XIV National School on Superconductivity, Ostrów Wielkopolski, October 13–17, 2009

Unconventional Superconducting States of an Almost Localized Fermionic Liquid with Nonstandard Quasiparticles: Generalized Gutzwiller Approach

J. Kaczmarczyk[a], J. Jędrak[a] and J. Spałek[a,b,*]

[a]Marian Smoluchowski Institute of Physics, Jagiellonian University
Reymonta 4, 30-059 Kraków, Poland

[b]Faculty of Physics and Applied Computer Science, AGH University of Science and Technology
Reymonta 19, 30-059 Kraków, Poland

We apply the concept of generalized (*almost localized*) Fermi liquid and associated with it unconventional superconductivity with Cooper pairs composed of quasiparticles with the spin dependent masses (in an applied field) and with the effective field, both induced by electron correlations. The pairing among quasiparticles takes place either in reciprocal space (Sect. 2) or in real space (Sect. 3) and is induced by the kinetic exchange of either superexchange (in the generic narrow-band situation) or Kondo-type interaction (in the Kondo-lattice limit of the periodic Anderson model). While the main features of this type of Fermi liquid have been introduced earlier, we present here a picture which is applicable to both heavy-fermion and high-T_c superconductivity within a single narrow-band representation of correlated states. Our approach introduces a set of additional concepts (spin-dependent masses, effective fields induced by electron correlations), for which the Landau concept of the Fermi liquid represents still a workable scheme. In the limit of the Kondo lattice, we present the phase diagram incorporating the Fulde–Ferrell–Larkin–Ovchinnikov phase within the BCS-type of pairing, whereas in that of the t–J model we show that the proper choice of renormalization factors and constraints is crucial for the mean-field description of the superconducting state.

PACS numbers: 74.20.−z, 71.27.+a, 71.10.Ca

1. Introduction

The strong correlations appear in the narrow-band situation, in which the intraatomic Coulomb interaction is comparable or much stronger than the particle kinetic (band) energy [1]. In that situation the interaction part cannot be treated as a perturbation of the single-particle states and we say that the *electron correlations* set in as new specific features of the corresponding quantum states and collective phases. A spectacular phenomenon marking the border between the weak/moderate and the strong-correlation regimes is the metal–insulator transition of the *Mott–Hubbard type* [2]. The properties near the Mott–Hubbard threshold are of particular interest, as then small changes in the system such as applied pressure, light doping or magnetic field, can alter decisively the nature of the physical ground state. These instabilities or quantum phase transitions are caused by the circumstance that the (negative) band energy and (positive) Coulomb repulsion energy almost compensate each other [1, 2]. These conditions define an *almost-localized-Fermi-liquid* (ALFL) regime which corresponds to a system with an almost half-filled band and with the repulsive (Coulomb) interaction U comparable or substantially larger than the bare bandwidth W (i.e. the limit $U/W \gtrsim 1$). The Fermi-liquid state may be stable then, albeit with nonstandard quasiparticles, as discussed below. One can say that ALFL represents the borderline situation for the ordinary (Landau) Fermi-liquid, near its instability, and as such is composed of nonstandard quasiparticles. Selected properties of such a liquid in the superconducting state are the main topic of this brief overview.

In connection with this one should mention that in the case of hybridized (heavy-fermion) systems, containing a coherent mixture of bare atomic (strongly correlated) and uncorrelated particles, the regime of applicability of ALFL concept extends to much larger values of intraatomic f–f interaction U ($U/W_{\mathrm{eff}} \gg 1$), where W_{eff} is the effective bandwidth of the emerging heavy quasiparticles (originating from f atomic states), principally of the $4f$ (mainly Ce compounds) or $5f$ (U compounds) types [3]. It is this limit, which we describe in this paper. We refer also to our recent original work [4, 5] on unconventional superconductivity in the Kondo-lattice limit. The same type of analysis, historically based on the *Gutzwiller ansatz*, has been used extensively in the

* corresponding author; e-mail: ufspalek@if.uj.edu.pl

description not only of heavy-fermion [4–6], but also of high-temperature superconductors within the t–J model [7–9] representing the correlated states in a generic single-band situation. We overview briefly here the main features of the superconducting state in both cases.

The concept of ALFL represents an extension of that of *Landau–Fermi liquid* and comprises the following novel factors: (i) very large effective masses of quasiparticles in the Kondo-lattice case, as exemplified by the large value of linear specific heat coefficient $\gamma \gtrsim 100$ mJ/(K^2 mole); (ii) quasiparticle mass which is spin-direction dependent in the magnetically polarized state (with spin polarization $\overline{m} = n_\uparrow - n_\downarrow \neq 0$ defined per site); (iii) correlation induced effective field h_{cor} and other fields (in the t–J model case); (iv) the chemical potential (the Fermi level position), that must be adjusted in each phase separately (in particular, it must be readjusted in each macrostate with broken symmetry). All these four factors should be taken into account concomitantly. Their inclusion leads to uncommon collective phenomena such as itinerant-electron metamagnetism, real space pairing, the Kadowaki–Woods scaling, and the Mott localization or other quantum critical behavior under the influence of various external factors.

Before turning to a detailed discussion, a methodological remark is in place. Namely, in analyzing theoretically the correlated systems, a few universal features should be mentioned, some of which are common to either slave-boson [10], Gutzwiller-ansatz [11], or the dynamic-mean-field [12] approaches.

First, the mass renormalization factor in the spin-polarized state is momentum-independent and is explicitly spin-dependent. This $\boldsymbol{k}$-independence of the mass renormalization factor has been interpreted [13] as the evidence for the spin-direction dependence of the quasiparticle effective mass itself, in direct analogy to the original Landau interpretation. Such generalization, however, leads to quite nontrivial consequences. Namely, if the mass depends on the spin polarization, then for the fixed direction of the spin polarization the quasiparticles with spin $\sigma =\uparrow$ and mass ($m^* = m_\uparrow$) and that with $\sigma =\downarrow$ ($m^* = m_\downarrow \neq m_\uparrow$) can be regarded as distinguishable in the quantum-mechanical sense, since the mass is one of the external factors that differentiates the particles in nonrelativistic wave mechanics. This question has been addressed in the context of forming a single Cooper pair elsewhere [4].

Second, the concept of an effective field induced by the correlations appeared for the first time in the slave-boson approach [14] and represents an additional feature to the Gutzwiller-ansatz approach. It can appear within the picture of correlated quasiparticle states naturally via constraints imposed by *statistical consistency* of the results [15], so it is of universal nature whenever the concept of renormalized mean-field Hamiltonian is introduced.

Third, the concept of real-space pairing induced by the kinetic exchange (either of superexchange or Kondo types [16]) can be applied in a natural manner to the ALFL that represents a generalized Fermi-liquid picture of a non-Fermi (non-Landau) liquid if the approach based on the Gutzwiller ansatz combined with the statistical consistency, is set at the outset.

The structure of the paper is as follows. In Sect. 2 we discuss the pairing for the nonstandard quasiparticles within the Bardeen–Cooper–Schrieffer (BCS) type of approach. In particular, we present an overall phase diagram on the applied magnetic field–temperature plane in the Pauli limiting case, incorporating also the Fulde–Ferrell–Larkin–Ovchinnikov (FFLO) state. In Sect. 3 we discuss the renormalized mean-field t–J model. Section 4 contains brief physical conclusions.

2. Simple version of renormalized mean-field theory with BCS-type pairing: FFLO state

2.1. Thermodynamics of almost localized Fermi liquid

The simplest extension of the Gutzwiller-type approach to the superconducting state relies on adding the BCS type of pairing to the Gutzwiller-projected effective Hamiltonian. Let us discuss here the simplest type of the so-called *mean-field renormalization scheme* for the correlated electron gas (i.e. with the quadratic dispersion relation). In the simplest approach [4], we start with the spin-direction ($\sigma = \pm 1$) dependent masses $m^* \equiv m_\sigma$ of quasiparticles and the effective field h_{cor} induced by the correlations. Quasiparticle energies in the applied field $h \equiv g\mu_{\mathrm{B}} H_{\mathrm{a}}$, when counted with respect to the chemical potential μ have the form

$$\xi_{\boldsymbol{k}\sigma} = \frac{\hbar^2 \boldsymbol{k}^2}{2m_\sigma} - \sigma(h + h_{\mathrm{cor}}) - \mu\,. \tag{1}$$

The spin dependence of the masses is taken in its simplest form for the narrow-band or the corresponding Kondo-lattice limits with the intraatomic Coulomb (Hubbard) interaction $U \to \infty$, i.e.,

$$\frac{m_\sigma}{m_{\mathrm{B}}} = \frac{1-n_\sigma}{1-n} = \frac{1-n/2}{1-n} - \sigma\frac{\overline{m}}{2(1-n)} \equiv \frac{1}{m_{\mathrm{B}}}\left(m_{\mathrm{av}} - \sigma\Delta m/2\right), \tag{2}$$

where m_{B} is the band (bare) mass, $\overline{m} \equiv n_\uparrow - n_\downarrow$ is the system spin polarization and $n = n_\uparrow + n_\downarrow$ is the total band filling (number of electrons per $\boldsymbol{k}$ state). Likewise, $\Delta m = m_\downarrow - m_\uparrow$ is the "spin splitting" of the mass and $m_{\mathrm{av}} = (m_\uparrow + m_\downarrow)/2$ is the average mass. Let us note that the convention is such that the state $\sigma = +1$ is regarded as that with magnetic moment along the applied field (H_{a}) direction.

The thermodynamic characteristics: $\overline{m}$, μ, h_{cor} must be determined self-consistently for given n, m_{B}, H_{a}, and temperature T. This is obtained from the free-energy functional $\mathcal{F}$, which in the present case has the following form:

$$\mathcal{F} = -k_{\mathrm{B}}T\sum_{\boldsymbol{k}\sigma}\ln(1+\mathrm{e}^{-\beta\xi_{\boldsymbol{k}\sigma}}) + \mu N + \frac{N}{n}\overline{m}h_{\mathrm{cor}}\,, \tag{3}$$

where N is the number of particles, N/n is the total number of atomic sites, and $\beta = (k_B T)^{-1}$. The quantities $h_{\rm cor}$, $\overline{m}$, and μ are determined from the minimization conditions ($\partial\mathcal{F}/\partial x_i = 0$, with $x_i = \overline{m}, h_{\rm cor}, \mu$), as in the Landau theory of phase transitions, i.e.,

$$h_{\rm cor} = -\frac{n}{N}\sum_{\boldsymbol{k}\sigma} f(\xi_{\boldsymbol{k}\sigma})\frac{\partial \xi_{\boldsymbol{k}\sigma}}{\partial \overline{m}}\,, \tag{4}$$

$$\overline{m} = \frac{n}{N}\sum_{\boldsymbol{k}\sigma} \sigma f(\xi_{\boldsymbol{k}\sigma})\,, \tag{5}$$

$$n = n_\uparrow + n_\downarrow = \frac{n}{N}\sum_{\boldsymbol{k}\sigma} f(\xi_{\boldsymbol{k}\sigma})\,, \tag{6}$$

where $f(\xi_{\boldsymbol{k}\sigma})$ is the Fermi–Dirac distribution. By inserting the solutions of (4)–(6) explicitly to the starting functional (3), it takes the form of the true free energy: $\mathcal{F}(T, H_{\rm a}; \overline{m}, \mu, h_{\rm cor}) \to \mathcal{F}(T, H_{\rm a})$. The physical properties obtained in this manner have been displayed explicitly and discussed in Ref. [4] for the case of a three-dimensional gas, so they will not be reproduced here. Instead, we discuss briefly the superconducting solution to demonstrate the novel features for the ALFL case.

2.2. BCS and FFLO superconducting phases of a gas with unconventional quasiparticles

We discuss next the three-dimensional condensed state of the quasiparticles introduced in the preceding subsection. Namely, we introduce the BCS Hamiltonian with a constant pairing potential (of s-wave symmetry), as well as allow for the possibility of nonzero center-of-mass momentum $\boldsymbol{Q}$ of a Cooper pair

$$\begin{aligned}\mathcal{H} = &\sum_{\boldsymbol{k}\sigma} \xi_{\boldsymbol{k}\sigma} a^\dagger_{\boldsymbol{k}\sigma} a_{\boldsymbol{k}\sigma} \\ &-\frac{V_0}{N}\sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{Q}} a^\dagger_{\boldsymbol{k}+\boldsymbol{Q}/2\uparrow} a^\dagger_{-\boldsymbol{k}+\boldsymbol{Q}/2\downarrow} a_{-\boldsymbol{k}'+\boldsymbol{Q}/2\downarrow} a_{\boldsymbol{k}'+\boldsymbol{Q}/2\uparrow} \\ &+\frac{N}{n}\overline{m} h_{\rm cor}\,.\end{aligned} \tag{7}$$

We consider here only the Pauli limit, as the Maki parameter is regarded high [17]. Carrying out the whole procedure detailed in [4], we obtain the system of self-consistent equations for $\boldsymbol{Q}$-dependent superconducting gap $\Delta_{\boldsymbol{Q}} \equiv \frac{V_0}{N}\sum_{\boldsymbol{k}}\langle a_{-\boldsymbol{k}+\boldsymbol{Q}/2\downarrow} a_{\boldsymbol{k}+\boldsymbol{Q}/2\uparrow}\rangle$, $h_{\rm cor}$, $\overline{m}$, and μ for fixed T, $H_{\rm a}$, $m_{\rm B}$, and n. The numerical procedure is cumbersome. In effect, we obtain the phase diagram on temperature-applied field plane shown in Fig. 1, where we have compared explicitly the results for the situation with the spin-dependent (SDM) and the spin-independent (SIM) masses of quasiparticles. The upper left-hand corner represents the state with $\boldsymbol{Q} \neq 0$, i.e. the FFLO state (of the simplest FF form, i.e. with $\Delta(\boldsymbol{r}) = \Delta_{\boldsymbol{Q}}\, {\rm e}^{{\rm i}\boldsymbol{Q}\boldsymbol{r}}$). One can see that the FFLO state becomes robust thermodynamically only in the situation with nonstandard quasiparticles (SDM). Also, one observes a weak metamagnetic behavior, pronounced at the lowest temperatures [4]. The situation in two dimensions with d-wave pairing is more involved, as different FFLO phases are observed [5].

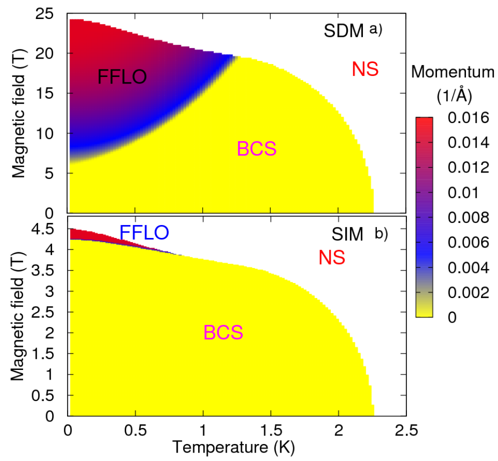

Fig. 1. Phase diagram for the cases with the spin-dependent (a) and the spin-independent masses (b). Light (yellow) region corresponds to $\boldsymbol{Q} = \boldsymbol{0}$ (BCS phase), the darker (blue-red) one to $\boldsymbol{Q} \neq \boldsymbol{0}$ (FFLO phase), and the white to normal state. Note that with the increasing temperature, the transition from BCS to FFLO state occurs at higher fields, in qualitative agreement with experimental results [17, 18]. The FFLO phase is stable in an extended $H_{\rm a}$-T regime only in the SDM case.

3. Real-space pairing and the paired states in the regime of almost localized fermions: *d*-RVB state

3.1. Effective t–J model with intersite repulsion and lattice distortion

The Gutzwiller-projection ansatz when applied in the regime of strongly correlated fermions, transforms the original t–J Hamiltonian [7, 8, 11] into that representing ALFL. This is because we replace the projected Fermi operators $b^\dagger_{i\sigma} \equiv a^\dagger_{i\sigma}(1 - n_{i\overline{\sigma}})$ and $b_{i\sigma} \equiv a_{i\sigma}(1 - n_{i\overline{\sigma}})$ back by the proper fermion operators $a^\dagger_{i\sigma}$ and $a_{i\sigma}$. To discuss the most general form of the narrow-band Hamiltonian, we start from the extended t–J or Hubbard Hamiltonian in the form

$$\begin{aligned}\mathcal{H} = P_{\rm G}\Bigg[&\sum_{ij\sigma}{}' t_{ij} a^\dagger_{i\sigma} a_{j\sigma} + U\sum_i n_{i\uparrow} n_{i\downarrow} + \frac{1}{2}\sum_{ij}{}' K_{ij} n_i n_j \\ &+\sum_{ij}{}' J_{ij}\left(\boldsymbol{S}_i\cdot\boldsymbol{S}_j - \frac{1}{4}n_i n_j\right)\Bigg] P_{\rm G}\,.\end{aligned} \tag{8}$$

In this Hamiltonian the first term expresses bare band energy in the form of particle intersite hopping ($\sum' \equiv \sum_{i\neq j}$), the second and the third represent, respectively, the intraatomic (Hubbard) and the intersite repulsive interactions, and the last expresses intersite antiferromagnetic exchange interaction containing the full exchange operator. $P_{\rm G}$ represents the Gutzwiller projection onto the state with a given double-occupation probability d^2 [19].

After expressing the intersite exchange via the real-space pairing operators

$$B_{ij}^{\dagger} \equiv \frac{1}{\sqrt{2}} P_{\mathrm{G}} \left(a_{i\uparrow}^{\dagger} a_{j\downarrow}^{\dagger} - a_{i\downarrow}^{\dagger} a_{j\uparrow}^{\dagger} \right) P_{\mathrm{G}} \,, \tag{9}$$

$$B_{ij} \equiv (B_{ij}^{\dagger})^{\dagger} \equiv \frac{1}{\sqrt{2}} P_{\mathrm{G}} \left(a_{i\downarrow} a_{j\uparrow} - a_{i\uparrow} a_{j\downarrow} \right) P_{\mathrm{G}} \,, \tag{10}$$

and the projected particle-number operators

$$\nu_i \equiv P_{\mathrm{G}} n_i P_{\mathrm{G}} \,, \quad \nu_{i\sigma} \equiv P_{\mathrm{G}} n_{i\sigma} P_{\mathrm{G}} \,, \tag{11}$$

we can rewrite (8) in the strong-correlation limit in the form [8, 20]:

$$\mathcal{H}_{\mathrm{G}} = \sum_{ij}{}' t_{ij} g_{\sigma}(d^2) a_{i\sigma}^{\dagger} a_{j\sigma} - \sum_{ij}{}' J_{ij} B_{ij}^{\dagger} B_{ij} + \frac{1}{2} \sum_{ij}{}' K_{ij} \nu_i \nu_j + NUd^2, \tag{12}$$

where N now is the number of atomic sites. One should note here that the intersite Coulomb repulsion can be destructive for the real-space pairing, particularly since we have that $U > K_{ij} > |t_{ij}| > J_{ij}$ in the strong-correlation limit (for the detailed estimate of the parameters $U = U(R_{ij})$, $K_{ij} \equiv K(R_{ij})$ and $t_{ij} \equiv t(R_{ij})$, where R_{ij} is the interatomic distance, see [21]). Therefore, one has to find a way of compensating K_{ij} so that it becomes negative. Namely, we have proposed recently [21b] a very simple model of bond distortion accompanying the coupled electron pair motion which leads to the effective t–J model with the pairing and with effective $K_{ij} < 0$. In the following simplified analysis we put $K_{ij} = 0$. We approximate the pairing operators (following mean-field renormalization scheme) as follows

$$B_{ij}^{\dagger} \simeq \sqrt{g^J} \frac{1}{\sqrt{2}} \left(a_{i\uparrow}^{\dagger} a_{j\downarrow}^{\dagger} - a_{i\downarrow}^{\dagger} a_{j\uparrow}^{\dagger} \right) \equiv \sqrt{g^J} A_{ij}^{\dagger} \,, \tag{13}$$

and similarly for B_{ij}. The factors $g_{\sigma}^{t}(d^2)$ and g^J express the restrictions on motion of single particles (g_{σ}^{t}) and bound spin-singlet pairs (g^J), respectively introduced by the constraint that, strictly speaking, no double occupancy is allowed during the charge hopping throughout the system. Let us note that here the Gutzwiller factor q_{σ} from the previous section has been replaced by the two factors g^t and g^J, not necessarily limited to their expression in the original Gutzwiller ansatz, as we consider here the paired states.

A methodological remark is in place here. The procedure leading to (12) and (13) seems ad hoc at first, as we introduce back the proper fermion operators out of the projected operators $P_{\mathrm{G}} a_{i\sigma} P_{\mathrm{G}}$, etc. It relies on the assumption that the renormalization factors play the role of restrictions imposed by the projection. It is obviously an approximate procedure, since the projected creation ($P_{\mathrm{G}} a_{i\sigma}^{\dagger} P_{\mathrm{G}}$) and annihilation ($P_{\mathrm{G}} a_{j\sigma} P_{\mathrm{G}}$) operators do not have the fermionic anticommutation relation, whereas $a_{i\sigma}^{\dagger}$ and $a_{j\sigma}$ do [8].

In effect, the effective starting t–J Hamiltonian can be recast to the simple form

$$\mathcal{H}_{\mathrm{G}} = \sum_{ij\sigma}{}' g_{\sigma}^{t}(d^2) t_{ij} a_{i\sigma}^{\dagger} a_{j\sigma} - \sum_{ij}{}' J_{ij} g^J A_{ij}^{\dagger} A_{ij} + NUd^2 \,. \tag{14}$$

The estimate of $g_{\sigma}^{t}(d^2)$ in the normal (including spin-polarized) phase is taken from the Gutzwiller ansatz [11]; the determination of g^J is prone to additional uncertainties. In the early formulation [22] $g_{\sigma}^{t}(d^2)$ was regarded as fraction of fermions with spin σ remaining itinerant in this almost localized system. For a paramagnetic ($\overline{m} = 0$) state $g_{\sigma}^{t} = g_{\overline{\sigma}}^{t} = g^t(d^2)$, and then g^t is the part of the electrons remaining itinerant in this roughly two-fluid (or itinerant-localized, two-phase) system. Likewise, $1 - g^t$ is the fraction of localized moments. In the Mott insulating state $g^t = 0$, whereas $g^t = 1$ in the metallic (Hartree–Fock) regime. Therefore, to encompass both "itinerant" and "localized" parts on the macro (mean-field) scale, we can replace g^J by g^t if we consider superconducting pairing (i.e. motion of the bound pairs) and $(1 - g^t)$ if we regard the antiferromagnetic exchange among their localized correspondants. This simple intuitive picture becomes in reality more complicated, since the part $-(1/4) \sum_{(ij)}' n_i n_j$ in (8) does not contribute to the mean-field exchange part leading to antiferromagnetism, whereas it does contribute to the real-space pairing.

3.2. d-wave RVB state and phase diagram

In the actual calculations we have used the $U \to \infty$ limit (i.e. $d^2 \equiv 0$) and the following simplified form of the effective Hamiltonian (14), which in the renormalized mean-field form for $H_{\mathrm{a}} = 0$ is

$$\begin{aligned} \hat{H} = {} & \sum_{\langle ij \rangle \sigma} \left(t_{ij} g_{ij}^{t} c_{i\sigma}^{\dagger} c_{j\sigma} + \mathrm{H.c.} \right) - \mu \sum_{i\sigma} c_{i\sigma}^{\dagger} c_{i\sigma} \\ & - \sum_{\langle ij \rangle \sigma} \frac{3}{4} J_{ij} g_{ij}^{J} \left(\chi_{ji} c_{i\sigma}^{\dagger} c_{j\sigma} + \mathrm{H.c.} - |\chi_{ij}|^2 \right) \\ & - \sum_{\langle ij \rangle \sigma} \frac{3}{4} J_{ij} g_{ij}^{J} \left(\Delta_{ij} c_{j\sigma}^{\dagger} c_{i-\sigma}^{\dagger} + \mathrm{H.c.} - |\Delta_{ij}|^2 \right) , \end{aligned} \tag{15}$$

where the summation is over neighboring pairs $\langle ij \rangle$, $\chi_{ij} = \langle c_{i\sigma}^{\dagger} c_{j\sigma} \rangle$ and $\Delta_{ij} = \langle c_{i\overline{\sigma}} c_{j\sigma} \rangle$ are respectively the hopping amplitude and the resonating-valence-bond parameter. The factor $(3/4)$ arises from the circumstance that not the full pairing is taken into account (only the $\boldsymbol{S}_i \cdot \boldsymbol{S}_j$ part [7, 9]).

This Hamiltonian, which replaces now the BCS-type Hamiltonian (7), contains χ_{ij} and Δ_{ij} as mean-field parameters and the chemical potential μ to be calculated self-consistently. However, a basic question arises exactly at this point and is caused by the circumstance that the renormalization factors contain also these mean-field parameters. For example, taking the form utilized before [23], we have

$$g_{ij}^t = \sqrt{\frac{4x_i x_j(1-x_i)(1-x_j)}{(1-x_i^2)(1-x_j^2)+8(1-x_i x_j)|\chi_{ij}|^2+16|\chi_{ij}|^4}}\,, \tag{16}$$

$$g_{ij}^J = \frac{4(1-x_i)(1-x_j)}{(1-x_i^2)(1-x_j^2)+8x_i x_j \beta_{ij}^-(2)+16\beta_{ij}^+(4)}\,, \tag{17}$$

with $x_i = 1 - n_i \equiv 1 - \sum_\sigma \langle c_{i\sigma}^\dagger c_{i\sigma}\rangle$, $\beta_{ij}^\pm(n) = |\Delta_{ij}|^n \pm |\chi_{ij}|^n$.

Because of the presence of the renormalization factors in the above form one cannot say that the Hamiltonian (15) has a typical mean-field form. Because of this, the equilibrium values of mean-field quantities calculated self-consistently may differ from those obtained variationally. To ensure an internal consistency of the whole approach, the following additional constraints have been added which redefine the Hamiltonian [9]:

$$\begin{aligned}\hat{H} \to \hat{H}_\lambda = \hat{H} &- \sum_i \lambda_i^{(n)}\Big(\sum_\sigma c_{i\sigma}^\dagger c_{i\sigma} - n_i\Big) \\ &- \sum_{\langle ij\rangle\sigma}\Big(\lambda_{ij}^{(\chi)}(c_{i\sigma}^\dagger c_{j\sigma} - \chi_{ij}) + \text{H.c.}\Big) \\ &- \sum_{\langle ij\rangle\sigma}\Big(\lambda_{ij}^{(\Delta)}(c_{i-\sigma} c_{j\sigma} - \Delta_{ij}) + \text{H.c.}\Big)\,,\end{aligned} \tag{18}$$

where the Lagrange multipliers $\lambda_{ij}^{(n)}, \lambda_{ij}^{(\chi)}, \lambda_{ij}^{(\Delta)}$ play the role of effective molecular fields. This effective Hamiltonian has been diagonalized via the Bogolyubov–Valatin transformation when all the parameters have been selected as spatially homogeneous [8]. Such procedure yields the energy of quasiparticles in the superconducting phase in the form

$$E_{\boldsymbol{k}} = \sqrt{\xi_{\boldsymbol{k}}^2 + D_{\boldsymbol{k}}^2}\,, \tag{19}$$

$$\xi_{\boldsymbol{k}} = -2\sum_\tau T_\tau \cos(k_\tau) - \mu - \lambda^{(n)}, \tag{20}$$

$$D_{\boldsymbol{k}} = \sqrt{2}\sum_\tau D_\tau \cos(k_\tau)\,, \tag{21}$$

with effective hopping in $\tau = x$ or y direction

$$T_\tau = -t_{1\tau} g_{1\tau}^t + \frac{3}{4} J_\tau g_\tau^J \chi_\tau + \lambda_\tau^{(\chi)}, \tag{22}$$

and the effective gap

$$D_\tau = \frac{3}{4} J_\tau g_\tau^J \Delta_\tau + \lambda_\tau^{(\Delta)}. \tag{23}$$

The numerical analysis has been performed for the isotropic case ($t_1 = t_{1\tau}$, $J = J_\tau$) as discussed next.

In Fig. 2a,b we plot the principal parameters of the model for the case of square lattice and the nearest-neighbor hopping only. The d-wave form of the solution for Δ_{ij} has been assumed, i.e. $\Delta_x = -\Delta_y$, where x and y are spatial directions. For the sake of comparison the renormalized gap parameter $g^t\Delta_x$ and that expressing renormalized hopping, $g^t\chi_x$, have also been displayed. Also, comparison with the results of self-consistent calculations when the additional constraints have been disregarded, was made. The important point, not detailed here, is that the present solution is stable thermodynamically, since it has a lower energy when compared to that obtained non-variationally. Obviously, having obtained these solutions which involves a simultaneous solution of six integral equations, we can calculate doping (x) and temperature dependences of other system properties. Detailed discussion of those points within a novel mean-field scheme is presented elsewhere [24]. This discussion contains also a renormalization scheme based on the recent Fukushima approach [25].

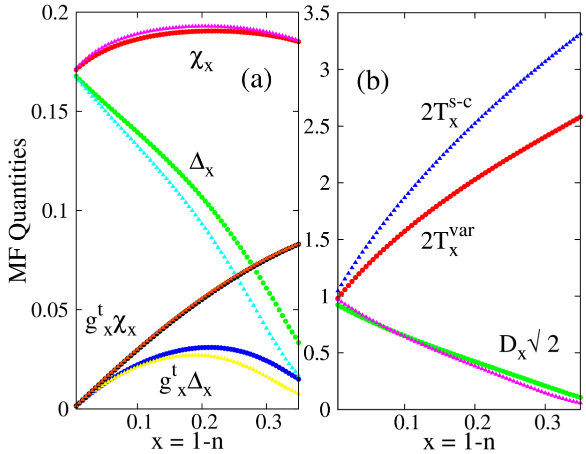

Fig. 2. (a) Doping dependence of the bond-order parameters $\chi_x = \chi_y$, the superconducting order parameters $\Delta_x = -\Delta_y$, their renormalized counterparts $g^t\chi_x = g^t\chi_y$ and $g^t\Delta_x = -g^t\Delta_y$, as well as (b) of the quantities $2T_x = 2T_y$ and $\sqrt{2}D_x = -\sqrt{2}D_y$ of Eq. (21), both for the self-consistent (s-c) calculations [23] (triangles) and the present variational (var) (circles) methods, respectively.

4. Conclusions

In this brief overview we have discussed the role of nonstandard quasiparticles on the form (and stability) of selected paired states: BCS and FFLO (Sect. 2) and d-wave resonating valence bond (RVB) state (Sect. 3), by taking into account the BCS or real-space type of pairing (t–J model), respectively. The former is more appropriate for heavy fermions in the Kondo-lattice limit, whereas the latter for high-temperature superconductors. The results are promising, but require a further detailed analysis. Among the problems to be tackled is the question concerning reliability of various mean-field renormalization schemes [24, 25]. Also, the coexistence of FFLO phase with antiferromagnetism has to be analyzed with care [22, 26]. Another important question is to what extent the single narrow-band representation of strongly correlated states reflects realistically those systems which, strictly speaking, contain minimally two types of orbitals. In general, a systematic approach going beyond the Gutzwiller approximation is needed to formulate a definite mean-field theory of strongly correlated superconducting states. We should be able to see progress along these lines in the near future.

Acknowledgments

The work was supported by Ministry of Higher Education and Science, grants Nos. N N202 128736 and N N202 173735. JK was also supported by the "Doctus" scholarship. Discussions with Prof. Maciej Maśka from the University of Silesia and Prof. Włodek Wójcik from Kraków University of Technology are appreciated. One of the authors (J.S.) dedicates this paper to his prematurely deceased former student Dr. Paweł Korbel, whose inquisitive mind helped him to understand better this and, in general, other scientific endeavors.

Note added

After this work was submitted, the present authors have completed a formal proof of equivalence between the generalized Gutzwiller ansatz (with statistical consistency conditions included) and the saddle-point approximation solution of the appropriate slave boson formulation (Kotliar-Ruckenstien or spin rotationally invariant approach). The results will be published separately. Thus the consistenst mean-field theory of an almost localized Fermi liquid, in our view, has been achieved.

References

[1] For a didactical overview see e.g. J. Spałek, *Eur. J. Phys.* **21**, 511 (2000).

[2] See e.g. F. Gebhard, *The Metal–Insulator Transition*, Springer Verlag, Berlin 1997; M. Imada, A. Fujimori, Y. Tokura, *Rev. Mod. Phys.* **70**, 1039 (1998).

[3] See e.g. Y. Kuramoto, Y. Kitaoka, *Dynamics of Heavy Electrons*, Clarendon Press, Oxford 2000; C.M. Varma, *Physica B* **378-380**, 17 (2006).

[4] J. Kaczmarczyk, J. Spałek, *Phys. Rev. B* **79**, 214519 (2009).

[5] J. Kaczmarczyk, J. Spałek, arXiv:0907.3589 (unpublished).

[6] J. Karbowski, J. Spałek, *Phys. Rev. B* **49**, 1454 (1994); *Acta Phys. Pol. A* **85**, 341 (1994).

[7] M. Ogata, H. Fukuyama, *Rep. Prog. Phys.* **71**, 036501 (2008).

[8] J. Spałek, *Acta Phys. Pol. A* **111**, 409 (2007).

[9] J. Jędrak, J. Spałek, *Phys. Rev. B* **81**, 073108 (2010).

[10] For recent review of the literature see: A. Camjayi, M.J. Rozenberg, R. Citra, *Phys. Rev. B* **76**, 195108 (2007). For earlier review see: J. Spałek, W. Wójcik, in: *Spectroscopy of Mott Insulators and Correlated Metals*, Springer Verlag, Berlin 1995, p. 41.

[11] M.C. Gutzwiller, *Phys. Rev.* **131**, A1726 (1965); J. Bünemann, F. Gebhard, R. Thul, *Phys. Rev. B* **67**, 075103 (2003). For extension of this method as applied to t–J model see e.g. M. Ogata, A. Himeda, *J. Phys. Soc. Jpn.* **72**, 374 (2003); N. Fukushima, *Phys. Rev. B* **78**, 115105 (2008).

[12] G. Kotliar, S.Y. Savrasov, K. Haule, V.S. Oudovenko, O. Parcollet, C.A. Marianetti, *Rev. Mod. Phys.* **78**, 865 (2006); H. Sakoda, Y. Ishii, *J. Phys. Soc. Jpn.* **79**, 041701 (2010).

[13] J. Spałek, *Physica B* **378-380**, 654 (2006), *Phys. Status Solidi B* **243**, 78 (2006); A.C. Hewson, J. Bauer, W. Koller, *Phys. Rev. B* **73**, 045117 (2006); S. Onari, H. Kontani, Y. Tanaka, *J. Phys. Soc. Jpn.* **77**, 023703 (2008); J. Bauer, A.C. Hewson, *Phys. Rev. B* **76**, 035118 (2007).

[14] P. Korbel, W. Wójcik, A. Klejnberg, J. Spałek, M. Acquarone, M. Lavagna, *Eur. J. Phys. B* **32**, 315 (2003); P. Korbel, J. Spałek, W. Wójcik, M. Acquarone, *Phys. Rev. B* **52**, R2213 (1995).

[15] J. Jędrak, J. Spałek, arXiv:0804.1376 (unpublished).

[16] The both types of pairing have been introduced with the exact projections respectively in: J. Spałek, *Phys. Rev. B* **37**, 533 (1988); ibid., **38**, 208 (1988); J. Karbowski, J. Spałek, ibid., **49**, 1454 (1994); for a brief review see: J. Spałek, in: *Encyclopedia of Physical Science and Technology*, 3rd ed., Vol. 16, Academic Press, San Diego 2002, p. 251.

[17] K. Maki, *Phys. Rev.* **148**, 362 (1966). The Maki parameter is high for heavy fermions, cf. K. Kumagai, M. Saitoh, T. Oyaizu, Y. Furukawa, S. Takashima, M. Nohara, H. Takagi, Y. Matsuda, *Phys. Rev. Lett.* **97**, 227002 (2006); C.F. Miclea, M. Nicklas, D. Parker, K. Maki, J.L. Sarrao, J.D. Thompson, G. Sparn, F. Steglich, *Phys. Rev. Lett.* **96**, 117001 (2006); K. Kakuyanagi, M. Saitoh, K. Kumagai, S. Takashima, M. Nohara, H. Takagi, Y. Matsuda, ibid., **94**, 047602 (2005).

[18] G. Koutroulakis, M.D. Stewart, Jr., V.F. Mitrović, M. Horvatić, C. Berthier, G. Lapertot, J. Flouquet, *Phys. Rev. Lett.* **104**, 087001 (2010); M. Kenzelmann, Th. Strässle, C. Niedermayer, M. Sigrist, B. Padmanabhan, M. Zolliker, A.D. Bianchi, R. Movshovich, E.D. Bauer, J.L. Sarrao, J.D. Thompson, *Science* **321**, 1652 (2008).

[19] For an explicit definition of the Gutzwiller projection operator see: K.A. Chao, J. Spałek, A.M. Oleś, *Phys. Rev. B* **18**, 3453 (1978).

[20] J. Spałek, *Condens. Matter Phys.* **11**, 455 (2008) [cf. arXiv: 0806.0773].

[21] (a) J. Kurzyk, W. Wójcik, J. Spałek, *Eur. Phys. J. B* **66**, 385 (2008); (b) J. Spałek, *Condens. Matter Phys.* **11**, 455 (2008).

[22] J. Spałek, A. Datta, J.M. Honig, *Phys. Rev. B* **33**, 4891 (1986); J. Spałek, J.M. Honig, M. Acquarone, A. Datta, *J. Magn. Magn. Mater.* **54-57**, 1047 (1986).

[23] M. Raczkowski, *Acta Phys. Pol. A* **114**, 107 (2008).

[24] J. Jędrak, J. Spałek, arXiv:1004.4282 (unpublished).

[25] N. Fukushima, *Phys. Rev. B* **78**, 115105 (2008).

[26] M. Mierzejewski, A. Ptok, M. Maska, *Phys. Rev. B* **80**, 174525 (2009); Y. Yanase, M. Sigrist, *J. Phys. Soc. Jpn.* **78**, 114715 (2009); A. Aperis, G. Varelogiannis, P.B. Littlewood, B. Simons, *J. Supercond. Nov. Magn.* **22**, 115 (2009).