asymmetry in the character of solutions of Eq. (12) with respect to the sign of the coupling constant.

The point of view[34] that there are incoherent electron or hole pairs in the pseudogap regime leads to a definite conclusion concerning the sign of the interaction energy which governs the pairing in HTSC cuprates. That is, neglecting the Friedel oscillations, one may propose that the only essential interaction between electrons is a screened Coulomb repulsion,

$$U(r) = \frac{e^2}{r} \exp\left(-\frac{r}{r_0}\right), \tag{26}$$

where r_0 is the screening length. Taking into account the explicit form of the Fourier transform of the screened Coulomb potential, one can write the coupling constant in the form $u_0 = r_0 \Xi_K a^2 / \pi a^*$ where $a^* = \hbar^2 / m e^2$ is an effective Bohr radius.[1] An increase of the carrier concentration due to doping leads to a decrease of the screening length and, as a result, to a decrease of the coupling constant. In Fig. 5, we represent a qualitative comparison of a typical HTSC cuprate phase diagram (Fig. 1) and Fig. 4 which we consider to show the dependence of the $\boldsymbol{K}$ pair energy ω, when increasing with doping, on the inverse value of the coupling constant u_0^{-1}. One can see that a crossover line $T^*(x)$, separating normal and pseudogap states in phase diagram, is in accordance with the line which determines the energy of the QSS with a positive infinitesimal decay, ω^+_{QSS}. In addition, there is accordance between the SC phase region bounded by the line $T_C(x)$ in the phase diagram and the line which determines the solution leading to the SC instability, ω^+_{SC}. Indeed, both functions of doping, $T_C(x)$ and $\omega^+_{SC}(x)$, have finite domains of definition bounded above and below.

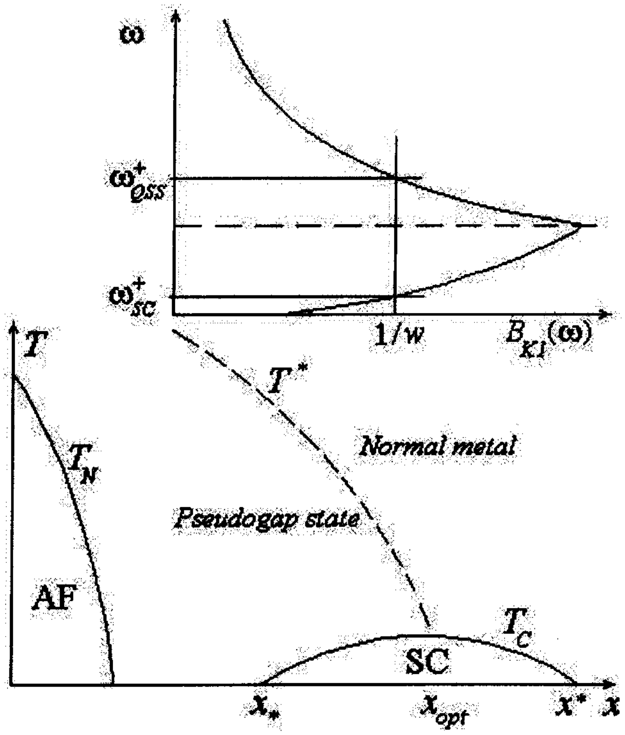

FIG. 5. A comparison of a typical HTSC cuprate phase diagram and the graphic solution of Eq. (12), determining the poles of the scattering amplitude (schematically).

An evaluation of Coulomb repulsion in an electron system with and without QSS's indicates that, provided that the QSS concentration exceeds a certain value, an energy gain is possible, and thus incoherent QSS's with different total momenta may exist not only as excitations but in the ground state, resulting in some suppression of one-particle density of states.[1] Therefore, a rise of such QSS's may be directly related to the pseudogap state. A spatial separation of the domains in which one can observe either a SC gap or a pseudogap[20] can be interpreted as an alternation of the regions with increased and decreased doping, respectively.

V. SUPERCONDUCTING PAIRING

The negative-decay poles in the scattering amplitude corresponding to the relative motion of an electron or hole pair with a large total momentum bears evidence of the possibility of SC pairing both during attraction and repulsion between the particles composing the pair. A consequence of the rise of a stripe structure is that a number of real $\boldsymbol{K}$ pairs belonging to the domain Ξ_K must leave this domain and form real pairs with a momentum $\boldsymbol{K}'$ ($\boldsymbol{K}'$ pairs) in a domain $\Xi_{K'}$ outside of the FC. The states inside Ξ_K and $\Xi_{K'}$, having become vacant and remaining filled, are separated from each other by a line which is, by our definition, the PFC. The values of the areas $\Xi_K^{(+)}$ and $\Xi_{K'}^{(-)}$ are dependent on the AF energy which determines the position of the chemical potential 2μ of pairs with respect to the edges of the energy bands corresponding to the domains Ξ_K and $\Xi_{K'}$. These energy bands and relevant densities of states, $g_K(\varepsilon)$ and $g_{K'}(\varepsilon)$, are represented schematically in Fig. 3. One part of the PFC, which is situated in the domain Ξ_K (the boundary between $\Xi_K^{(-)}$ and $\Xi_K^{(+)}$), may be related to the AF part of a stripe, whereas another part, separating $\Xi_{K'}^{(-)}$ and $\Xi_{K'}^{(+)}$, belongs to the M part of a stripe. An excitation of carriers (a rise of holes above and electrons below the chemical potential level) leads to the possibility of their pairing. Formally, one can consider (1) a scattering of pairs in the AF part of a stripe (in the domain Ξ_K), (2) a scattering of pairs in the M part of a stripe (in the domain $\Xi_{K'}$), and also (3) a scattering which includes transfers of pairs between the AF part of a stripe (the domain Ξ_K) and the M part of a stripe (the domain $\Xi_{K'}$). In such a case (3) pairs are spatially separated, and the interaction leading to their scattering is reduced. As already mentioned, the condition $|\boldsymbol{K}'-\boldsymbol{K}|\gg\delta k_c$ allows us, in a first approximation, to consider pairing in the domains Ξ_K and $\Xi_{K'}$ independently of each other, thus restricting ourselves to one of the cases (1) or (2). In this section, we restrict ourselves to case (1) and consider SC pairing near the part of the PFC belonging to the AF part of a stripe. Thus we suppose that rather thin M parts of stripes do not affect the superconductivity, essentially due to the proximity effect.

In the general case, considering a pairing of carriers with the momentum $\boldsymbol{K}$ along an antinodal direction, it is necessary to take into account all excited states arising due to transfers of carriers across the PFC, namely, $\Xi_K^{(-)}\leftrightarrow\Xi_K^{(+)}$. As a result, we have a pair with a large total momentum along one of the antinodal directions. As mentioned above, in the case of antinodal directions, there exists a quadruple of equivalent pairs with total momenta $\hat{g}\boldsymbol{K}$ where, due to symmetry, $\Sigma_{\hat{g}}\hat{g}\boldsymbol{K}=0$. The interaction leading to a scattering of such equivalent pairs turns out to be weaker as compared to the interaction which results in a rise of a bound state of a pair with given $\boldsymbol{K}$. This may mainly be due to an essential increase of the scattering momentum in spite of the fact that the scattering region in the momentum space also increases. The scattering of pairs with equivalent total momenta leads to a state of the form of Eq. (5) which, due to the condition that $\Sigma_{\hat{g}}\hat{g}\boldsymbol{K}=0$, corresponds to a currentless state. In this sense, a pair state, such as quadruple pairs with equivalent large total momenta, is similar to a conventional Cooper pair; however, it is clear that the internal structure of pair states discussed here differs essentially from the rather simple structure of Cooper pair.

For a simple one-dimensional stripe structure, a $\boldsymbol{K}$- ($\boldsymbol{K}'$-) pair state arises due to a mixing of only two $\boldsymbol{K}$ states corresponding to either [100] (k_1 axis) or [010] (k_2 axis) directions. Thus one may expect a rise of an array of alternating conducting planes with 1D stripes which are perpendicular to each other in the neighboring planes. Pair states formed by quadruples of $\boldsymbol{K}$ pairs correspond to a more complicated periodic 2D stripe structure.

In the zero-temperature limit, the equation determining the SC order parameter is similar to the conventional BCS equation, and can be written in the form

$$\Delta_{Kk}=-\frac{1}{2S}\sum_{k'}\frac{\tilde{U}_K^*(\boldsymbol{k}-\boldsymbol{k}')\Delta_{Kk'}}{\sqrt{\xi_{Kk'}^2+\Delta_{Kk'}^2}}. \qquad (27)$$

It is obvious that, in the case of repulsion between particles composing a $\boldsymbol{K}$ pair, a BCS-like solution, independent of $\boldsymbol{k}$, is absent.

The solutions of Eq. (27) for a SC energy gap in the cases of attraction ($\tilde{U}_K^*<0$) and repulsion ($\tilde{U}_K^*>0$) between particles composing a $\boldsymbol{K}$ pair differ from each other essentially. First of all, we consider the case of attraction and restrict ourselves to the simplest approximation, namely, $\tilde{U}_K^*(k)\equiv U_K=$const. Such an approximation, like the BCS approximation, enables one to obtain an explicit expression for the SC energy gap. A magnitude of the coupling constant U_K depends on the pairing mechanism, which is not under discussion here. The only circumstance we have to take into account is that one may neglect the predominance of repulsion as compared to attraction in a comparatively narrow energy region corresponding to a vicinity of the PFC. Let $2\bar{\xi}$ be the characteristic energy width of such a region and suppose, for the sake of simplicity, that $\bar{\xi}$ is more less than any characteristic energy scale relating to each of the subdomains $\Xi_K^{(-)}$ and $\Xi_K^{(+)}$. The approximation $\tilde{U}_K^*(k)=$const results in that there is a solution of Eq. (27) independent of the momentum of the relative motion of the $\boldsymbol{K}$ pair, that is, $\Delta_{Kk}\Rightarrow\Delta_K$. We restrict ourselves to a consideration of such a solution only. Reducing, as usual, the sum in Eq. (27) into an integral over ξ_{Kk}, and introducing an average density of states g_K related to unit area, one can obtain the order parameter in the form

$$\Delta_K\approx\bar{\xi}\exp\left(-\frac{1}{g_KU_K}\right). \qquad (28)$$

That is, a solution which formally coincides with the BCS solution. It should be noted that g_K is more less as compared with the total density of states on the Fermi level. Therefore, in the case of a typical phononic pairing mechanism coupling constant value, one obtains the energy gap [Eq. (28)], which should be certainly more or less in comparison with the gap that arises due to conventional Cooper pairing on the full FC.

Now, let us consider the case when a repulsion between particles composing ***K***-pair dominates. In this case, one has not to take into account the existence of any bosonic degree of freedom (phononic, electronic, magnetic or something else) as a necessary condition of a rise of a bound state of ***K***-pair. Screened Coulomb repulsion becomes the only essential interaction.

As one can see from Eq. (27) there is no solution of constant signs inside the domain Ξ_K, provided that $U_K > 0$. Therefore, to obtain an approximate solution of Eq. (27), we suppose that the order parameter dependence on the momentum of the relative motion of the ***K*** pair is given by a discontinuous function changing its sign on the PFC. We restrict ourselves to a consideration of the simplest case when the order parameter is independent of ***k*** and different from other values inside the subdomains $\Xi_K^{(-)}$ and $\Xi_K^{(+)}$. That is, omitting the label K in the definition of the order parameter, we assume that $\Delta_K \equiv -\Delta_- < 0$ inside $\Xi_K^{(-)}$ and $\Delta_K \equiv \Delta_+ > 0$ inside $\Xi_K^{(+)}$.

This assumption allows us to rewrite Eq. (27) in the form of a system of two equations for Δ_- and Δ_+. In this connection, one should take into account the above-mentioned remark that the effective interaction matrix element $\tilde{U}_K^* \sim 2\Xi_K^{(-)}$ when both ***k*** and ***k***′ belong to the subdomain $\Xi_K^{(-)}$, that is, a scattering due to the interaction is restricted to this subdomain (the factor 2 takes into account the fact that the scattering is possible both from ***k*** into ***k***′ and from ***k***′ into ***k***). However, if ***k*** belongs to $\Xi_K^{(-)}$ and ***k***′ belongs to $\Xi_K^{(+)}$ and hence the scattering is possible in the whole of the domain Ξ_K, we have $\tilde{U}_K^* \sim \Xi_K$ (scattering from $\Xi_K^{(-)}$ into $\Xi_K^{(+)}$ only). One can rewrite Eq. (27) in the forms

$$(1-\alpha)\Delta_- + \Delta_+ = \frac{U_K \Xi_K a^2 h_\alpha}{2S} \sum_{k \in \Xi_K^{(-)}} \frac{\Delta_-}{\sqrt{\xi_k^2 + \Delta_-^2}},$$

$$\Delta_- + \alpha\Delta_+ = \frac{U_K \Xi_K a^2 h_\alpha}{2S} \sum_{k \in \Xi_K^{(+)}} \frac{\Delta_+}{\sqrt{\xi_k^2 + \Delta_+^2}}. \tag{29}$$

Here we denote $h_\alpha \equiv (1/2-\alpha)^2$ and $\alpha \equiv \Xi_K^{(-)}/\Xi_K$.

The dependence of the AF energy on the doping level allows us to hunt down the evolution of the PFC due to a variation of doping. If $I(x) < \delta\varepsilon_{KK'} \equiv I_m$, the PFC is absent and the energy width of the subdomain is $\Xi_K^{(-)}$, $\varepsilon_{K-} = \varepsilon_0$ whereas the energy width of the subdomain is $\Xi_K^{(+)}$, $\varepsilon_{K+} = 0$ where ε_0 is an energy width of the domain Ξ_K. At $I(x_2) = I_m$, there is an "opening" of the PFC at two points a and a', which are situated on the k_1 axis, as shown in Fig. 2. A decrease of doping, $x < x_2$, leads, first of all, to a rise, and then to an extension, of the subdomain $\Xi_K^{(+)}$ which is accompanied by a corresponding decrease of the subdomain $\Xi_K^{(-)}$. Thus the PFC length increases and then, after reaching the maximal length value corresponding to a certain doping level, begins to decrease, shrinking at two points b and b' on the k_2 axis (Fig. 2). Such a shrinking corresponds to a value of the doping level related to, the AF energy $I(x_1) = I_M$. If one assumes that the pair condensate density is directly connected to the PFC length, one can qualitatively explain both the rather small superfluid density and the peculiar doping dependence of T_C observed in cuprates. One can take such a dependence into account by assuming that it is explicitly included in AF energy $I(x)$ and the screening length $r_0(x)$. An evolution of the PFC length with a variation of doping has to determine, in the main, the doping dependence of both the superconducting transition temperature and the superfluid density.

For the sake of simplicity we suppose that ε_{K-} and ε_{K+} are linear functions of doping: $\varepsilon_{K-}(y) = \varepsilon_0 y$ and $\varepsilon_{K+}(y) = \varepsilon_0(1-y)$. Here $y = (x-x_1)/(x_2-x_1)$ is a "reduced" doping level varying within the limits of interval $0 \leqslant y \leqslant 1$ when $x_1 \leqslant x \leqslant x_2$. As another simplification, we assume that the density of states is constant inside the whole of the domain Ξ_K, $g_K = \Xi_K/(2\pi)^2\varepsilon_0$. From this assumption, it follows immediately that $\Xi_K^{(-)}/\Xi_K = \varepsilon_{K-}/\varepsilon_0$, that is $\alpha \equiv y$.

Reducing the summation over momenta in Eq. (27) to an integration over the energy of the relative motion of the ***K*** pair, one can rewrite the system of equations (27) in the forms

$$(1-y)\delta_- + \delta_+ = w_K(y) h_y \delta_- \ln\left|\frac{y}{\delta_-}\right|,$$

$$\delta_- + y\delta_+ = w_K(y) h_y \delta_+ \ln\left|\frac{(1-y)}{\delta_+}\right|, \tag{30}$$

where $h_y \equiv (1/2-y)^2$, $\delta_\pm \equiv \Delta_\pm/\varepsilon_0$ [we suppose, for the sake of simplicity, that $y \gg \delta_-, (1-y) \gg \delta_+$], and

$$w_K(y) = \frac{\pi e^2 r_0(y) \Xi_K a^2}{\varepsilon_0 a^2 (2\pi)^2}. \tag{31}$$

The screening length $r_0 = r_0(y)$ is a decreasing function of the doping level; therefore, we use a linear approximation for the coupling parameter, $w_K(y) = w_K(1-y/y_b)$ where $y_b > 1$.

It should be noted that the chemical potential μ as a point of reference of kinetic energy of the relative motion of the ***K*** pair changes due to a rise of the SC order as compared with its value in the normal (nonsuperconducting) state. However, the corresponding shift of the chemical potential is quite small (of the order of the SC gap). Thus, calculating the values of the parameters δ_- and δ_+ one need not consider the chemical potential shift arising due to the SC condensation of ***K*** pairs. Thus we assume approximately that μ is determined by the only parameter *I*, and equal to a value which corresponds to the PFC at given *I* in the normal state. However, in contrast to BCS theory, in our case just the chemical potential shift determines the SC condensation energy, and thus a doping dependence of the superconducting transition temperature.

By definition, both unknown quantities δ_- and δ_+ in Eq. (30) are non-negative: $\delta_- \geqslant 0$ and $\delta_+ \geqslant 0$. Nontrivial solutions turn out to be possible under the condition that the coupling parameter [Eq. (31)], is large enough. The dependence of this parameter on doping [Eq. (31)] leads to an asymmetry of the functions $\delta_-(y)$ and $\delta_+(y)$, that is, in the general case (except as some special values of doping level), $\delta_-(y) \neq \delta_+(y)$. The doping dependence of $\delta_-(y)$ and $\delta_+(y)$ are represented schematically in Fig. 6.

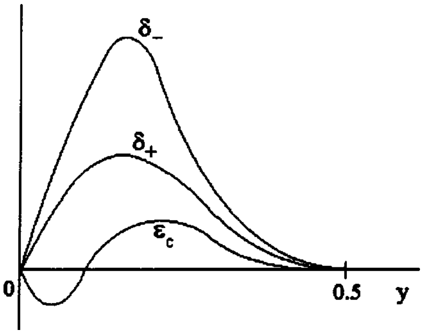

FIG. 6. Solutions δ_- and δ_+ of the system of equations [Eq. (29)] and the condensation energy [Eq. (41)], plotted schematically as functions of the reduced doping level.

VI. CHEMICAL POTENTIAL SHIFT

In a spatially homogeneous system, the value $2E_F$ of the chemical potential of pairs indicates that the whole of the domain Ξ_K is filled, whereas all of the states inside any domain $\Xi_{K'}$ are vacant. A rise of a stripe structure leads to a hole redistribution between Ξ_K and $\Xi_{K'}$, with the result that the PFC arises. Thus the PFC may be treated, in the zero-temperature limit, as a line separating filled and vacant pair states in momentum space. The possibility of pairing itself resulting in an opening of the SC gap on the PFC arises just as a result of such a redistribution which may be, for example, due to above discussed partial restoration of AF order. The numbers of vacant states inside Ξ_K and, on the other hand, filled states inside $\Xi_{K'}$ are governed by the value I of AF energy which determines the position 2μ of the chemical potential of pairs with respect to the edges of the energy bands corresponding to the domains Ξ_K and $\Xi_{K'}$. The densities of states $g_K(\varepsilon)$ and $g_{K'}(\varepsilon)$, corresponding to these domains, are represented in Fig. 3.

To evaluate the chemical potential shift μ' due to a condensation of $\boldsymbol{K}$ pairs belonging to the domain Ξ_K, one has to take into account that a formal definition of an average number of particles inside Ξ_K,

$$\langle N_K\rangle = 2\sum_{k\in\Xi_K} v_{Kk}^2 \equiv \sum_{k\in\Xi_K}\left(1-\frac{\xi_{Kk}}{\sqrt{\xi_{Kk}^2+\Delta_{Kk}^2}}\right), \qquad (32)$$

takes into consideration the particles which may pass from Ξ_K into $\Xi_{K'}$. Such a passage is compensated for by the particles passing from $\Xi_{K'}$ into Ξ_K. Therefore, the conserving quantity is a sum $\langle N_K\rangle + \langle N_{K'}\rangle$, where the second term is an average number of particles inside $\Xi_{K'}$. The condensation may be considered in each of the domains Ξ_K and $\Xi_{K'}$ independently if, as accepted above, $|\boldsymbol{K}'-\boldsymbol{K}| \gg \delta k_c$. In such a case, one has to take into account only the passages of particles from $\Xi_K^{(-)}$ into $\Xi_K^{(+)}$ if one considers a condensation of $\boldsymbol{K}$ pairs only, bearing in mind that the position of the PFC in the normal state is determined by the AF energy I which is considered here as an external parameter. As far as the chemical potential shift due to SC condensation of pairs is also small together with Δ_{Kk}, such an approximation only slightly affects the introduced below coefficients λ and τ. Thus $\langle N_K\rangle$ may be considered as an approximately conserving average number of particles inside the domain Ξ_K, provided that the AF energy I has a certain given value. In the normal states $v_{Kk}^2=1$, when $k\in\Xi_K^{(-)}$, and $v_{Kk}^2=0$, when $k\in\Xi_K^{(+)}$ in zero-temperature limit, therefore, the condition that $\langle N_K\rangle = \text{const}$ can be rewritten in the form[2]

$$\sum_{k\in\Xi_K^{(+)}} 1 - \sum_{k\in\Xi_K^{(-)}} 1 = \sum_{k\in\Xi_K} \frac{\xi_{Kk}}{\sqrt{\xi_{Kk}^2+\Delta_{Kk}^2}}. \qquad (33)$$

Let us consider the case of repulsion between particles composing the $\boldsymbol{K}$ pair. Since $\Delta_- \ll \varepsilon_{K-}$ and $\Delta_+ \ll \varepsilon_{K+}$ in any case, and the chemical potential shift μ' measured from the PFC position at $\Delta_\mp \to 0$ is small together with $\Delta_\mp$, one can, reducing the summation over the momentum to an integral over ξ_{Kk}, approximately rewrite Eq. (33) as

$$\sqrt{\mu'^2+\Delta_-^2}-\sqrt{\mu'^2+\Delta_+^2} \approx 2\mu' + \frac{1}{2}\frac{\Delta_-^2}{\varepsilon_{K-}} - \frac{1}{2}\frac{\Delta_+^2}{\varepsilon_{K+}}. \qquad (34)$$

Assuming that $\mu' = \mu_1' + \mu_2'$ where μ_1' (μ_2') is a quantity of the first (second) order with respect to $\Delta_\mp$, Eq. (34) may be solved with the use of the method of successive approximations. Two values of the order parameter, δ_- and δ_+, are not independent, as follows from the Eq. (30). Their ratio $\gamma \equiv \delta_+/\delta_-$ is a function of doping, $\gamma = \gamma(y)$. The chemical potential shift can be written as

$$\mu' = \varepsilon_0 \delta[\lambda + \tau\delta], \qquad (35)$$

where we denote $\delta_- \equiv \delta$, and

$$\lambda \equiv \frac{1}{2\sqrt{2}} \frac{1-\gamma^2}{\sqrt{1+\gamma^2}}. \qquad (36)$$

One can easily obtain an explicit expression of the second parameter τ from Eq. (34).

It should be noted that in the case of attraction between particles composing a $\boldsymbol{K}$ pair, we have only the value of the order parameter [Eq. (28)], which is independent of the momentum of the relative motion. Therefore, to obtain the chemical potential shift due to SC condensation one should formally write $\delta_+ = -\delta_-$. Then we have

$$\mu' = -\frac{\varepsilon_0}{4}\frac{(1-2y)}{y(1-y)}\delta^2. \qquad (37)$$

Thus the approximation we use here leads to the absence of a term which is linear in δ, and the chemical potential shift turns out to be proportional to δ^2.

It should be noted that the necessity of the k dependence of the SC gap and a corresponding displacement of the chemical potential from its value in the normal state was established phenomenologically by Hirsch[35] in his theory of hole superconductivity. It is clear that “the gap slope” introduced by Hirsch is directly related to our simple discontinuous solution of the gap equation, whereas the linear term in the chemical potential shift, arising just in the case when $\Delta_- \neq \Delta_+$, corresponds to Hirsch’s “electron-hole symmetry-breaking term” the difference μ' being between the chemical potential values in the superconducting and the normal state. One can see quite easily that, in the case of electron-hole asymmetry observed in tunnel current-bias characteristics, such a chemical potential shift is a direct consequence of the particle conservation law. Indeed, if one considers a redistribution of particles due to SC condensation inside the domain Ξ_K only, it becomes obvious that in the case when $\Delta_- \neq \Delta_+$, the value 1/2 of the factor v_{Kk}^2 cannot correspond to the position of the chemical potential relating to the normal state. Thus some chemical potential shift is needed to satisfy the condition that the number of transfers of holes from $\Xi_K^{(-)}$ must be equal to the number of transfers into $\Xi_K^{(+)}$. The sign of such a shift is determined by the sign of the difference $\Delta_- - \Delta_+$. Thus Hirsch's statement that $\mu' > 0$ is valid, generally speaking, in the case when $\Delta_- > \Delta_+$. One can also note that the so-called superconducting "Fermi surface," introduced in Ref. 35 as the locus in k space of quasiparticle states of minimum energy, in a sense, plays the role which, indeed, the PFC plays in the analysis of ARPES spectra and some other phenomena typical of HTSC cuprates.

VII. CONDENSATION ENERGY

The existence of the solution of Eq. (28) for a SC order parameter in a doping interval $x_1 < x < x_2$ does not mean that the SC state arises throughout, or at least in some part of, this interval. A phase transition from the N state into the SC state occurs under a necessary condition: namely, the condensation energy defined as a difference between N and SC state values of the ground state energy must be positive.

A contribution into the ground state energy which is associated with a condensation of $\boldsymbol{K}$ pairs inside the domain Ξ_K may only be written, as usual, in the form

$$E_{0S} = \sum_{k \in \Xi_K} \xi_{Kk} - \frac{1}{2} \sum_{k \in \Xi_K} \frac{2\xi_{Kk}^2 + \Delta_{Kk}^2}{\sqrt{{\xi_{Kk}^2}^2 + \Delta_{Kk}^2}}. \tag{38}$$

Reducing the summation over momentum in Eq. (38) to the integration over ξ_{Kk}, one has to take into account that the energy ξ_{Kk} measured from the chemical potential of the N phase varies within the interval $-\varepsilon_{K-} \leq \xi_{Kk} \leq \varepsilon_{K+}$. Therefore, taking into account the above-discussed chemical potential shift due to SC condensation, μ', and the fact that the SC order parameter has a discontinuity on the PFC, the condensation energy, correct to the terms of the order of Δ^2, can be represented in the form

$$E_{0S} = E_{0N} - S4g_K\varepsilon_0^2\delta(\overline{\lambda} + c\delta), \tag{39}$$

where $E_{0N} = -Sg_K\varepsilon_K^2 y^2$ is the corresponding contribution into the ground state energy of the N phase. The parameters $\overline{\lambda}$ and c are connected with λ and τ in Eq. (35), in accordance with the relations $\overline{\lambda} = 2y\lambda$ and $c = 2y\tau + (1+\gamma^2)/4$.

The term $(1+\gamma^2)/4$ may be formally related to a direct contribution of the pairing interaction into the condensation energy, whereas the contributions associated with the coefficients λ and τ may be related to a renormalization of kinetic energy of the relative motion of $\boldsymbol{K}$ pairs, being a result of SC condensation (it should be noted, however, that both contributions vanish when the coupling constant tends to zero).

As it follows from Eq. (39), an energy gain due to the condensation of $\boldsymbol{K}$ pairs is possible when

$$\overline{\lambda} + c\delta > 0. \tag{40}$$

It can be seen from Eq. (39) that this gain is mainly due to a renormalization of the kinetic energy of the relative motion of the $\boldsymbol{K}$ pair. Indeed, the chemical potential shift due to a rise of a condensate of $\boldsymbol{K}$ pairs results in a corresponding shift of the position of the PFC. Provided that the condition (40) is satisfied the PFC is shifted in a way that there is an extension of the part $\Xi_K^{(-)}$ of the domain Ξ_K in which the energy of the relative motion of the $\boldsymbol{K}$ pair is negative. The ground state energy decreases due to a filling of the states which arise as a result of such a PFC shift.

In this connection, one relevant optical experiment[36] consistent with the conception elaborating here should be noted. An estimation of the superfluid density ρ_s, which is directly connected with the IR reflection, indicates that, in several HTSC cuprates, ρ_s significantly exceeds the value obtained from optical conductivity by means of Kramers-Kronig relations under the condition that one takes into account an energy interval comparable to the SC gap.[36] This contradiction may be eliminated if one considerably extends the interval of integration. In conventional superconductors, as follows from the BCS theory, each Cooper pair leads to an energy gain of the order of Δ. The energy width of the condensation region in the vicinity of the FC is of the same order. Therefore, the condensation energy turns out to be of the order of Δ^2. This explains the fact that, using Kramers-Kronig relations, we can restrict ourselves to a finite interval of integration having a character energy width of about Δ. The presence of the linear term ($\sim\Delta$) in the condensation energy in Eq. (39) clearly indicates that each $\boldsymbol{K}$ pair also leads to an energy gain of the order of Δ, but that the contribution to this gain is due to the vicinity of the PFC, giving a character energy width of about μ' which is usually larger compared to Δ.

Let us define the condensation energy per unit area as

$$\varepsilon_c \equiv (E_{0N} - E_{0S})/4g_K\varepsilon_0^2 S = \delta(\overline{\lambda} + c\delta), \tag{41}$$

and qualitatively study its dependence on the doping level. In Fig. 6, we represent a plot of the function [Eq. (41)] calculated numerically for some values of the coupling parameter. It is obvious that there exists a certain minimal value of this parameter which corresponds to the beginning SC condensation. This conclusion is in agreement with a finite value of the scattering amplitude at $\omega = \omega_1$ obtained in Sec. IV.

As one can see from Fig. 6, the calculated condensation energy has a negative sign inside some region of the doping level. This fact is due mainly to the negative sign of the chemical potential shift μ', leading to a kinetic energy increase. One may believe that such a result is a consequence of a special choice of the gap equation solution being discontinuous on the PFC and leading to an energy gain in a doping region where the condensation energy turns out to be positive. At another choice of the gap equation solution, which varies with a momentum of the relative motion continuously within an energy scale of the order of Δ near the PFC inside both $\Xi_K^{(-)}$ and $\Xi_K^{(+)}$, the values of Δ_- and Δ_+ are supposed to be unaffected; therefore, one may expect a gain in the condensation energy in the whole of the reduced doping interval, $0<y<1$, in which the solution of the gap equation exists. In this connection, it should be noted that such a choice of the parameters Δ_- and Δ_+ has to correspond to more symmetric tunnel current-bias characteristics in an extremely underdoped regime in comparison with the optimal one.

The condensation energy and the transition temperature corresponding to an extremely underdoped regime are rather small, whereas the superconducting gap value is finite and large enough. Therefore, one must not consider as striking the large value of the ratio $2\Delta/T_C$ observable in underdoped HTSC cuprates.[37]

VIII. SUMMARY AND CONCLUSIONS

The total energy increase which is due to a rise of PFC and a corresponding redistribution of carriers in momentum space may be compensated for when (as appears to be just the case related to hole–doped HTSC cuprates) there is an energy decrease due to a partial restoration of AF ordering in hole-depleted regions. An alternation of hole–depleted and -enriched regions in real space forms charge and spin spatial structures. Under definite conditions (in particular, in an underdoped regime), this structure, associated closely with short-range AF order fluctuations, becomes apparent as a quasiregular static or dynamic 1D stripe structure. Such a phase separation,[38] accompanied by a change in the filling of hole states in momentum space, may correspond to the minimum of total energy of the electron system. Short-range AF ordering, stabilizing stripes due to a redistribution of hole pairs, is an intrinsic but possibly not unique attribute of such a self-organization. For example, long-range orbital magnetic ordering,[39] known as a flux phase state, may play the same role as well. This phase is perhaps associated with the so-called hidden-order-parameter region in the phase diagram.[40]

A redistribution of carriers in momentum space may result in the rise of a zero-excitation-energy line separating occupied and vacant states in a 2D Brillouin zone. We believe that, first of all, a rise of vacant states inside and occupied states outside of the parent FC must lead to the formation of pairs with total momenta corresponding to the largest areas Ξ_K and $\Xi_{K'}$ with $\boldsymbol{K}$ and $\boldsymbol{K}'$ along the antinodal directions. Such pairs have the largest binding energies and exist up to the temperature T^* of the beginning of the pseudogap regime. Then the lowering of the temperature from T^* to T_C results in a gradual rise of electron and hole pairs with total momenta having different values and directions and corresponding to some set of domains Ξ_K and $\Xi_{K'}$. Finally, at $T=T_C$, there is the beginning of a SC condensation of pairs into the state with the largest binding energy. SC condensation gives a start to transfers of different $\boldsymbol{K}$ pairs into the the state corresponding to the ‘‘antinodal’’ domain Ξ_K, only accompanied by a rise of the phase coherence of the ‘‘antinodal’’ $\boldsymbol{K}$ pairs. Thus, as a final result, the zero-energy line for pair excitations arises inside the domain Ξ_K (similarly, such a line arises inside the corresponding domain $\Xi_{K'}$ outside of the FC as well). Just this line may be treated as ‘‘pair’’ Fermi contour (PFC).

The conception of the PFC and hyperbolic pairing enables one to explain qualitatively some general features of phase diagrams and many surprising experimental data relating to HTSC cuprates. In particular, the rise of both SC and pseudogap states may be considered as a manifestation of hyperbolic metrics of momentum space and screened Coulomb repulsion between holes. Therefore, both the SC gap and the pseudogap must have one and the same energy scale, and their *d*-type ‘‘orbital’’ symmetry, in fact, is determined by the crystal symmetry. A character spatial scale of a pair both in QSS and SC states (the coherence length) is of the order of a few interatomic distances.[1]

Thus we believe that the SC gap and the pseudogap have one and the same origin in the sense that they may be associated with pairs with large total momentum. Nevertheless, one can think that the pseudogap regime has a nonsuperconducting character because it is due to a rise of pairs with different total momenta, whereas the SC regime arises after the condensation of these pairs into a state with a definite total momentum and a rise of the phase coherence. In this connection, it should be emphasized that our point of view relating to the origin of the pseudogap does not contradict the conclusion[20] concerning the different natures of the SC gap and the pseudogap.

As evidence in favor of the PFC conception, one may consider an interpretation of two interesting experiments, relating to an examination of the electronic spectrum of several HTSC cuprates with the help of the ARPES technique. In this case, when the energy of an excited electron is near the Fermi level E_F (less than about 100 meV), ARPES data[41] indicate unequivocally that the electronic structure has a 2D character and the FC remains in the well-known form of a square with rounded corners.[7] If an electron is excited far from E_F (about 500 meV) the electronic structure becomes 1D rather than 2D. It should be noted that a simple cross-shaped form of the FC, in fact, is derived not directly from experimental data but offered as a result of motivated speculations based on the simplest 1D stripe model. Such a fairly surprising conclusion is entirely consistent with the concept of the PFC introduced here. In fact, if the SC pairing conditions are satisfied on the isoline of the kinetic energy of the relative motion of the $\boldsymbol{K}$ pair as a continuation of the PFC, and if some piece of this isoline is situated close enough (about 500 meV) to the FC, just this piece provides an excitation energy minimum outside the FC.

One can believe that the so-called ‘‘dip-hump structure’’ in the ARPES spectra[42] is more evidence in favor of the concept of the PFC: a hump, arising (just in the case of the antinodal direction corresponding to the maximal value of Ξ_K) at energies which are essentially more than the energy related to the quasiparticle peak, may be associated with the excitations in the form of pairs near the PFC.

Another one unusual feature of HTSC cuprates with a

d-type symmetry of the SC gap can be qualitatively interpreted in the framework of the PFC conception. It is believed that impurity scattering has to lead to an essential reduction of T_C, because the scattering of a pair into regions of momentum space corresponding to nodal directions means, in fact, a break of the pair. In this sense, nonmagnetic impurities play a role similar to that which play magnetic impurities in conventional superconductors. However, the experimental fact is that the HTSC cuprates are weakly sensitive to impurity content. Thus there are no experimental data which were confirmed such a ''destructive'' influence of impurities on the SC state. In this connection, it should be noted that, to reconcile such a statement with the experiment, one has to suppose that any interaction resulting in a scattering of Cooper pair in a d-type superconductor, including the interaction which leads to a binding in the pair itself, must possess a peculiar feature, namely, the scattering into ''nodal regions'' has to be more weak in comparison with the scattering into ''antinodal regions'' (the so-called ''forward scattering'').[43] Using the PFC conception, it is not necessary to consider any peculiar feature of scattering as far as there are kinematic constraints which forbid the scattering into the region of momentum space outside the domain Ξ_K, in particular, into regions which correspond to the nodes of the SC gap.

A problem connected with a strong anisotropy of reversed relaxation times, that is the existence of so-called ''hot'' and ''cold'' spots on the Fermi surface,[43,44] can also be qualitatively solved in the framework of the PFC conception. Indeed, a rise of $\boldsymbol{K}$ pairs results in their free in-plane motion without a change of charge density, whereas a character of the interaction of paired carriers may be changed essentially: this interaction, being inside antinodal regions, turns out to be more weak as compared to the interaction of unpaired carriers inside nodal regions.[1]

The idea we use here is based, in the main, on the fact that the PFC should be ''opened''; that is, due to a rise of stripes and hyperbolic metrics of momentum space, some piece of the FC turns out to be the same as a line of zero kinetic energy of the relative motion of a hole pair with a large momentum. If such a line corresponding to a certain $\boldsymbol{K}$ is close enough to a rather large piece of the real FC (such a case may occur, for example, just at $\nu \ll 1$ and $|2k_F - K| \ll k_F$) the pairing mechanism discussed here may also be possible even without any hole redistribution both in momentum space (between the domains Ξ_K and $\Xi_{K'}$) and in real space (that, is without a rise of a stripe structure). In this case, the value of ε_{K+} plays the role of a cutoff parameter, since it must appear in the arguments of the logarithmic functions in Eq. (30) together with the SC gap parameters Δ_- and Δ_+. In a sense, the pairing problem becomes analogous to that which arises in the case of Cooper pairing in weak ferromagnets.[6] This statement is consistent with the results presented in Secs. III and IV. That is, at $\nu \to 0$ and $\omega_1 \to 0$ (it is obvious that the parameter $\omega_1 \to 0$ plays the role of an energy distance between the FC and the line of zero energy of pair relative motion), the imaginary part of the SC pole of the scattering amplitude (which is proportional to the SC gap parameter) necessarily exceeds the real part of the pole due to a logarithmic singularity of $B_{K2}(\omega)$ at $\omega \to 0$. Thus one can assume the possibility of the existence of crystals with such a form of the FC which optimally conforms to the form and energy position of a line of zero kinetic energy of the relative motion of a hole pair with certain large total momentum (one can consider simple hyperbolic lines used here as a certain limiting case). As a simple example in behalf of such a statement, one can consider a two-band model of a cuprate compound[45] in which the FC consists of two simply connected parts. If one part of a doubly connected FC is the same as a piece of the boundary of the domain Ξ_K for a certain $\boldsymbol{K}$, this mutual line just is the PFC for given Ξ_K. As a result, in such crystals, the pairing mechanism discussed here may dominate (possibly even without the AF state in the neighborhood of the SC state, and thus without a rise of stripes as may occur in cuprate compounds with more than one CuO$_2$ plane in the unit cell[46]). Note that, in the framework of the model,[45] the order parameter changes sign at a transfer between the bands. In real space it corresponds to different signs of the order parameter on the two conducting planes, taking into account in the model. Apparently, this is a general property of any two-band model with repulsion between particles composing a pair.[47] It should also be noted that the consideration of the so-called η pairing[48] in the framework of a one-dimensional Hubbard model with pair hopping interaction (the Penson-Kolb-Hubbard model)[49] results in a sign alternation of SC order parameter defined on the sites of atomic linear chain.

It should be noted that a superconducting state with a large ($K \approx 2k_F$) total pair momentum was previously studied[50] in the framework of the microscopic model of the coexistence of superconductivity and antiferromagnetism or the charge-density-wave (a structural phase transition; in such a case, the momentum $K \approx 2k_F$ turns into a vector of the reciprocal lattice). In this model, a state with a large pair momentum arises as a result of the coexistence of AF ordering and Cooper pairs with zero total momentum. Phenomenologically, such transitions may be considered as a break of corresponding symmetry. Zhang[51] assembled AF and d-wave SC order parameters into a five-dimensional vector, and postulated the symmetry of order parameter unified in such a way under rotations of an SO(5) group. However, to obtain the closed Lie algebra of fermion pairing and particle-hole operators describing antiferromagnetism and superconductivity, one has to consider a more general symmetry than SO(5) symmetry, for example, the SU(4) symmetry.[52] Such a more general approach leads directly to a rise of the components of the unified order parameter corresponding to pairs with large (of the order of the AF vector) total momentum.[52] Thus one may conclude that the $\boldsymbol{K}$ pairs introduced in our paper in a microscopic way are fully consistent with rather general symmetry constraints. Note that if the vector $\boldsymbol{K}$ coincides with the AF vector exactly, the SC order parameter, due to the rise of $\boldsymbol{K}$ pairs, and the AF (triplet) order parameter turn out to be connected to another SC order parameter corresponding to pairs with zero total momentum. A small difference between $\boldsymbol{K}$ and the AF vector leads to a small total momentum of these pairs. Such pairs may be a in singlet spin state (conventional Cooper pairs) or in a triplet spin state. The case we discuss in this paper corresponds just to the latter of the two possibilities, namely, triplet AF order coexists with singlet SC order due to ***K*** pairs and triplet SC order due to the pairs with small total momentum.

The phenomenological approach used here to take account of the influence of AF fluctuations on carrier pairing enables one to interpret qualitatively the key experimental data relating to HTSC cuprates. We believe that the principal conception of hyperbolic pairing and a rise of the pair Fermi contour is an inherent feature of a cuprate electron system, which has become apparent both in the band scheme and in appropriate models of strongly correlated systems, such as the t-J model[53] with regard for next-nearest-neighbor interactions (the so-called t-t'-J model[54]).

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