Exchange interaction as the source of pairing in correlated electron systems: a brief overview

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Abstract. We address the question of real space pairing induced by exchange interaction, customarily associated with the presence of the broken-symmetry magnetism. For such mechanism of pairing, the appearance of superconductivity (or superfluidity) without magnetism presents itself still as a highly nontrivial problem and it seems, it can be practically realized only when the kinetic energy of individual-particle motion is comparable or even smaller than the magnitude of exchange interaction that takes place among strongly correlated fermions, where the kinetic exchange and/or the Hund’s rule coupling can become relatively strong in the vicinity of the onset of the Mott insulating state. In that situation, the pairing arises from a coherent correlated pair motion rather than from a free motion of a tightly bound pair. We elaborate on this question in general terms, as well as provide selected results in the mean-field approximation in concrete situations.

1. Introduction
The original Heisenberg-Dirac exchange interaction concept [1] reflects the transposition symmetry of the many-particle systems and has been applied to atomic [2], solid state [3], and nuclear [4] systems of fermions. In the case of atomic physics, it allows to define the high- and low-spin multiplets of 3d and 4f shells according to the Hund’s rule. In the condensed matter physics it is customarily used to describe symmetry-broken magnetic states (ferromagnetism, antiferromagnetism, spin density or spin-glass states) [5], whereas in nuclear physics it serves to classify high angular-momentum states, as well as to introduce the pairing corrections to the nuclei bound energy in the filled-shell systems [6]. In brief, the exchange interaction is instrumental in explaining the magnetism of magnetic insulators and other systems with localized magnetic moments. In real systems, it may be augmented with anisotropy, spin-orbit, crystal field, and other interactions [5]. It is also crucial as one of the principal factor in classifying the high-spin states of finite Fermi systems such as a quantum dots or nuclei.

A related but highly nontrivial question concerns the role of exchange interactions in itinerant-fermion (metallic) systems, particularly when describing ferromagnetic metals, heavy-fermion and high-temperature superconductors, where magnetism either coexists or is intimately connected with the onset of superconductivity, and involves the same set of electrons responsible for the appearance of both phenomena [7]. The natural question is then whether the spin correlations in real space and induced by the short-range exchange interaction, can also
become the mechanism of pairing resulting in either superfluid or superconducting state of fermion systems. This is an involved problem, since the magnetic ordering is described by the (staggered) magnetization and the superconducting order is described by the off-diagonal correlation function (in the simplest Hartree-Fock limit by the binding of electron and hole of opposite momentum and spin). So, in principle, those two types of ordering are not directly related, as they are described by different type of correlations. In particular, it must by noted that while the magnetism of localized spins reflects the static long-range spin-spin correlations, in the superfluid state the spin-spin correlations contain a coherent translational motion of thus mutually correlated pairs of particles with spin. Therefore, in the latter situation the strength of the exchange interaction must represent a sizable portion of the kinetic (band) energy of the particles, so the coherent (or bound) moving pair states can be sustained, not necessarily in the milieu of already ordered spins. This is the reason why this type of pairing can be effective only in the strongly correlated systems, where the kinetic energy of individual particles is drastically reduced by the correlations resulting from strong repulsive Coulomb interaction as is the case in e.g. t-J model [8] (in the extreme case of the Mott-Hubbard insulators the kinetic energy is reduced to zero by the correlations).

The magnetic mechanism of pairing interesting us here and induced by exchange interaction in real space differs from the superconducting or superfluid states induced by paramagnons (spin fluctuations), which represent collective boson (paramagnon) virtual excitations in either spin disordered or weakly ordered systems [9]. In the latter situation, we deal with pairing analogous to that induced by phonons [10], except that in the case of paramagnons spin-triplet (high-spin) pairing may be preferred, as is in the case of superfluid $^3$He [11], neutron stars [6], and possibly, in UGe$_2$ [12] and Sr$_2$RuO$_4$ [13]. In the case of exchange-interaction induced pairing the spin-correlations in real space are instrumental in the pairing, i.e. there is no “boson glue” to produce a coherent superfluid state of pairs [14]. Nonetheless, as we shall see below, any mechanism of pairing, must eventually be brought to the ”effective” BCS form, since the condensed state is either metallic (for superconductors) or liquid (for superfluids), which is described by paired (quasi)particles, with well defined momentum (in nuclear physics, the angular momentum).

The purpose of this paper is to overview briefly the role of the real-space magnetic pairing as the driving force of superconductivity. Such mechanism must be first considered for strongly correlated systems: heavy fermions, high temperature superconductors, and selected magnetic systems, particularly close to the Mott-Hubbard localization of relevant particles, i.e. when their kinetic energy is drastically reduced and the purely magnetic states are on the verge of (in) stability. In Section 2 we characterize briefly the strongly correlated system with their kinetic exchange interaction leading to spin-singlet-pairing, whereas in Section 3 we characterize briefly the mean-field solution for them. The case of spin-triplet pairing will not be discussed here. One of the conclusions (cf. Sec. 4) is that the topic announced in the title is by no means a finished story. We provide some reasons for that opinion, as well as point out to a possibility of further development.

2. Kinetic exchange and spin-singlet pairing: narrow band case

The role of the so-called kinetic [15] exchange interaction in spin-singlet-pairing case was raised for the first time in the context of high temperature superconductivity [16] and a bit later, in the context of heavy-fermion superconductivity [17]. In the former case, the superconducting state evolves from antiferromagnetic Mott insulator and in the latter, it can also coexist with a very weak antiferromagnetic state of the spin-density-wave type. Under such circumstances, a natural question to be posed is whether the source of the magnetism can also become simultaneously the mechanism of pairing. Models of these two types should be considered first in the absence of evidence for any other pairing mechanism such as the electron-phonon interaction. This last presumption seems to be legitimate, since the superconducting state in those systems is highly
unconventional in many respects not to be discussed here [18]. We introduce first the idea of kinetic exchange for strongly correlated metals [8] and then discuss the paired states.

2.1. Kinetic exchange for strongly correlated metals

The relevant for our purposes here history of antiferromagnetic exchange interactions in strongly correlated and insulating magnetic oxides bears its origin from the pioneering work of Anderson [14] who introduced the idea of kinetic exchange between the neighboring atomic 3d states of transition metal cations, say Ni$^{2+}$ each of which has an admixture of 2p states of surrounding O$^{2-}$ anions. The Anderson’s superexchange interaction via the nonmagnetic anions is effectively expressed by that between the magnetic 3d cations dressed with an admixture of the 2p oxygen states. The Anderson’s kinetic exchange, applicable first of all to the Mott insulators, has been applied also to the charge-transfer insulators [19].

The idea of kinetic exchange was extended subsequently to strongly correlated metals [17]. Its essence can be summarized as follows. In the simplest situation, we start from the Hubbard model representing a single narrow band and expressed in the Wannier representation, which has the form

$$H = \sum_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + U \sum_i n_i \nabla_i,$$

where the summation means that we take only the sites $i \neq j$ in the hopping part with the hopping integral $t_{ij}$ between them. The hopping range is determined by the number of coordination spheres of 3d ions, for which $t_{ij} \neq 0$. The second term represents the intraatomic part of the Coulomb interaction only between the two particles with opposite spins ($\sigma = \uparrow$ and $\sigma = \downarrow$) located on the same orbital. Here $i$ denotes symbolically the Wannier state $|w_i(t)\rangle = |w(t - R_i)\rangle$ centered on site $i$. In the strong-correlation limit, we have $|t_{ij}| \ll U$ and hence the kinetic (bare band) energy, as represented by the first term, is much smaller than $U$ and thus can be regarded as a perturbation. In effect, the Hubbard Hamiltonian may be transformed in the (second) order in $t_{ij}/U$ to the following form [17, 20] including exchange interaction in an explicit form:

$$H_{ij} = \sum_{ij\sigma} t_{ij} b_{i\sigma}^\dagger b_{j\sigma} + \sum_{ij} J_{ij} \left( S_i \cdot S_j - \frac{1}{4} c_1 \nu_i \nu_j \right) + c_2 \sum_{ijk} \frac{t_{ij} t_{jk}}{U} \left( b_{i\sigma}^\dagger S_{ij}^\sigma b_{j\bar{\sigma}} - b_{i\sigma}^\dagger \nu_{j\bar{\sigma}} b_{j\sigma} \right),$$

where normally $c_1 = c_2 = 1$ for their role see below. The processes representing the dynamical processes are sketched in Fig. 1. In the above expression the projected fermions operators are:

$$b_{i\sigma}^\dagger \equiv a_{i\sigma} \left( 1 - n_i \nu \right), \nu_i \equiv n_i \nu_i \left( 1 - n_i \nu \right), \nu_i \equiv \sum_{\sigma} \nu_i \sigma, \text{ and } S_i^\sigma \equiv b_{i\sigma}^\dagger b_{i\bar{\sigma}}.$$

The kinetic - exchange integral is $J_{ij} = 2t_{ij}^2/U$. In this Hamiltonian, we project out the local (site) double occupancies, as well as include both the two-site (virtual-exchange) and the three-site hopping terms, the second and the third terms, respectively. In the Mott-Hubbard insulating limit we have the conservation of particle number at each site, i.e. $n_i + n_i \nu = 1$, and hence the effective Hamiltonian reduces to that of Anderson [15] in this single-band situation (with spin $S = 1/2$). One has also to note that the intersite Coulomb interaction $\sum_{ij} K_{ij} n_i n_j$ has been neglected in (1). This term can be included in the analysis [21]. In general, the first term describes a nontrivial form of single-particle hopping, with the particles avoiding each other (no double occupancy), while the third term represents the nontrivial three-site hopping $j \rightarrow i$, with and without spin flip on the intermediate site $j$, respectively. In effect, one can say that in the metallic state (with the band filling $n = \langle n_i \rangle \neq 1$), we have $nN$ moving spins (or equivalently, of $N - Nn = N(1 - n)$ holes among the spins of the N-site system) that are correlated via the antiferromagnetic exchange interaction, with its range equal to the number of coordination spheres we take, for which $t_{ij} \neq 0$. The state describing such liquid of moving spins and holes in between them is customarily called the resonating valence bond (RVB) state [16] although,
Figure 1. On the left: schematic representation of the Hubbard subbands. The virtual hopping processes correspond to the virtual transitions lower → upper → lower Hubbard subbands (process a)). On the right: three possible intersite hopping processes (in real space) determining the dynamics of Hamiltonian (2) in the lower Hubbard subband (i.e. for the band filling $n \leq 1$): a) virtual hopping between single occupied neighboring sites that leads to their antiferromagnetic (kinetic) exchange interaction; b) two-site single-particle hopping between the single occupied and the empty sites; and c) three-site hopping between the singly occupied and the empty site via on intermediate single occupied site with opposite spin.

strictly speaking, in the present situation the various pair spin-singlet configurations, taken into account in the RVB theory of Mott insulator [6], are intermixed with the hopping processes, due to the presence of holes. So, strictly speaking we should speak about a quantum spin liquid (no double occupancies!) with antiferromagnetic correlations.

2.2. Kinetic exchange as real space pairing

The effective Hamiltonian (2) contains essentially the intertwined hopping (kinetic motion) and the explicit spin correlations (kinetic exchange and 3-site hopping), as any pair of the terms do not commute with each other. So quite few nontrivial types the behavior may appear, since minimally the band and the frozen spin-ordering effects compete *viciously*, as they become comparable near the Mott insulating limit [16]. Therefore, it was totally surprising at first (at least for the author), that the Hamiltonian (2) contains also an essentially new physics connected with the real space pairing [6], which effectively can be reduced to some form of the BCS theory. A systematic approach to the concept of this new type of pairing starts with definition of the local pairing operators [19] in the form:

$$
B^\dagger_{ij} = \frac{1}{2} \left( b_{i\uparrow}^\dagger b_{j\downarrow}^\dagger - b_{i\downarrow}^\dagger b_{j\uparrow}^\dagger \right),
$$

$$
B_{ij} = \frac{1}{2} \left( b_{i\uparrow} b_{j\downarrow} - b_{i\downarrow} b_{j\uparrow} \right) = \left( B^\dagger_{ij} \right)^\dagger.
$$

(3)
In effect, one can rewrite the kinetic-exchange energy part in the completely equivalent forms as follows:
\[ S_i \cdot S_j - \frac{1}{4} \nu_i \nu_j \equiv -B_{ij}^\dagger B_{ij}. \] (4)

What is even more surprising, the Hamiltonian (2), even with inclusion of the three-site terms, can be rewritten in the following closed form [19] for \( c_1 = c_2 = 1 \), namely:
\[ H_{tJ} = \sum_{ij\sigma} t_{ij} b_{i\sigma}^\dagger b_{j\sigma} - \sum_{ijk} \frac{4t_{ij}t_{jk}}{U} B_{ij}^\dagger B_{kj}. \] (5)

This is the full form of the so-called \( t-J \) model. In this form we see that the effective Hamiltonian contains in a direct manner an individual spin hopping (the first term) and the local pair binding (the \( i = k \) part), as well as the 3-site hopping (and spin-flip) processes for \( i \neq k \). The beauty (and the complication) of the problem is that the two terms composing the above Hamiltonian can become comparable right at the lower (lower critical) concentration for the transition from an insulating antiferromagnetic to the superconducting state in representing high temperature superconductors [17]. This is the reason why the superconductivity and antiferromagnetism can become intimately connected in the \( t-J \) model if only \( B_{ij} \) are the forerunners of a condensed spin-singlet superconducting state. Parenthetically, because of the exclusion of the double-occupied site configurations we have \( B_{ii}^\dagger = B_{ii} \equiv 0 \), and the pairing in the superconducting will have a nontrivial momentum \( \hbar k \) dependence (\( d \)-wave) of the superconducting gap. The superconducting state emerging out of this representation of the kinetic-exchange part is discussed in the next Section. We should mention that the ideas of real-space pairing have been extended also to the case with orbital degeneracy in [22], and to the case of hybridized systems as we discuss next.

### 2.3. Kondo-interaction in hybridized-band case

The Anderson-lattice model represents another example and the simplest two-band situation, in which (originally) atomic and strongly correlated states (of 3d or 4f type, for example) are intermixed with the conduction (4s or d5-6s type, respectively), which form correlated and hybridized bands. This is easy to understand, since the valence states as more extended collectivize first. The specific feature of the Anderson-lattice model is that the outermost valence states loose their atomic parity due to their band character, so it is possible to have a nonzero hybridization (e.g. the interatomic mixing between the atomic (4f) and the Wannier 5d-6s states). This last circumstance constitutes the physical origin of the model. Its formal structure from the first-quantization point of view is not so simple. However, in the second - quantization language it is easy to formulate the microscopic Hamiltonian, as the qualitative argument provided above is contained in the microscopic parameters. In effect, the starting Hamiltonian in the Wannier representation has the form

\[ H = \sum_{mn\sigma} t_{mn} c_{m\sigma}^\dagger c_{n\sigma} + \epsilon_f \sum_{i\sigma} N_{i\uparrow} + U \sum_{i\downarrow} n_{i\uparrow} n_{i\downarrow} + \sum_{im\sigma} V_{im} \left( f_{i\sigma}^\dagger c_{m\sigma} + c_{m\sigma}^\dagger f_{i\sigma} \right) \]
\[ -\mu \left( \sum_{i\sigma} N_{i\sigma} + \sum_{m\sigma} n_{m\sigma} \right), \]

where \( i \) labels correlated atomic (\( f=3d \) or 4f) states, \( (m,n) \) label delocalized \( c \) states, \( N_{i\sigma} \equiv f_{i\sigma}^\dagger f_{i\sigma} \), and \( V_{im} \) represents the hybridization magnitude. In the limit when \( |V_{im}| \ll |\epsilon_f|, U \), the above periodic Anderson Hamiltonian transforms into the Kondo Hamiltonian with the antiferromagnetic (kinetic-exchange) Kondo coupling between itinerant and localized electrons [23]. In this limit, the numbers of correlated and of the itinerant electrons are conserved.
Figure 2. On the left: the possible interband hopping process in real space involving virtual hopping process to the double occupied f-level a) and the three-state (site) hopping process (b) and c), 2 and 2’ alternative steps). The arrow (labels) by $\tilde{t}_{ij}$ represents the resulting intersite f–f hopping process. On the right: schematic representation of hybridization-induced process as f-level occupation dependent hopping process and its division into the low- and the high-energy processes. The former (I) corresponds to the presence of the residual hybridization term in (8); the other (II) leads to the Kondo-type coupling which in turn is expressed as a real-space hybrid pairing in (11) in the second order in $V/\epsilon_f$.

separately. This limit of the Anderson-lattice Hamiltonian, the so-called Kondo-lattice limit, does not concern us here, even though it has been also discussed in the context of pairing.

The situation of interest to us here is provided by the condition that $|V_{in}| \ll U$, but $|V_{in}| \lesssim |\epsilon_f|$, as represented schematically in Fig 2.

This means that we transform out only the high-energy terms of the order $\sim V_{in}/U$ and replace them with the effective kinetic-exchange interactions of the Kondo type, but leave at the same time the residual hybridization term $\sim V_{im} (1 - N_{\bar{\sigma}}) f_{im}^\dagger c_m + H.c.$, untouched. In result, the effective Hamiltonian in the second order acquires the following form [24]

$$
\mathcal{H} = \sum_{mn\sigma} t_{mn} c_{m\sigma}^\dagger c_{n\sigma} + \epsilon_f \sum_{i\sigma} n_i + \sum_{im\sigma} V_{i\sigma} (1 - N_{i\bar{\sigma}}) (f_{i\sigma}^\dagger c_{m\sigma} + c_{m\sigma}^\dagger f_{i\sigma})
$$

$$
+ \sum_{im} \frac{2V_{im}^2}{\epsilon_f + U} \left( \mathbf{S}_i \cdot \mathbf{s}_m - \frac{1}{4} \nu_i n_m \right) + \frac{1}{\epsilon_f + U} \sum_{imn\sigma} V_{im} V_{in} S_{i\sigma}^\dagger c_{m\sigma}^\dagger c_{n\bar{\sigma}},
$$

where now $t_{mn} \equiv t_{mn} - \mu \delta_{mn}$, and $\epsilon_f \equiv \epsilon_f - \mu$. As in the single-narrow-band case, we have projected out completely the double occupancies on f-site, as well as have defined the
quantities $\nu_{i\sigma} \equiv N_{i\sigma} (1 - N_{i\bar{\sigma}})$, $\nu_i = \sum_{\sigma} \nu_{i\sigma}$, $S_i \equiv (S_i^x, S_i^y) \equiv \left[f_{i\bar{\sigma}}^\dagger f_{i\sigma}^\dagger (1/2)(n_{m1} - n_{m\bar{1}})\right]$, and $s_m = (s_m^x, s_m^y) = \left[e_{m\sigma}^\dagger c_{m\bar{\sigma}}, (1/2)(n_{m1} - n_{m\bar{1}})\right]$. The third and the fourth terms represent the Kondo coupling the truncated a-c mixing respectively. The Kondo antiferromagnetic exchange integral here is $J_{im}^{(K)} = 2V_{im}^2/(\epsilon_f + U)$. The dynamical process leading to the above Hamiltonian have been sketched in Fig. 2. In this situation, the antiferromagnetic Kondo coupling corresponds to the kinetic exchange in the narrow-band case. Note that in this form a second-order renormalization of the hopping part has been neglected.

2.4. Kondo interaction as hybrid pairing

In analogy to the Section 2.2 we introduce here the so-called hybrid pairing operators in real space

$$
\begin{align*}
A_{im}^\dagger &= \frac{1}{2} \left[f_{i\bar{\sigma}}^\dagger c_{m\bar{\sigma}}^\dagger (1 - N_{i\bar{\sigma}}) - f_{i\sigma}^\dagger c_{m\sigma}^\dagger (1 - N_{i\sigma})\right] \\
A_{im} &= \left(A_{im}^\dagger\right)^\dagger.
\end{align*}
$$

Note that the f-electron operators contain the same type of projections as those in Subsection 2.1. In that situation, the hole effective Hamiltonian can be cast in a bit more compact form as follows

$$
\mathcal{H} = \sum_{m\sigma} t_{mn} c_{m\sigma}^\dagger c_{n\sigma} + \sum_{im\sigma} \left[V_{im} (1 - N_{i\bar{\sigma}}) f_{i\sigma}^\dagger c_{m\sigma} + H.c.\right] - \sum_{imn} \frac{2V_{im}V_{in}^*}{\epsilon_f + U} A_{im}^\dagger A_{in}.
$$

In this form we have taken into account the fact, that the hybridization matrix element $V_{im}$ can be complex. In principle, we can also include the higher order terms. In the fourth order the pairing part between f-electrons takes the form (5). The basic question when the Hamiltonian for e.g. magnetic oxides can be taken in the simpler single-band form (5). The question has not answered definitely as yet, although there exist a subdivision into Mott- and charge-transfer insulators [19].

2.5. Specific features of the magnetic real-space pairing

The pairing operators $B_{ij}^\dagger B_{ij}$ and $A_{im}^\dagger A_{im}$ have not a direct relation to the diagonal particle-number operator $a_{i\sigma}^\dagger a_{j\bar{\sigma}}^\dagger a_{j\bar{\sigma}} a_{i\sigma} = n_{i\sigma} n_{j\bar{\sigma}}$, as the latter represents intersite (for $i \neq j$) particle-particle, density-density correlation function, whereas the former represent the pair spin-singlet correlations. However, the pairing part of the total energy diminishes if the average $\langle B_{ij}^\dagger B_{ij}\rangle$ is nonzero. This average has a nontrivial structure, namely $B_{ii}^\dagger B_{ii} \equiv 0$. The last property follows from the circumstance that the double occupancies are strictly projected out on each site. This circumstance leads in turn, to a nontrivial structure of the superconducting gap, as we shall see below. Both of the above properties follow from fact that the pairing operators are composed of the projected fermion operators $b_{i\sigma}^\dagger \equiv a_{i\sigma} (1 - n_{i\bar{\sigma}})$and $b_{i\bar{\sigma}} \equiv a_{i\bar{\sigma}} (1 - n_{i\sigma})$, and similarly for $f$ operators. Obviously, there is a long way to go from forms (3) and (9), representing the real-space correlations to the condensed paired state.

The second characteristic feature of the whole approach is that the projected Fermi operators have non-fermionic anticommutation relations. For example,

$$
\left\{b_{i\sigma}, b_{j\bar{\sigma}}^\dagger\right\} = \left[(1 - n_{i\bar{\sigma}}) \delta_{\sigma\bar{\sigma}} - S_i^\sigma (1 - \delta_{\sigma\bar{\sigma}})\right] \delta_{ij}.
$$

This introduces a completely new feature of resulting quantum-liquid states, although this property has not been explored in full. Additionally, the hopping and the exchange-interaction
terms do not commute with each others, so the motion of electrons and the spin-interaction (e.g. the spin-flip processes) are entangled with each other and result in a strongly correlated (non-Fermi liquid) metallic state. What is equally important, the kinetic-energy \( \sim t_{ij} \) and the exchange \( \sim t_{ij}^2 / U \) can easily become comparable for filing close to the half filling \( n \) and we can have a transformation form such metal to the localized antiferromagnetic state (or vice versa) or to the phase separation into antiferromagnetic islands immersed in the sea of \( (1 - n)N \) holes with ferromagnetic ordering of the spin inside the sea. The second state is rather unstable as the Coulomb repulsion introduced by the hole condensation in part of the system will charge the system and destabilize such phase-separated state. Nonetheless, an itinerant antiferromagnetic (or spin density wave) state may coexist with the paired state. Such possibility arises from the identity which for the single narrow-band case reads

\[
S_i \cdot S_j - \frac{1}{4} \nu_i \nu_j \equiv -B_{ij}^\dagger B_{ij},
\]

and hence, the nonzero averages of the type \( \langle B_{ij} \rangle \) may imply at the same time nonzero average of magnetic moment \( \langle S_i^z \rangle \) and vice versa. Likewise, from the analogous identity for the \( f-c \) system, i.e.

\[
S_i \cdot s_m - \frac{1}{4} \nu_i m_m \equiv -A_{im}^\dagger A_{im},
\]

it follows, that the nontrivial structure of magnetic correlations expressed via \( \langle S_i \cdot s_m \rangle \) may implicate nontrivial structure of the averages \( \langle A_{im}^\dagger \rangle \) (and vice versa) in some sort of mean field approximation. Obviously, there is a problem, to what extent the magnetic and the paired states can be regarded as different states in view of the identities (11) and (12). This question can be answered in a way empirically only when studying relative stability of different states obtained from an approximate treatment, as the exact solution of any of these models is not available.

3. Renormalized mean-field solution: pure paired states
We concentrate here next on the analysis of the so-called renormalized mean-field solution [25-30] for both t-J model (5) and the Anderson-lattice with the Kondo-type pairing (9) in the narrow-band limit. The standard method of approach is either the Gutzwiller approximation (GA) or the slave-boson approach, the latter constructed in such a manner that it reduces to the Gutzwiller approximation for the cases of the simplest normal and paramagnetic states. However, in the case of magnetic and/or superconducting state, the SB approach additionally introduces specific effective fields which also renormalize the chemical potential. Recently, we have proposed a new method of approach [28] which combines the feature of the GA and SB methods in the mean-field approximation. We called it the statistically-consistent Gutzwiller approximation (SGA). We discuss this method on two examples of the models introduced above leaving the detailed elaboration of the method to separate publications.

3.1. General features of mean-field approximation for strongly correlated electrons in a narrow band
Hamiltonian (5) (or its equivalent form (2)), contains principal features two principal features. First of them is the restriction on motion (hopping) of the single particles due to the exclusion of double occupied sites (it is called the projection). The second is a kind of real-space correlations, which are composed of the pairing part (for \( k = i \)) and the pair-hopping processes (\( k \neq i \)). Both the Gutzwiller projection and the real-space pairing must be treated jointly. The treat the first of them a certain type of approximation has to be used which starts back to the original Gutzwiller considerations for the Hubbard model (1) [20], and in the present context, applied to t-J and related models was developed later [25, 27]. Its essence relies in replacing the operator part of
3.2. Results

In general, with the help of the above procedure we get the renormalized hopping probability and the pairing gap magnitude. Namely, if we define $\chi_{ij} \equiv \langle a_{i\sigma}^\dagger a_{j}\rangle$ and $\Delta_{ij} \equiv \langle a_{i\sigma} a_{j\sigma}\rangle$, then the corresponding physical quantities have the renormalized form: $g_{ij}^t \chi_{ij}$ and $g_{ij}^J \Delta_{ij}$.

The second factor is to make some sort of mean-field (Hartree-Fock) approximation on the pairing part. In the simplest version, it is decomposed in the following manner

$$B_{ij}^1 B_{ij} \equiv \langle B_{ij}^1 \rangle + B_{ij}^1 \langle B_{ij} \rangle - \langle B_{ij}^1 \rangle \langle B_{ij} \rangle.$$  (13)

This type of the decoupling $\lambda_{\sigma}$ a real space version of the Bogoliubov-Valatin approximation commonly utilized in BCS theory. In practice, the H-F approximation scheme is much more involved, as it comprises both using a more sophisticated than Gutzwiller method [22], as well as including in the Hartree-Fock scheme all possible decoupled terms [23] and the so-called statistical consistency conditions [27] ensuring agreement between the self-consistently and variationally obtained results for mean fields and other parameters. There is no need for repeating this quite involved analysis here. Therefore, we only illustrate the final results and discuss them briefly in physical terms.
In Fig. 3a we plot the renormalized gap value $\Delta_c = g^d \Delta_{(ij)}$ for nearest neighbors $\langle ij \rangle$ in the square lattice as a function of hole number (doping) $x \equiv 1 - n$. This dependence reflects the overall trend of the experimental data for $La_{2-x}Sr_xCuO_4$ displayed in Fig. 4. Before explaining various curves (i.e. specifying the microscopic parameters and different versions of the model leading to the curves 1-7) let make the following note. The presence of the upper critical concentration is in our view a crucial factor to be reproduced by any approach pretending to describe correctly the phenomenon of high temperature superconductivity. This is because can appear only in the situation with the real space pairing. Explicitly, as the kinetic energy of particle is roughly $\sim tx$ and the exchange energy $\sim t(1 - x)^2$ and for parameters chosen (see below) they are comparable for $x \sim 0.1$. For $x \geq 0.3$ the kinetic energy is already substantially larger than the pairing part, so the pairing correlations between neighboring spin is radically reduced. On the other hand, the hopping is reduced to zero in the complementary limit $x \rightarrow 0$ and the metallic paired state cases to exist (the Mott insulating state becomes stable).

What concerns detailed information concerning the calculation of the curves 1-7 the situation $i$ as follows. The ratio $T/|t| = 0.3$, which in the Hubbard model terminology means $U/|t| = 12$. Taking into account the fact that the experimental value of $T = 1500K$, we obtained that $|t| \simeq 400$ meV $\simeq 5000K$. The last value is important since the magnitude $\Delta_c$ of the calculated renormalized super-conducting gaps (of the $d$-wave $\Delta_k = \Delta_c (\cos k_x - \cos k_y)$); this means that its maximum value at the optimal doping (the dotted vertical line) is $\Delta_c \simeq 150K$. The group labels 1-3 and 4-6 correspond respectively to the two situation: the second-neighbor hopping $t'/|t| = 0$ and 0.25. Additionally, the curves within 1-3 ($t' = 0$) and 4-6 ($t' = 0.25|t|$) represent three additional conditions imposed, namely $1(4): c_1 = c_2 = 0; 2(5): c_1 = 1, c_2 = 0; and 3(6): c_1 = c_2 = 1$. We can now thus explain the meaning of the extra constants $c_1$ and $c_2$. The full $t$-$J$ model is that with $c_1 = c_2 = 1$. The situation with $c_1 = c_2 = 0$ [25] and $c_1 = 1, c_2 = 0$ [26] are also used. Hence with the help of those extra parameters we can single out the particular role of particular terms of (2) in the pairing. One can see clearly that the presence of the three-site terms suppresses both the concentration range in which the superconducting solution exists (i.e. reduces the upper critical concentration), as well as reduces the superconducting gap. The role of term $\sim c_2$ is minor even though it express an attractive density-density interaction between the neighbors, the reason being it does not differentiate between the singlet and the triplet of diagonal correlations $\langle c_{i\sigma}^\dagger c_{j\sigma} \rangle$. Note also that the curve labeled as 7 comprises the fit closest to experiment and corresponds to slightly changed values of parameters. The detailed discussion of quasiparticle energies, their Fermi velocity, and of the upper critical concentration is provided elsewhere [27].

The summarize this Section, we can say that from the day of the complete $t$-$J$ model derivation for strongly correlated metals [20] to its reinterpretation in terms of real-space pairing operators for cuprate superconductors [17], we have reaching the (semi) quantitative stage of description the concrete single plane high-$T_c$ systems [27] in the overdoped regime. However, we still require the detailed interpretation of the underdoped regime $x \leq 0.15$ and in particular the coexistence of magnetic density order with superconductivity the understanding evaluation of the Fermi-surface topology with the doping [32], and the quantitative explanation of the pseudogap appearance [33]. We should be able to see a progress along those lines soon.

### 3.3. Kondo-interaction induced pairing: spin-dependent effective masses and Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase

In this Section we concentrate on a novel state discovered in strongly correlated system, namely on the Fulde-Ferrell-Larkin-Ovchinnikov state proposed theoretically many years ago [34]. The motivation for us for carrying out the overviewed below work was the discovery that this state has been observed in the heavy-fermion system $CeCoIn_5$ [35]. The interesting thing is that in the same system the spin-dependent masses have been observed earlier [36]. This last discovery was
predicted earlier theoretically [37] and leads to rather strong Zeeman spin splitting of distortion induced by correlations of the band states. Therefore, it seems natural to combine the two effects appearing simultaneously when the electronic correlations are considered. However, one has to include then also the appearance of the effective field driven by the correlations and the real space pairing introduced in Section 2.2 when the correlations are strong. All of these factors have been included the recent series of papers for both electron-gas [38, 39] and two-dimensional-band systems [40].

Spin-dependent masses

For a quasiparticle gas of correlated particles, their energy in the applied field \( h = \frac{1}{2} g \mu_B H_a \), when the Landau quantization is neglected, is expressed as [38, 39]

\[
\xi_{k\sigma} = \frac{\hbar^2 k^2}{2m_\sigma} - \sigma h - \mu - \sigma h_{corr},
\]

(14)

where \( h_{corr} \) is the field induced by the correlations and spin-dependent mass enhancement \( m_\sigma/m_B \) is of the form in the limit of \( U \to \infty \) for a single narrow band [37]

\[
\frac{m_\sigma}{m_B} = \frac{1 - n_\sigma}{1 - n} = \frac{1 - n/2}{1 - n} - \frac{\sigma m}{2(1 - n)} \equiv \frac{1}{m_B} \left( m_{av} - \frac{\sigma}{2} \Delta m \right),
\]

(15)

where \( m_B \) is the bare (band) mass, \( m = n_\uparrow - n_\downarrow \) is the system spin polarization, and \( n \) is the band filling \( (n = n_\uparrow + n_\downarrow) \). Also, \( \Delta m = m_\uparrow - m_\downarrow \) is the mass difference and \( m_{av} = (m_\uparrow + m_\downarrow)/2 \) is the average quasiparticle mass. It is interesting to note that in the magnetic-saturation limit we recover the band limit for the spin-majority subband, i.e. \( m_\uparrow/m_B = 1 \), whereas the heavy quasiparticles in the spin-minority band (with \( m_\downarrow/m_B = 1/(1 - n) \)) disappear. Two features are important here: (i) the masses are high in the almost-localized limit \( (1 - n) \ll 1 \) and (ii) the mass \( m_\downarrow \) in the spin-minority band is the heaviest, since due to the spin imbalance, those quasiparticles scatter very strongly (due to the presence of the large-magnitude Hubbard term \( \sim U \sum_{i} n_{\uparrow i} n_{\downarrow i} \)). Additional features follows from the circumstance that we can “switch-off” completely the Hubbard interaction by applying the magnetic field and saturating magnetically the system. This is possible only (and is the case) because the field induced by the correlations enhances strongly the effect of applied magnetic field.

The brief analysis provided above delineates the principal message about what we mean by nonstandard quasiparticles in a (strongly) correlated system. First, they can become quite heavy, i.e. \( m_{av}/m_B \gg 1 \). Second, they depend on spin direction, what makes them distinguishable in the quantum-mechanical sense, since the mass in nonrelativistic quantum mechanics is an external (input) characteristic in the problem at hand. Third, the effective field driven by correlations can become very strong i.e. much stronger than any molecular field appearing in traditional magnetism. All these microscopic properties must be determined self-consistently. This feature of nonstandard quasiparticles distinguishes the way they are introduced, as compared to that they are defined within the original phenomenological Landau- Fermi-liquid theory, where the enhancement of the effective mass and of the magnetic susceptibility is expressed in terms of interaction parameters, which are not determined within the scheme. Additionally, in the Landau scheme the enhancement factors are determined by including the interaction only among the quasiparticles at and/or in close vicinity of the Fermi surface. Here, all the particles mutually influence each other, what is expressed via an integration over all occupied states when solving appropriate self-consistent equations.

Superconducting state: Fulde-Ferrell-Larkin-Ovchinnikov state

We will describe next the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state for the model heavy-fermion system starting from Hamiltonian (9) with the hybrid pairing. This Hamiltonian in the
simplest Gutzwiller approximation yields the following effective BCS-type Hamiltonian

$$\mathcal{H} = \sum_{k\sigma} \left[ \epsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} + \tilde{\epsilon}_{f\sigma} f_{k\sigma}^\dagger f_{k\sigma} + \tilde{V}_{k\sigma} f_{k\sigma}^\dagger c_{k\sigma} + \tilde{V}_{k\sigma}^* c_{k\sigma}^\dagger f_{k\sigma} \right] - \frac{2}{\epsilon_f + U} \sum_{kk'Q} V_{k\sigma} V_{k'\sigma}^* A_{kQ}^\dagger A_{k'Q},$$

(16)

with

$$A_{kQ} = \frac{1}{\sqrt{2}} \left[ f_{k+Q/2\uparrow} c_{-k+Q/2\downarrow}^\dagger - f_{k+Q/2\downarrow} c_{-k+Q/2\uparrow}^\dagger \right].$$

(17)

The single-particle part can be easily diagonalized by moving to the hybridized basis, whereas the pairing part is represented by a separable pairing potential. We proceed with the transformation to the hybridized basis first, which yields the following transformed pairing part among the quasiparticles in the lower hybridized band (appropriate for $\langle f_{i\sigma} f_{i\sigma} \rangle + \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle \leq 1$)

$$\mathcal{H} = \sum_{k\sigma} E_{k\sigma} a_{k\sigma}^\dagger a_{k\sigma} - \frac{4}{\epsilon_f + U} \sum_{kk'Q} \frac{|V_{k\sigma} V_{k'\sigma}|^2 (q_{\sigma} q_{\sigma})^{1/2}}{[|\epsilon_{k\sigma} - \tilde{\epsilon}_{f\sigma}|^2 + |V_{k\sigma}|^2]^{1/2} [(|\epsilon_{k\sigma} - \tilde{\epsilon}_{f\sigma}|^2 + |\tilde{V}_{k\sigma}|^2)^{1/2} \times \alpha_{k+Q/2\uparrow} \alpha_{-k+Q/2\downarrow}^\dagger \alpha_{-k'+Q/2\downarrow} \alpha_{k'+Q/2\uparrow}^\dagger},$$

(18)

where the quasiparticle energy in the normal state is given by

$$E_{k\sigma} \equiv \frac{\epsilon_{k\sigma} + \tilde{\epsilon}_{f\sigma}}{2} - \left( \frac{\epsilon_{k\sigma} + \tilde{\epsilon}_{f\sigma}}{2} \right)^2 \left( |\epsilon_{k\sigma} - \tilde{\epsilon}_{f\sigma}|^2 + |\tilde{V}_{k\sigma}|^2 \right)^{1/2}.$$

(19)

In all these equations $\epsilon_{k\sigma} = \epsilon_{k} - \sigma \hbar - \mu$, $\epsilon_{f\sigma} = \epsilon_{f} - \sigma \hbar - \mu$, $\tilde{V}_{k\sigma} = V_{k} g_{\sigma}^1$, where the normalization factor is takes in the Gutzwiller approximation [31]. For the constant (intraatomic) form of the hybridization $V_k = V = -|V|$, we obtain effectively single-band model discussed in detail in [36], with heavy electrons of primary $f$ type, i.e $\alpha_{k\sigma} \simeq f_{k\sigma}$ if $1 - n \ll 1$. Below we present only the principal features of the phase diagram leaving the details for the full papers [36, 37, 38]. Note that in general we have here the center-of-mass momentum of the Cooper pair $Q \neq 0$ to include a possibility of the FFLO phase appearance (strictly speaking, we consider only the Fulde-Ferrell case).

In the standard Hartree-Fock approximation with anomalous averages, Hamiltonian (18) in the narrow band limit reduces to the form

$$\mathcal{H} = \sum_{k\sigma} \left( \epsilon_{k\sigma} - \mu \right) f_{k\sigma}^\dagger f_{k\sigma} - g_{\mu B} H \sum_{k} \left( f_{k\uparrow}^\dagger f_{k\downarrow} - f_{k\downarrow}^\dagger f_{k\uparrow} \right) + \sum_{k} \left( \Delta_{kQ}^* f_{k\downarrow} f_{-k+Q\uparrow} + H.c. \right) + N \frac{|\Delta_{kQ}|^2}{V_0},$$

(20)

with the single-particle energy parameterized in the hight-binding approximation, which in for the case of square lattice takes the form

$$\epsilon_{k\sigma} \equiv q_{\sigma} [-2t (\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y],$$

(21)

and $q_{\sigma}$ is, as before, the Gutzwiller band narrowing factor (the spin-dependent mass enhancement) and the superconducting gap is determined from the self-consistent equation

$$\Delta_{kQ} = -\frac{V_0}{N} \sum_{k'} \gamma_k \gamma_{k'} \langle f_{-k'+Q\downarrow} f_{k\uparrow} \rangle.$$

(22)
Figure 4. Phase diagram for the cases with the spin-dependent (a) and the spin-independent masses (b). Yellow region corresponds to $Q = 0$ (BCS phase), the darker one to $Q \neq 0$ (FFLO phase) and the white to normal state. Note that with increasing temperature, the transition from BCS to FFLO state occurs at higher fields, in qualitative agreement with experimental results [28]. The FFLO phase is stable in an extended $H_a$-$T$ regime only in the spin-dependent-masses (SDM) case.

Additionally, $V_0$ is the pairing magnitude which for the constant hybridization has the form

$$V_0 = -\frac{4V^2(q_0q_f)^{1/2}}{\epsilon_f + U},$$

and the factors $\gamma_k$ and $\gamma_k^\prime$ correspond to the separable $k$-dependent factors in (18) divided by $V^2$.

Next, we carry out the approximate form of the Bogoliubov transformation which in the meantime acquired the name of the Bogoliubov-Valatin-de Gennes-Nambu transformation! For that purpose we represent (20) in the matrix form [38-40]

$$\mathcal{H} = \sum_k (f_{k+Q}^\dagger f_{-k}^\dagger - f_{-k}^\dagger f_{k+Q}^\dagger) \begin{pmatrix} \epsilon_{k+Q} - g\mu_B H - \mu & \Delta_{k,Q} \\ \Delta_{k,Q}^* & -\epsilon_k - g\mu_B H + \mu \end{pmatrix} \begin{pmatrix} f_{k+Q}^\dagger \\ f_k^\dagger \end{pmatrix} + \sum_k (\epsilon_k + g\mu_B H - \mu) + N \frac{\Delta^2}{V_0}. \quad (24)$$

The transformation to the quasiparticle representation has the usual form

$$\begin{pmatrix} \tilde{\alpha}_k \\ \tilde{\beta}_k^\dagger \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ -v_k & u_k \end{pmatrix} \begin{pmatrix} f_{k+Q}^\dagger \\ f_k^\dagger \end{pmatrix}, \quad (25)$$

with the Bogoliubov coherence factors given now by the relations

$$u_k = \left[ \frac{1}{2} \left( 1 + \frac{\epsilon_k + \epsilon_{-k+Q} - 2\mu}{\sqrt{(\epsilon_k + \epsilon_{-k+Q} - 2\mu)^2 + 4\Delta^2_{k,Q}}} \right) \right]^{1/2}, \quad (26)$$

$$v_k = \left[ \frac{1}{2} \left( 1 - \frac{\epsilon_k + \epsilon_{-k+Q} - 2\mu}{\sqrt{(\epsilon_k + \epsilon_{-k+Q} - 2\mu)^2 + 4\Delta^2_{k,Q}}} \right) \right]^{1/2}. \quad (27)$$
Phase boundaries for a two-dimensional \(d\)-wave superconductor with both the spin-independent masses (SIM) (a) and with the spin-dependent masses (SDM) (b). The FFLO-BCS transition line is of discontinuous nature. The dashed line marks the stability limit of the BCS state as determined by the value of the second critical field \(H_{c2}\) for the BCS state. The values of parameters are \(n = 0.97\) and \(V_0 = 12.5\, K\). For these values of the parameters, the superconducting transition temperature is \(T = 2.5\, K\) and the uppermost critical field for the FFLO phase is above \(6T\). Note that the FFLO state is robust in the situation with SDM and this result is one of the principal features of the present discussion.

The quasiparticle energies in the phase with \(Q \neq 0\) are

\[
E_{kQ\alpha} = \frac{1}{2} (\epsilon_{k\uparrow} - \epsilon_{-k+Q\downarrow}) - g\mu_B H + \alpha \frac{1}{2} \left[ (\epsilon_{k\uparrow} + \epsilon_{-k+Q\downarrow} - 2\mu)^2 |\Delta_{kQ}|^2 \right]^{1/2},
\]

where sign factor \(\alpha = \pm\) corresponds to the electron or hole excitations, respectively.

Having discussed the explicit expression for the fermionic quasiparticle excitations, we can construct the free energy functional, as well as determine the system of self-consistent equations for \(\Delta_{kQ}, \mu, \) and \(\bar{n}\); we also optimize the energy with respect to the magnitude of the wave vector \(Q\). One should also mention that for the electron-gas situation we have included explicitly in the effective Hamiltonian the correlation field \(h_{corr}\), which we optimize, whereas for the two-dimensional band structure (21) we have been able so far to carry out only the whole analysis in the Gutzwiller approximation for the Hamiltonian (24), before the pairing is included. In Fig. 4 and 5 we provide the exemplary phase diagrams on the plane temperature \(T\) - applied magnetic field \(H\) for the three-dimensional gas [38] and square-lattice cases [40], respectively.

The most important feature coming out of these Figures are: (i) the BCS state (i.e. that with \(Q = 0\)) is quite robust in the lower fields and higher temperatures, (ii) the inclusion of the effective-mass spin dependence leads to a remarkable extension of regime of the FFLO stability, (iii) in the FFLO phase the upper critical field of the transition to the normal phase is much higher than that for the BCS superconducting state, and (iv) the first-order BCS→FFLO transition can be accompanied by a weak metamagnetic transition. One should also not that the detailed analysis of the FFLO state is carried out separately. Also, the full SGA analysis
of the superconducting states within the full statistically-consistent Gutzwiller approach (SGA) for the present model is still to be finalized.

4. Concluding remarks

In this brief review we have tried to demonstrate the usefulness of the concept of an unconventional Fermi liquid for such diverse phenomena as high temperature superconductivity (as represented by t-J model) and heavy-fermion superconductivity (represented by the Kondo-type pairing) and particularly, the Fulde-Ferrell-Larkin-Ovchinnikov-state stability the latter (on the example of narrow-band limit with the Kondo-interaction induced pairing). The statistically-consistent (SGA) method proposed by us [28] is probably the most general Fermi-liquid approach possible for almost localized correlated systems, as we renormalize all relevant quantities: introduce the spin-dependent mass renormalization, as well as the effective field and the chemical-potential shift, all induced by the interparticle correlations. In addition to that, specific purely electronic mechanism of pairing in real space, leads to the BCS-type of Hamiltonian for all electrons and with a nontrivial (d-wave) form of the superconducting gap. Inclusion of quantum fluctuations in the mean-field SGA solution may be possible [27], but first one has to implement the SGA method completely by incorporating in it also the possibility of coexistence of superconductivity with antiferromagnetism. Also, the role of the intersite Coulomb (for the t-J model) and of the interorbital Coulomb (for the model with Kondo pairing) has to clarified, as the form works against real-space pairing driven by the electronic correlations. We should be able to see a progress along these lines in the near future.

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