New Journal of Physics
The open access journal at the forefront of physics
Deutsche Physikalische Gesellschaft DPG | IOP Institute of Physics

Even-parity spin-triplet pairing by purely repulsive interactions for orbitally degenerate correlated fermions

M Zegrodnik[1], J Bünemann[2] and J Spałek[3]

[1] AGH University of Science and Technology, Academic Centre for Materials and Nanotechnology, Al. Mickiewicza 30, 30-059 Kraków, Poland
[2] Max-Planck Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany
[3] Marian Smoluchowski Institute of Physics, Jagiellonian University, ul. Reymonta 4, 30-059 Kraków, Poland
E-mail: michal.zegrodnik@gmail.com, buenemann@gmail.com and ufspalek@if.uj.edu.pl

Received 12 September 2013, revised 20 January 2014
Accepted for publication 3 February 2014
Published 03 March 2014
New Journal of Physics **16** (2014) 033001
doi:10.1088/1367-2630/16/3/033001

Abstract

We demonstrate the stability of the spin-triplet paired s-wave (with an admixture of extended s-wave) state for the limit of purely repulsive interactions in a degenerate two-band Hubbard model of correlated fermions. The repulsive interactions limit represents an essential extension of our previous analysis (2013 *New J. Phys.* **15** 073050), regarded here as I. We also show that near the half-filling the considered type of superconductivity can coexist with antiferromagnetism. The calculations have been carried out with the use of the so-called *statistically consistent Gutzwiller approximation* (SGA) for the case of a square lattice. We suggest that the electron correlations in conjunction with the Hund's rule exchange play the crucial role in stabilizing the real-space spin-triplet superconducting state. A sizable hybridization of the bands suppresses the homogeneous paired state.

Keywords: correlated fermions, orbitally degenerate Hubbard model, spin-triplet superconductivity, Hund's rule pairing, antiferromagnetism-superconductivity coexistence, even-parity spin-triplet pairing

Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.

© 2014 IOP Publishing Ltd and Deutsche Physikalische Gesellschaft

1. Introduction

Spin-triplet superconductivity was suggested to occur in Sr_2RuO_4 [1, 2], in uranium compounds [3–5], and in iron pnictides [6, 7]. All these multi-band systems have moderately (Sr_2RuO_4 and the pnictides) or strongly correlated (URhGe, UPt_3) electrons, *d* and *f* respectively. Previously, the spin-triplet pairing has been used successfully to describe the superfluidity of liquid ^{3}He [8, 9] and that of the neutron-star crust [10]. In the last two cases of continuous fermionic systems, which are regarded as paramagnets with an enhanced magnetic susceptibility, a single-component (single-band) Landau Fermi-liquid picture was taken as a starting point and the pairing of the odd parity (p-wave type) was due to the exchange of paramagnons when combined with the Pauli exclusion principle. Such an approach is limited to weak correlations and was also applied to weakly ferromagnetic superconductors [11] and to the paramagnetic Sr_2RuO_4 [12].

In the case of correlated and orbitally degenerate lattice systems the intra-atomic ferromagnetic (Hund's rule) exchange interaction of magnitude $J \gtrsim 0.1\,\mathrm{eV}$, appears naturally and is essential to the description of ferromagnetism, for moderately and strongly correlated electrons. Furthermore, its significance to the spin-triplet pairing has been emphasized in general [13–17], as well as for both the pnictides [6] and Sr_2RuO_4 [18, 19]. In most cases, the Hund's rule in conjunction with remaining local Coulomb interactions are either treated in the Hartree–Fock approximation [20] or a semi-phenomenological negative-U intersite attraction [21] is introduced. Moreover, magnetism is robust (i.e. that with a substantial static magnetic moment) in most of the mentioned systems, at least at and near the half filling of the relevant bands, and thus the spin-fluctuation mechanism may be insufficient to describe the magnetism-superconductivity coexistence. In effect, it is very important to scrutinize a global stability of the spin-triplet phase against an onset of either pure magnetism or coexistent states within the orbitally degenerate Hubbard model (the canonical model of correlated electrons) when both the magnetism and the pairing in real space are treated on an equal footing. Analysis of such states is possible only by including the local interelectronic correlations. By correlated systems we understand those for which the kinetic (band) energy of fermions is either comparable or even smaller than the interaction energy among them. In such systems, starting from the Hartree–Fock approximation combined with BCS-type approach, is ruled out.

We have very recently analyzed a microscopic model with the Hund's-rule induced magnetism and spin-triplet pairing, in both the Hartree–Fock [20] and the modified Gutzwiller approximations [22] (hereinafter referred to as I). In the Hartree–Fock–BCS approach, the paired states (often coexisting with magnetism) appear only in the limit $U' - J \equiv U - 3J < 0$, where U' (U) is the intra-atomic interorbital (intra-orbital) magnitude of the direct Coulomb repulsion and J is the Hund's-rule exchange integral. This limit can be named as that with attractive interactions. In the correlated Gutzwiller state and under the same conditions, superconductivity, both pure and coexistent with antiferromagnetism, is also stable [22]. The stability of the superconducting phases does not come as a surprise in this parameter regime, since it resembles a single band model with negative U.

In the course of our study reported in I [22] it became apparent to us that the spin-triplet paired state can also become stable in the regime of purely repulsive interactions $U' - J > 0$, which represents a typical situation for the correlated $3d$ and $4d$ electrons considered in the discussion of pure magnetic phases. In this manner, we essentially extend the regime of applicability of our approach by encompassing superconductivity within the context of correlated itinerant magnetism in its canonical regime of interaction parameters [23]. This regime has been considered for a similar model with the use of the dynamical mean-field theory in [16], where only the normal-state instability with respect to the spin-triplet pairing was analyzed. Here we show explicitly that the s-wave (with an admixture of an extended s-wave) symmetry solution for the paired state, i.e. that with even parity, is stable (also against ferromagnetism) and therefore should be included in the analysis of the spin-triplet superconductivity in the orbitally degenerate and correlated systems. We would like to underline that this is a generic microscopic approach in which the electronic correlations play a decisive role in stabilizing the orbital-singlet spin-triplet state. The spin-fluctuation contribution represents in the present analysis a higher order effect and will not be considered here. One should note that the possibility of the spin-triplet pairing by purely repulsive interactions has been discussed a long time ago [24], though the authors considered only the case with odd-parity.

In connection with our analysis one should also note the studies of analogous pairing in multicomponent cold-atom fermionic systems (see e.g. [25–27]) where the phenomenon of superfluidity is investigated in general terms but not with an explicit reference to this particular microscopic mechanism.

It should be emphasized that the model considered here is not as yet material specific. Nonetheless, it allows for an analysis of general features of the proposed pairing mechanism. One should also notice some similarities between the considered pairing mechanism and the single-band real space spin-singlet pairing considered for the Hubbard [28] and *t-J* models [29, 30] of correlated systems. In this respect, the present work contributes to the universality of the exchange-interaction induced local pairing since the concept of exchange interaction is tied in a fundamental manner to the antisymmetry of the many-fermion wave function [31] (for the case of orbitally degenerate electrons see e.g. [32, 33]).

The paper is composed as follows. In section 2, we provide a brief description of our theoretical approach, within the SGA method, for the spin-triplet superconducting phase of type A ($\Delta_{\uparrow,\uparrow} = \Delta_{\downarrow,\downarrow}$) with both inter- and intrasite pairing components included. Details of the method in use are provided in appendices A and B. Similar description with only intrasite pairing is shown in I for the same phase, as well as for the spin-triplet paired phase coexisting with antiferromagnetism, for which the results will be also analyzed here but in the purely repulsive interactions regime. In section 3 we analyze the stability of considered phases as a function of band filling n and the effective pairing parameter $J_{\mathrm{eff}} = U' - J$, as well as discuss the influence of hybridization on the paired states, whereas section 4 contains the concluding remarks.

2. Model and method: Effective Hamiltonian in statistically consistent Gutzwiller approximation (SGA)

The starting Hamiltonian, as in I, has the form of the extended Hubbard model, i.e.

$$\begin{aligned}\hat{\mathcal{H}} &= \sum_{ij\,(i\neq j)ll'\sigma} t_{ij}^{ll'}\hat{c}_{il\sigma}^{\dagger}\hat{c}_{jl'\sigma} + U'\sum_{i}\hat{n}_{i1}\hat{n}_{i2} \\ &+ U\sum_{il}\hat{n}_{il\uparrow}\hat{n}_{il\downarrow} - J\sum_{ill'\,(l\neq l')}\left(\hat{S}_{il}\cdot\hat{S}_{il'} + \frac{1}{4}\hat{n}_{il}\hat{n}_{il'}\right),\end{aligned} \tag{1}$$

where $l = 1, 2$ labels the orbitals. The first term includes intraband ($l = l'$) and interband (hybridization, $l \neq l'$) hopping terms, the second and the third represent the interorbital and intra-orbital Coulomb repulsion interactions, whereas the last represents the full form of the interorbital (Hund's rule) ferromagnetic exchange interaction. The Hamiltonian (1) can be rewritten in an alternative form by introducing the real-space pairing representation for the interaction part

$$\begin{aligned}\hat{\mathcal{H}} &= \sum_{ij\,(i\neq j)ll'\sigma} t_{ij}^{ll'}\hat{c}_{il\sigma}^{\dagger}\hat{c}_{jl'\sigma} + U\sum_{il}\hat{n}_{il\uparrow}\hat{n}_{il\downarrow} \\ &+ (U'+J)\sum_{i}\hat{B}_{i}^{\dagger}\hat{B}_{i} + (U'-J)\sum_{im}\hat{A}_{im}^{\dagger}\hat{A}_{im}\,,\end{aligned} \tag{2}$$

where the spin-triplet $\hat{A}_{im}$ and the spin-singlet $\hat{B}_i$ pairing operators are defined as follows

$$\hat{A}_{i,m}^{\dagger} \equiv \begin{cases} \hat{c}_{i1\uparrow}^{\dagger}\hat{c}_{i2\uparrow}^{\dagger} & m = 1, \\ \hat{c}_{i1\downarrow}^{\dagger}\hat{c}_{i2\downarrow}^{\dagger} & m = -1, \\ \dfrac{1}{\sqrt{2}}(\hat{c}_{i1\uparrow}^{\dagger}\hat{c}_{i2\downarrow}^{\dagger} + \hat{c}_{i1\downarrow}^{\dagger}\hat{c}_{i2\uparrow}^{\dagger}) & m = 0, \end{cases} \tag{3}$$

$$\hat{B}_{i}^{\dagger} \equiv \frac{1}{\sqrt{2}}(\hat{c}_{i1\uparrow}^{\dagger}\hat{c}_{i2\downarrow}^{\dagger} - \hat{c}_{i1\downarrow}^{\dagger}\hat{c}_{i2\uparrow}^{\dagger}). \tag{4}$$

As one can see, for $U' > J$ the interaction energy that corresponds to the creation of a local pair in either spin-triplet or spin-singlet states, is positive. The factor favoring the triplet configuration is the Hund's rule exchange, but as we show, the interelectronic correlations are of primary importance to stabilize this spin-triplet paired state globally. Below we present only briefly the essential ingredients of the approach already discussed in I, but point out those elements not detailed there (cf appendix A).

As stated above, electronic correlations turn out to be crucial in the present situation. To account for them in our study we use the Gutzwiller approach modified by us [22]. In this method, one assumes that the correlated state $\left|\Psi_G\right\rangle$ of the system can be expressed in the following manner

$$\left|\Psi_G\right\rangle = \hat{P}_G\left|\Psi_0\right\rangle, \tag{5}$$

where $|\Psi_0\rangle$ is the normalized non-correlated state to be defined below, whereas $\hat{P}_G$ is the Gutzwiller correlator, which we have selected in the form

$$\hat{P}_G = \prod_i \hat{P}_{Gli} \equiv \prod_i \sum_{I,I'} \lambda_{I,I'} \, |I\rangle_{ii} \langle I'|. \tag{6}$$

Here, $\{|I\rangle\}$ is a basis of the local (atomic) Fock space ($4^2 = 16$ states, corresponding to $N_e = 0, 1, \ldots, 4$) and $\lambda_{I,I'}$ are the variational parameters, which we assume to be real and symmetric. In the subsequent discussion, we write the expectation values with respect to $\left| \Psi_0 \right\rangle$ as $\langle \hat{O} \rangle_0 \equiv \left\langle \Psi_0 \right| \hat{O} \left| \Psi_0 \right\rangle$, while the expectation values with respect to $\left| \Psi_G \right\rangle$ will be denoted by

$$\langle \hat{O} \rangle_G \equiv \frac{\left\langle \Psi_G \right| \hat{O} \left| \Psi_G \right\rangle}{\left\langle \Psi_G \right| \left. \Psi_G \right\rangle} = \frac{\left\langle \Psi_0 \right| \hat{P}_G \hat{O} \hat{P}_G \left| \Psi_0 \right\rangle}{\left\langle \Psi_0 \right| \hat{P}_G^2 \left| \Psi_0 \right\rangle} \, . \tag{7}$$

We focus on the pure superconducting phase of type A defined as $\langle \hat{A}_{i,1} \rangle_G = \langle \hat{A}_{i,-1} \rangle_G \neq 0$, and $\langle \hat{A}_{i,0} \rangle_G \equiv 0$. This is because one would expect that the equal-spin state (ESP) is favored by the local ferromagnetic exchange. Note that the expectation values in the correlated state, $|\Psi_G\rangle$ of the respective pairing operators are nonzero only if the corresponding expectation values in the noncorrelated state $|\Psi_0\rangle$ are also nonzero. For simplicity as in I, we assume that $t^{11} = t^{22} \equiv t$ and $t^{12} = t^{21} \equiv t'$ for the nearest neighbors. The expectation value of the grand Hamiltonian $\hat{\mathcal{K}} = \hat{\mathcal{H}} - \mu \hat{N}$ in the correlated state now takes (cf appendix A for details) the following form

$$\begin{aligned} \langle \hat{\mathcal{K}} \rangle_G \; = \; & \sum_{ijl\sigma} Q \; t_{ij} \langle \hat{c}^{\dagger}_{il\sigma} \hat{c}_{jl\sigma} \rangle_0 + \sum_{ijll'\sigma} Q \; t_{ij}{}' \langle \hat{c}^{\dagger}_{il\sigma} \hat{c}_{jl'\sigma} \rangle_0 \\ & + \sum_{ij\sigma} \tilde{Q} \; t_{ij} (\langle \hat{c}^{\dagger}_{i1\sigma} \hat{c}^{\dagger}_{j2\sigma} \rangle_0 + \langle \hat{c}_{j2\sigma} \hat{c}_{i1\sigma} \rangle_0) \\ & + L \sum_{I,I'} \bar{E}_{I,I'} \langle \hat{m}_{I,I'} \rangle_0 - \mu \sum_{il\sigma} q^s_{l\sigma} \langle \hat{n}_{il\sigma} \rangle_0 \, , \end{aligned} \tag{8}$$

where Q and $\tilde{Q}$ are the band renormalization factors (cf appendix A), μ refers to the chemical potential, and $q^s_{l\sigma} = \langle \hat{n}_{il\sigma} \rangle_G / \langle \hat{n}_{il\sigma} \rangle_0$ (for the case considered here $q^s_{l\sigma} \equiv q^s$). The expression for $\langle \hat{\mathcal{K}} \rangle_G$ can be rewritten as the expectation value of the effective single-particle Hamiltonian $\hat{\mathcal{K}}_{GA}$, evaluated with respect to $|\Psi_0\rangle$. This effective Hamiltonian is defined within the subspace of broken-symmetry single-particle states in the following manner

$$\begin{aligned} \hat{\mathcal{K}}_{GA} \; \equiv \; & \sum_{ijl\sigma} Q \; t_{ij} \hat{c}^{\dagger}_{il\sigma} \hat{c}_{jl\sigma} + \sum_{ijll'\sigma} Q \; t'_{ij} \hat{c}^{\dagger}_{il\sigma} \hat{c}_{jl'\sigma} \\ & + \sum_{ij\sigma} \tilde{Q} \; t_{ij} (\hat{c}^{\dagger}_{i1\sigma} \hat{c}^{\dagger}_{j2\sigma} + \hat{c}_{j2\sigma} \hat{c}_{i1\sigma}) \\ & + L \sum_{I,I'} \bar{E}_{I,I'} \langle \hat{m}_{I,I'} \rangle_0 - \mu \sum_{il\sigma} q^s \hat{n}_{il\sigma} \, . \end{aligned} \tag{9}$$

The first three terms of (9) originate from the single particle part of (2), whereas the fourth originates from its interaction part. The intra-atomic interaction appears only through its average, in accordance with the general philosophy of the Gutzwiller approach. This amounts to saying that physically the configurations dictated by the macroscopic parameters (number of orbital double occupancies, component-band occupancies, spin-subband magnetic polarization) are fixed and form the background for the quasiparticle dynamics. Thus, Q and $\tilde{Q}$ are the

renormalization factors of the respective quasiparticle hopping processes. The first of them refers to the narrowing of the component quasiparticle bands, whereas the second corresponds to the intersite pairing amplitude. In other words, Q and $\tilde{Q}$ can be regarded as $\mathbf{k}$-independent renormalization factors of the hopping and pairing-potential matrix elements respectively. It should be emphasized that in our initial Hamiltonian (1) there are no intersite interaction terms and so the intersite pairing that is present in (9) is due to correlations (a non-BCS factor). Also, the off-diagonal factor $\tilde{Q}$ is nonzero only when the local expectation values $\langle \hat{A}_{i,\pm 1} \rangle_G$ (and the corresponding $\langle \hat{A}_{i,\pm 1} \rangle_0$) are also nonzero. As a result, the intersite pairing appears concomitantly with the intrasite one. The Hamiltonian (9) now can be solved without invoking an explicit form of $|\Psi_0\rangle$, since it will be specified by the type of averages $\langle \ldots \rangle_0$ we assume as nonzero (i.e. selected type of the symmetry-broken state).

As discussed in detail in [22, 34–37], in the Gutzwiller approximation the mean fields entering the problem should be treated as variational parameters to obtain the fully minimized energy of the system. This is due to the fact that the renormalization factors depend explicitly on those mean fields. However, to assure the statistical-consistency during the minimization procedure, one has to impose additional constraints so that the mean values obtained from a self-consistent procedure coincide with those determined variationally. This is the principal additional ingredient to the Gutzwiller approximation (GA) to make the whole approach mutually (statistically) consistent. In this statistically consistent Gutzwiller approach (SGA) [22, 34–37] the constraints are introduced with the help of the Lagrange-multiplier method which leads to supplementary terms in the effective Hamiltonian so that now it takes the final form

$$\begin{aligned} \hat{\mathcal{K}}_{\lambda} \equiv\ & \hat{\mathcal{K}}_{GA} - \lambda_n \left(\sum_{il\sigma} q^s \hat{n}_{il\sigma} - L \langle \hat{n} \rangle_G \right) \\ & - \sum_{m=\pm 1} \left[\lambda_m \left(\sum_i \hat{A}_{im} - L \langle \hat{A}_m \rangle_0 \right) + H.\,C. \right], \end{aligned} \tag{10}$$

where

$$\langle \hat{n} \rangle_G \equiv \sum_{l\sigma} \langle \hat{n}_{il\sigma} \rangle_G \,, \qquad \langle \hat{A}_m \rangle_0 \equiv \left\langle \hat{A}_{im} \right\rangle_0, \tag{11}$$

since we consider a spatially homogeneous situation. The global Lagrange multipliers λ_m and λ_n are introduced to ensure that the spatially homogeneous averages $\langle \hat{A}_m \rangle$ and $\langle \hat{n} \rangle$ calculated either from the corresponding self-consistent equations or variationally, coincide with each other. One should also note that it is natural to fix $\langle \hat{n} \rangle_G$ instead of $\langle \hat{n} \rangle_0$ during the minimization procedure. That is why we put the term $-\mu \hat{N}$ already at the beginning of our derivation. This assumption is typical in the whole approach and represents a simplified procedure; a full treatment requires that the two particle numbers ($\langle \hat{n} \rangle_G$ and $\langle \hat{n} \rangle_0$) should coincide, what leads only to quantitative corrections [38]. The values of the mean fields, the variational parameters, and the Lagrange multipliers, are all found by minimizing the free energy functional $\hat{\mathcal{F}}_{\lambda}$ that is derived with the help of the effective Hamiltonian $\hat{\mathcal{K}}_{\lambda}$ in a standard statistical-mechanical manner. For the

considered two-band model there can be up to 256 variational parameters $\lambda_{I,I'}$. Fortunately, for symmetry reasons, one can reduce their number significantly. In effect, we have to minimize only 16 variables in this pure superconducting state of type A. We should emphasize that the SGA method does not introduce any additional approximations in comparison to the standard Gutzwiller approximation. Moreover, by setting $\lambda_{I,I'} = \delta_{I,I'}$ we reproduce the Hartree–Fock–BCS results which constitutes a test for the applied method. Additionally, it can be shown that our treatment is fully equivalent to the saddle-point slave-boson approach but does not contain the spurious condensed slave Bose fields [37].

From equations (9) and (10) it can be seen that the Lagrange multipliers λ_m have an interpretation of the intrasite gap parameters, while the symmetry of the intersite gap parameter is fully determined by the bare band dispersion relation that results from (9). By assuming the dispersion relation for a square lattice with nonzero hopping t between nearest neighbors only

$$\epsilon_{\mathbf{k}} = -2t\,(\cos k_x + \cos k_y), \tag{12}$$

one obtains the following form of the gap parameter

$$\Delta_{\mathbf{k}} = \Delta^{(0)} + \Delta^{(1)}\,(\cos k_x + \cos k_y), \tag{13}$$

where $\Delta^{(0)} \equiv \lambda_1 = \lambda_{-1}$ (as we are considering an ESP state) while $\Delta^{(1)} \equiv 2\tilde{Q}t$ is the intersite pairing amplitude. In this manner, we have obtained a mixture of the s-wave and the extended s-wave pairing symmetry. To obtain the expression for the free energy, which is minimized when carrying out calculations, one has to first transform the Hamiltonian (10) into the reciprocal space and then carry out the diagonalization in order to obtain the renormalized quasiparticle energies. This procedure is detailed in appendix B.

In order to check if the stable spin-triplet paired phases can indeed appear in the repulsive-interaction regime, we have first performed the calculations, taking into account only the intrasite pairing for the following selection of phases: type A superconducting (**A**), pure ferromagnetic (**FM**), paramagnetic (**NS**), superconducting coexisting with antiferromagnetism (**SC+AF**), and pure antiferromagnetic (**AF**). The antiferromagnetic ordering considered by us has a simple two-sublattice form. We have also considered the so-called A1 superconducting phase, i.e. with $\langle \hat{A}_1 \rangle_G \neq 0$ and $\langle \hat{A}_{-1} \rangle_G = \langle \hat{A}_0 \rangle_G \equiv 0$, coexisting with ferromagnetism. However, this phase turned out not to be stable in the whole range of the model parameters examined. Therefore, it is not included in the subsequent discussion. Detailed information concerning the above phases can be found in Part I, where we have analyzed the intrasite paired states only in the regime of attractive interaction, i.e. for $U' - J < 0$. Below we present results from the repulsive-interaction regime first and subsequently analyze the evolution from the attractive to the repulsive regime by plotting the gap parameter as a function of $J_{\mathrm{eff}} = U' - J$ from negative to positive values.

Note that the renormalized single-particle properties, Fermi surface topology, etc, have been discussed separately [38], so here we concentrate only on the detailed discussion on stability of the superconducting state and its coexistence with antiferromagnetism in the regime of purely repulsive interactions.

3. Results in the purely repulsive interactions limit: $U' - J > 0$

The numerical analysis has been performed assuming that the hybridization matrix element has the simplest form $\epsilon_{12\mathbf{k}} \equiv \beta_h \epsilon_{\mathbf{k}}$, where $\beta_h \in [0, 1]$, specifies the interband hybridization strength. The interorbital Coulomb repulsion constant U' was set to $U' = U - 2J$. All the energies have been normalized to the bare band-width, $W = 8|t|$ for a two-dimensional square lattice, and the results were obtained for $k_B T/W = 10^{-4}$ emulating the $T = 0$ state.

In figure 1 we show that the superconducting phases, both pure and coexisting with antiferromagnetism, are stable for purely repulsive interactions regime ($U' - J > 0$). With the increasing Coulomb repulsion U, the regions of stability of the paired phases are becoming narrower. Note that the Hartree–Fock calculations lead only to the stability of magnetically ordered phases in this regime. The appearance of the paired states is therefore a genuine correlation-induced effect taken into account within the SGA method. One can say that out of the 2, 3, and 4-particle configurations possible locally, all with positive interaction energies, those representing the spin-triplet are selected as the ones for which the relative system energy is lowered by the amount of J on a local scale and subsequently stabilized globally by including the renormalized band energy. What is interesting is that, within the parameter range analyzed, the coexistence of ferromagnetism and superconductivity does not appear even though both are stabilized by the Hund's-rule exchange.

Next, we analyze the superconducting A phase with inclusion of the intersite part of the pairing. In figure 2 we plot the superconducting gap components $\Delta^{(0)}$ and $\Delta^{(1)}$ as a function of the effective pairing parameter $J_{\text{eff}} \equiv U' - J$ and for a representative value of the band filling $n = 1.2$. As the J_{eff} parameter changes sign to positive, the intrasite interaction corresponding to the spin-triplet-pair creation on a single atomic site changes from the attractive to the repulsive. As one could expect, according to the Hartree–Fock–BCS results, the intrasite gap parameter vanishes before J_{eff} reaches zero (from the negative-side values) and the intersite pairing does not appear at all. The situation is different in the SGA. Namely, the paired solution survives for $J_{\text{eff}} > 0$ and the pairing has both the intra- and the intersite components. However, the $\Delta^{(1)}$ parameter is an order of magnitude smaller than $\Delta^{(0)}$. The phase A has a lower value of energy than the normal phase for the whole range of J_{eff} presented in figure 2. The evolution of the gap components is smooth when the sign of J_{eff} changes. This speaks again for the decisive role of correlations in stabilizing globally this pairing induced by local interaction. Exemplary values of the order parameters, the renormalization factors, and the free energy for $T \to 0$, are all listed in table 1.

So far we have put $\beta_h = 0$. In figure 3 we show the J dependences of the gap parameters for $J_{\text{eff}} = 0.1$ and the influence of the hybridization on the considered type of superconductivity. The superconducting gaps are not affected by the increase of the β_h parameter up to the critical value $\beta_h^C \approx 0.0379$ at which both of them suddenly drop to zero. Therefore, a sizable hybridization is detrimental to the homogeneous spin-triplet pairing. This result represents a rather stringent condition ($\beta_h \ll 1$) imposed on the observability of a pure homogeneous A-SC state. It is caused by the fact that the hybridization introduces inequivalence of the bands which results in a Fermi wave-vector mismatch between $\mathbf{k}_{F1}$ and $-\mathbf{k}_{F2}$ and thus leads to a collapse of the interband paired phase at a critical value of β_h. Such a destructive role of hybridization

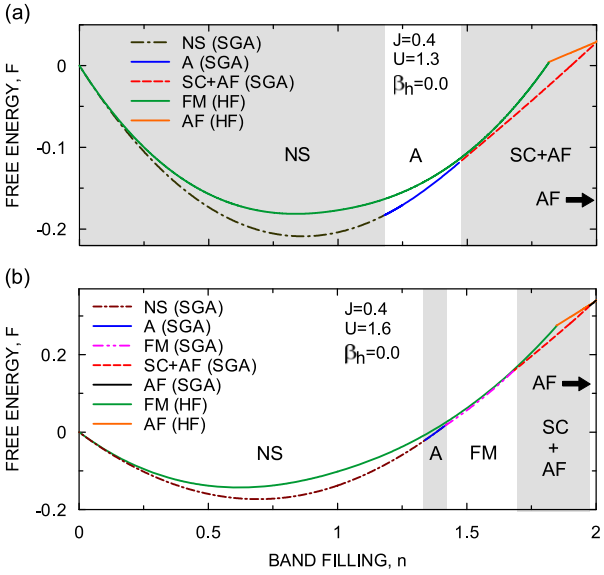

Figure 1. Ground-state energy of stable phases as a function of the band filling for two values of U for the case when only the intrasite pairing is included (i.e. for $\Delta^{(1)} \equiv 0$). For comparison, plots obtained in the H-F approximation are also shown. The shaded regions mark the stability of corresponding phases according to the SGA method. A pure AF state is stable for $n = 2$ in a and $n \approx 2$ in b (marked by arrow). Note the appearance of the pure FM and A-SC states, next to each other in b. No stable coexisting FM+SC state appears in this range of parameters.

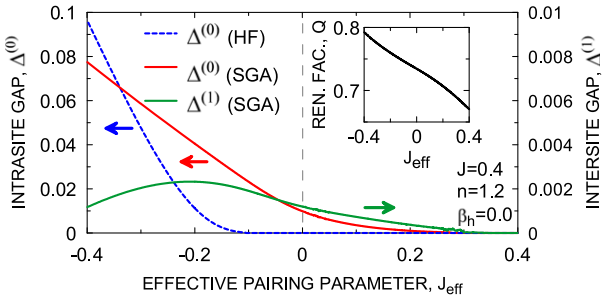

Figure 2. The intrasite (left scale) and the intersite (right scale) gap components as a function of the effective coupling constant $J_{\text{eff}} \equiv U' - J$. For comparison, we provide also the results obtained in the Hartree–Fock approximation (blue dotted line). Additionally, the band renormalization factor Q is shown in the inset. Note that $\Delta^{(1)} \equiv \tilde{Q}/4$. The HF-BCS paired solution is stable only for $J_{\text{eff}} < 0$, whereas that in the correlated state evolves smoothly to the $J_{\text{eff}} > 0$ regime.

appears also in the attractive interactions limit (cf I) but for a substantially larger amplitude of $\beta_h \sim 0.1$.

4. Outlook: meaning of the pairing mechanism

As this paper provides an essential extension of the idea of spin-triplet pairing to the nontrivial situation of real-space pairing with repulsive interactions, a methodological remark is in place

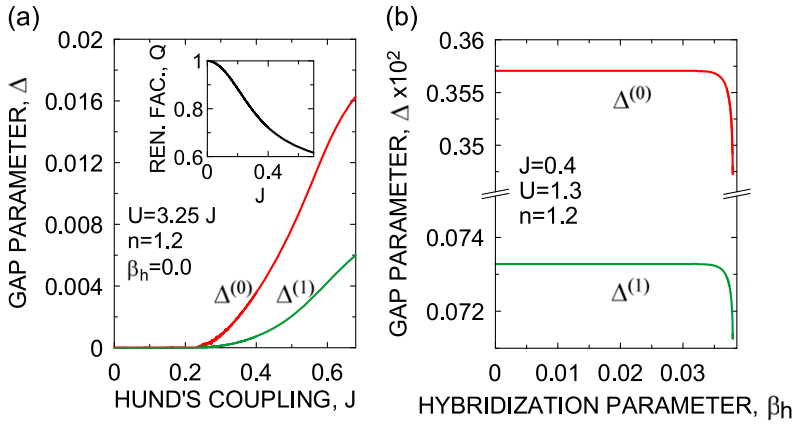

Figure 3. Intrasite ($\Delta^{(0)}$) and intersite ($\Delta^{(1)}$) gap amplitudes as a function of the Hund's exchange integral (a) and the hybridization parameter (b). In the inset of (a) the J dependence of the band narrowing factor is shown. In the repulsive limit, the hybridization is rapidly destructive to the SC stability (cf I, where the influence of hybridization in the attractive limit is analyzed).

Table 1. Representative values of the gap parameters, the renormalization factors and the free energies for $J = 0.4$, $n = 1.2$ and $\beta_h = 0.0$, for three different values of the effective pairing constant, J_{eff}. For comparison, we have provided the values of the renormalization factor and the free energy for the superconducting phase of type A and the normal phase, NS. The subscripts refer to these two phases. The numerical accuracy is better that the last digit specified.

J_{eff}	$\Delta^{(0)}$	$\Delta^{(1)}$	Q_A	Q_{NS}	F_A	F_{NS}
−0.1	0.02325	0.00191	0.74669	0.74401	−0.255481	−0.255067
0.1	0.00357	0.00073	0.72164	0.72157	−0.179725	−0.179705
0.15	0.00200	0.00054	0.71454	0.71453	−0.161874	−0.161867

here. First, the standard concept of spin-triplet superconductivity involves pairing among quasiparticles in **k** space near the Fermi surface, in a single band. This situation forces an odd parity in connection with the antisymmetry of the orbital part of the pair wave function. The pairing potential within, e.g., the spin-fluctuation mechanism is explicitly **k**-dependent as it contains the appropriate dynamic susceptibility. Such pairing mechanism contains also the retardation effects [8, 9, 11, 12].

In the present situation we introduce the pairing potential already at the model level in real space. This is because we consider the system locally strongly correlated in an extreme situation even close to the Mott (or Mott–Hubbard) localization. The obtained quasiparticles as a rule contain strong renormalization effects. Nevertheless, in the limit of weak correlations our results reduce to those coming from the Hartree–Fock–BCS approximation and this limit represents a sort of implicit checkout that our approach has a solid basis. Here the pairing operates between electrons from two different bands and leads to an orbital-singlet spin-triplet pairing. As a result, the superconducting gap is an even function of **k** but the wave function of the Cooper pair as a whole is antisymmetric as it should be. Furthermore, the pairing potential is **k**-independent and contains no retardation effects. However, it involves all electrons, i.e. is not

limited to the vicinity of the Fermi surface, as would be the case in BCS theory. The last circumstance requires the specific variational (self-consistent) evaluation of both the quasiparticle properties as well as the magnitude of the pairing within a single framework. Finally, the **k**-dependent component of the pairing obtained in our approach is an effect of correlations and, from the technical point of view, appears during the construction of the effective Hamiltonian. Explicitly, the intersite pairing term in this Hamiltonian originates from the hopping part of the initial Hamiltonian and as a result the intersite pairing symmetry (in our case the extended s-wave) is determined by the dispersion relation of the bare electrons.

By using the statistically consistent Gutzwiller approach (SGA), we have shown that the real-space spin-triplet paired states, both pure (A-type) and coexistent with antiferromagnetism (SC+AF phase) become stable in the orbitally degenerate Hubbard model, in the limit of purely repulsive interactions ($U' - J > 0$) near the half filling. One can say that both the Hund's rule and the correlation-induced change of the band energy contribute to the spin-triplet pairing; they correspond to the BCS (potential energy gain) and the non-BCS (kinetic energy gain) factors stabilizing the paired state, respectively. Also, the intersite (extended s-wave) component of the pairing is directly related to the intrasite (s-wave) counterpart. This can be seen from figures 2 and 3(a), where $\Delta^{(0)}$ and $\Delta^{(1)}$ reach zero for the same values of the model parameters. One should note that the present model does not lead to a stable SC+FM state. Therefore it cannot account for such a coexistence observed in e.g. UGe_2 or URhGe. However, in that group of uranium compounds the proper starting point is the orbitally degenerate Anderson-lattice model in which principally quasi-atomic 5f states due to U are strongly hybridized with those electrons from uncorrelated conduction bands. In other words, a strongly inequivalent-band structure must be assumed from the start even before the hybridization is taken into account. In that situation the interband Kondo exchange, as well as the f-f superexchange leading to the spin-triplet pairing, compete with the contribution arising from the Hund's rule counterpart.

The intersite hybridization suppresses the homogeneous paired states and this is ascribed to the Fermi wave-vector mismatch in the bands ($\mathbf{k}_{F1} \neq \mathbf{k}_{F2}$), that appears when the bands become inequivalent. This band inequivalency introduced by the hybridization has been discussed elsewhere [38]. However, when the mismatch is not very large, the homogeneous paired phase is still stable, which means that such paired state should appear in some realistic situations. One of the possibilities is the compound $LaFeAsO_{1-x}F_x$, for which a two-band model has been used in [6] for the description of the triplet superconducting state. In the case of strongly inequivalent bands (like the α and β bands in Sr_2RuO_4), the large Fermi wave vector mismatch of the Cooper pair partners can be compensated by introducing a nonzero center-of-mass momentum of the Cooper pair which could lead to a spontaneous creation of a Fulde–Ferrell–Larkin–Ovchinnikov type of phase. This kind of inhomogeneous SC state has not been analyzed in detail as yet. Furthermore, the application of the pairing mechanism analyzed here to the ultracold atom fermionic systems in optical lattices, where the simplest two-equivalent-band situation can be realized, should also be considered.

At the end, one must emphasise that the present pairing mechanism by purely repulsive interactions is of similar type as the spin-singlet pairing in the correlated single-band Hubbard [28] and *t-J* models [29, 30]. As the *t-J* model is derived from the one band Hubbard model in the large-*U* limit, one can say that in both approaches the intra-atomic repulsion leads to the intersite pairing, as in our case. In the mentioned models, the spin-fluctuation induced pairing appears as a higher order contribution to the renormalized mean-field or SGA approaches,

which in turn can be regarded as saddle-point solutions within a statistical-field-theoretical approach.

Acknowledgments

MZ has been partially supported by the EU Human Capital Operation Program, Polish Project No. POKL.04.0101-00-434/08-00. This work has been partially supported by the Foundation for Polish Science (FNP) within project TEAM and partially by the National Science Center (NCN), through scheme MAESTRO, Grant No. DEC-2012/04/A/ST3/00342. We are also grateful to Karol I Wysokiński for helpful discussions and comments. This work represents a part of the PhD thesis of MZ, submitted to the Faculty of Physics and Applied Computer Science of the AGH University of Science and Technology in Kraków.

Appendix A. Derivation of the effective Hamiltonian in the correlated state

In order to construct the effective Hamiltonian within the Gutzwiller approach one has to derive the formula of the expectation value of the initial Hamiltonian $\hat{\mathcal{K}} = \hat{\mathcal{H}} - \mu\hat{\mathcal{N}}$, in the correlated state defined by (5). This can be done by the use of the diagrammatic approach in the limit of infinite dimensions [33, 39]. By applying this method to the two-site term that originates from the hopping part of the Hamiltonian, one obtains

$$\langle \hat{c}^{\dagger}_{il\sigma}\hat{c}_{jl'\sigma}\rangle_G = \frac{\left\langle \Psi_0 \right| \left[\prod_{m\neq i,j}\hat{P}^2_{G|m}\right]\hat{P}_{G|i}\hat{P}_{G|j}\hat{c}^{\dagger}_{il\sigma}\hat{c}_{jl'\sigma}\hat{P}_{G|i}\hat{P}_{G|j}\left|\Psi_0\right\rangle}{\left\langle \Psi_0 \right| \prod_m \hat{P}^2_m \left|\Psi_0\right\rangle}. \tag{A1}$$

The sites with $m \neq i, j$ play the role of inner vertices and as it can be shown the contribution of all diagrams with those inner vertices vanishes, at least proportional to $1/\sqrt{d}$, where d is the spatial dimensionality. As a result in the $d = \infty$ limit we obtain

$$\langle \hat{c}^{\dagger}_{il\sigma}\hat{c}_{jl'\sigma}\rangle_G = \left\langle \Psi_0 \right| \hat{P}_i\hat{P}_j\hat{c}^{\dagger}_{il\sigma}\hat{c}_{jl'\sigma}\hat{P}_i\hat{P}_j \left|\Psi_0\right\rangle . \tag{A2}$$

In executing our diagrammatic approach we demand that at least four lines meet at every inner vertex which can be fulfilled by putting restrictions on the $\lambda_{I,I'}$ parameters. This leads to a set of constraints that have to be obeyed during the calculations (see equation (26) in I [22]). The right hand side of equation (A2) can be further simplified due to the fact that in the case of infinite dimensions only a single line can join the two external vertices $i \neq j$. In such a situation the contraction at i can be done with the creation operator $\hat{c}^{\dagger}_{il\sigma}$ when it meets the annihilation operator $\hat{c}_{jl'\sigma}$ at j (the inverse situation is also considered). However, when the superconducting pairing correlations are possible in $\left|\Psi_0\right\rangle$, the line between i and j can also be an anomalous propagator. The resulting one particle density operator takes the form

$$\begin{aligned}\langle \hat{c}^{\dagger}_{i\gamma}\hat{c}_{j\gamma'}\rangle_G &= \sum \tilde{\gamma}\tilde{\gamma}' t^{\gamma\gamma'}_{ij}\left(q_{\gamma\tilde{\gamma}}q_{\gamma'\tilde{\gamma}'} - \bar{q}_{\gamma\tilde{\gamma}}\bar{q}_{\gamma'\tilde{\gamma}'}\right)\langle \hat{c}^{\dagger}_{i,\tilde{\gamma}}\hat{c}_{j,\tilde{\gamma}'}\rangle_0 \\ &+ \sum \tilde{\gamma}\tilde{\gamma}' t^{\gamma\gamma'}_{ij}\left(q_{\gamma\tilde{\gamma}}\bar{q}_{\gamma'\tilde{\gamma}'}\ \langle \hat{c}^{\dagger}_{i,\tilde{\gamma}}\hat{c}^{\dagger}_{j,\tilde{\gamma}'}\rangle_0 + \bar{q}_{\gamma\tilde{\gamma}}q_{\gamma'\tilde{\gamma}'}\ \langle \hat{c}_{i,\tilde{\gamma}}\hat{c}_{j,\tilde{\gamma}'}\rangle_0\right),\end{aligned} \tag{A3}$$

where we have introduced for simplicity the index $\gamma = 1, 2, 3, 4$ which labels the four spin-orbital states (in the $l\sigma$ notation: $1\uparrow$, $1\downarrow$, $2\uparrow$, and $2\downarrow$). The second sum of equation (A3), which corresponds to the anomalous propagator, leads to the intersite pairing terms in the Gutzwiller effective Hamiltonian, as discussed below. The interaction term of Hamiltonian (2), which consists of only one-site operators, can be expressed by using the diagrammatic approach in the following way

$$\hat{\mathcal{H}}^{at} = L\sum_{I,I'} \bar{E}_{I,I'} \langle \hat{m}_{I,I'} \rangle_0, \tag{A4}$$

where $\hat{m}_{I,I'} \equiv |I\rangle\langle I'|$ and L is the number of atomic sites. The factors q and $\bar{q}$, as well as $\bar{E}_{I,I'}$, can be expressed with the use of the variational parameters $\lambda_{I,I'}$, the local single particle density matrix elements $\langle \hat{c}^{\alpha}_{il\sigma} \hat{c}^{\alpha'}_{il'\sigma'} \rangle_0$, and the matrix elements of the atomic part of (1) represented in the local basis, $\langle I | \hat{H}^{at} | I' \rangle$. Here $\hat{c}^{\alpha}_{il\sigma}$ represents either creation or annihilation operators. The explicit formulas for q, $\bar{q}$, and $\bar{E}_{I,I'}$ are provided in I.

By using (A3) and (A4) we can easily derive the expression for $\langle \hat{\mathcal{K}} \rangle_G$ which is given by (8) for the case of superconducting phase of type A, for which the q and $\bar{q}$ parameters fulfill the following relations

$$\begin{aligned} q_{l\sigma,l\sigma} &\equiv q, \\ \bar{q}_{2\sigma,1\sigma} &= -\bar{q}_{1\sigma,2\sigma} \equiv \bar{q}. \end{aligned} \tag{A5}$$

In (8) we have introduced the so-called renormalization factors which are defined by

$$\begin{aligned} Q &= q^2 - \bar{q}^2, \\ \tilde{Q} &= 2q\bar{q}. \end{aligned} \tag{A6}$$

Having the formula for $\langle \hat{\mathcal{K}} \rangle_G$ one can construct $\hat{\mathcal{K}}_{GA}$ and the final effective Hamiltonian (10) which is the subject of our analysis.

Appendix B. Diagonalization of the effective Hamiltonian

The effective Hamiltonian (9) transformed to the reciprocal space has the following form

$$\begin{aligned} \hat{\mathcal{K}}_{GA} &= \sum_{\mathbf{k}l\sigma} (Q\epsilon_{\mathbf{k}} - q^s\mu)\hat{n}_{\mathbf{k}l\sigma} + \sum_{\mathbf{k}ll'(l\neq l')\sigma} Q\epsilon_{\mathbf{k}12} \hat{c}^{\dagger}_{\mathbf{k}l\sigma} \hat{c}_{\mathbf{k}l'\sigma} \\ &\quad + \sum_{\mathbf{k}\sigma} \tilde{Q}\epsilon_{\mathbf{k}} (\hat{c}^{\dagger}_{\mathbf{k}1\sigma} \hat{c}^{\dagger}_{-\mathbf{k}2\sigma} + \hat{c}_{-\mathbf{k}2\sigma} \hat{c}_{\mathbf{k}1\sigma}) + L\sum_{I_1,I_4} \bar{E}_{I_1,I_4} \langle \hat{m}_{I_1,I_4} \rangle_0 \ , \end{aligned} \tag{B1}$$

where $\epsilon_{\mathbf{k}}$ is the bare band dispersion relation, which in our case corresponds to electrons on a square lattice with nearest neighbors hopping only

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y). \tag{B2}$$

The renormalization (Q) of the electron hopping, which is visible in the first two terms of the effective Hamiltonian, is caused by the interelectronic correlations. Moreover, within our approach an additional term appears which is also due to the correlation effect, and it corresponds to the intersite pairing—the third sum of equation (B1). One can see explicitly, that in the considered case the momentum dependence of the intersite component of the

superconducting gap is fully determined by the bare band dispersion relation $\epsilon_{\mathbf{k}}$, which leads to an extended s-wave symmetry. This comes as a result of the fact that the intersite pairing appears during the renormalization procedure (A3) of the electron hopping term from the initial Hamiltonian.

Transforming the complete effective Hamiltonian $\hat{K}_{\lambda}$, given by (10), to the reciprocal space one obtains

$$\begin{aligned}\hat{\mathcal{K}}_{\lambda} &= \hat{\mathcal{K}}_{GA} - \lambda_n\left(\sum_{\mathbf{kl}\sigma} q^s \hat{n}_{kl\sigma} - L\langle\hat{n}\rangle_G\right) \\ &\quad - \sum_{m=\pm 1}\left[\lambda_m\left(\sum_{\mathbf{k}}\hat{A}_{\mathbf{km}} - L\langle\hat{A}_m\rangle_0\right) + H.C.\right].\end{aligned} \tag{B3}$$

As it can be seen the intrasite pairing term from (10) leads to a momentum independent superconducting gap (s-wave symmetry). To diagonalize $\hat{\mathcal{K}}_{\lambda}$ we introduce the four-component representation of the single particle operators

$$\hat{f}^{\dagger}_{\mathbf{k}\sigma} = (\hat{c}^{\dagger}_{\mathbf{k}1\sigma}, \hat{c}^{\dagger}_{\mathbf{k}2\sigma}, \hat{c}_{-\mathbf{k}1\sigma}, \hat{c}_{-\mathbf{k}2\sigma}), \tag{B4}$$

and write down $\hat{\mathcal{K}}$ in the following manner

$$\begin{aligned}\hat{K}_{\lambda} &= \frac{1}{2}\sum_{\mathbf{k}\sigma}\hat{f}^{\dagger}_{\mathbf{k}\sigma}\hat{M}_{\mathbf{k}\sigma}\hat{f}_{\mathbf{k}\sigma} + 2\sum_{\mathbf{k}}\tilde{\epsilon}_{\mathbf{k}\sigma} + 2L\sum_{m=\pm 1}\lambda_m\langle\hat{A}_m\rangle_0 + L\lambda_n\langle\hat{n}\rangle_G \\ &\quad + L\sum_{I_1,I_4}\bar{E}_{I_1,I_4}\langle\hat{m}_{I_1,I_4}\rangle_0,\end{aligned} \tag{B5}$$

where $\hat{M}_{\mathbf{k}\sigma}$ is a 4 x 4 orthogonal matrix

$$\hat{M}_{\mathbf{k}\sigma} = \begin{pmatrix} \tilde{\epsilon}_{\mathbf{k}} & Q\epsilon_{\mathbf{k}12} & 0 & \Delta_{\mathbf{k}} \\ Q\epsilon_{\mathbf{k}12} & \tilde{\epsilon}_{\mathbf{k}} & -\Delta_{\mathbf{k}} & 0 \\ 0 & -\Delta_{\mathbf{k}} & -\tilde{\epsilon}_{\mathbf{k}} & -Q\epsilon_{\mathbf{k}12} \\ \Delta_{\mathbf{k}} & 0 & -Q\epsilon_{\mathbf{k}12} & -\tilde{\epsilon}_{\mathbf{k}} \end{pmatrix}. \tag{B6}$$

In the above expression we have introduced the following notation

$$\tilde{\epsilon}_{\mathbf{k}} = Q\epsilon_{\mathbf{k}} - q^s(\mu + \lambda_n)\ , \tag{B7}$$

$$\Delta_{\mathbf{k}} = \Delta^{(0)} + \Delta^{(1)}(\cos k_x + \cos k_y), \tag{B8}$$

where $\Delta^{(0)} \equiv \lambda_1 = \lambda_{-1}$ (as we are considering an ESP state), which has an interpretation of the intrasite gap parameter, while $\Delta^{(1)} \equiv 2\tilde{Q}t$ is the intersite pairing amplitude. In this manner, we have obtained a mixture of the s-wave and the extended s-wave pairing symmetry. By diagonalizing (B6) one obtains the quasiparticle eigen-energies in the paired states

$$E^{SC}_{\mathbf{k}} = \pm\sqrt{\tilde{\epsilon}^2_{\mathbf{k}} + \Delta^2_{\mathbf{k}}} + Q\left|\epsilon_{\mathbf{k}12}\right|, \tag{B9}$$

which correspond to quasiparticle (+) and quasihole (−) excitations. These renormalized quasiparticle energies represent the input quantities to construct the free energy functional of the Landau type (cf I) and carry out the minimization procedure with respect to all mean field,

variational and Lagrange parameters in order to determine the equilibrium properties and the phase diagram discussed in the main text.

References

[1] Mackenzie A P and Maeno Y 2003 *Rev. Mod. Phys.* **75** 657
[2] Rice T M and Sigrist M 1994 *J. Phys.: Condens Matter* **7** L643
[3] Saxena S S *et al* 2000 *Nature* **406** 587
[4] Huxley A, Sheikin I, Ressouche E, Kemovanois N, Braithwaite D, Calemczuk R and Flouquet J 2001 *Phys. Rev.* B **63** 144519
[5] Tateiwa N, Kobayashi T C, Hanazono K, Amaya K, Haga Y, Settai R and Onuki Y 2001 *J. Phys.: Condens. Matter* **13** 117
[6] Dai X, Fang Z, Zhou Y and Zhang F-C 2008 *Phys. Rev. Lett* **101** 057008
[7] Lee P A and Wen X-G 2008 *Phys. Rev.* B **78** 144517
[8] Anderson P W and Brinkman W F 1973 *Phys. Rev. Lett.* **30** 1108
[9] Anderson P W and Brinkman W F 1978 *The Physics of Liquid and Solid Helium: Part 2 (Interscience Monographs and Texts in Physics and Astronomy)* ed K H Bennemann and J B Ketterson (New York: Wiley) pp 177–286
[10] Pines D and Alpar A 1985 *Nature* **316** 27
[11] Fay D and Appel J 1980 *Phys. Rev.* B **22** 3173
[12] Mazin I I and Singh D I 1997 *Phys. Rev. Lett.* **79** 733
[13] Spałek J 2001 *Phys. Rev.* B **63** 104513
[14] Klejnberg A and Spałek J 1999 *J. Phys.: Condens. Matter* **11** 6553
[15] Han J E 2004 *Phys. Rev.* B **70** 054513
[16] Sakai S, Arita R and Aoki H 2004 *Phys. Rev.* B **70** 172504
[17] Puetter C M and Kee H-Y 2012 *Eur. Phys. Lett.* **98** 27010
[18] Takimoto T 2000 *Phys. Rev.* B **62** R14641
[19] Koikegami S, Yoshida Y and Yanagisawa T 2003 *Phys. Rev.* B **67** 134517
[20] Zegrodnik M and Spałek J 2012 *Phys. Rev.* B **86** 014505
[21] Annett J F, Györffy B L, Litak G and Wysokiński K I 2003 *Eur. Phys. J.* B **36** 301
Annett J F, Györffy B L and Wysokiński K I 2009 *New J. Phys.* **11** 055063
Wysokiński K I, Annet J F and Györffy B L 2012 *Phys. Rev. Lett.* **108** 1077004
[22] Zegrodnik M, Spałek J and Bünemann J 2013 *New J. Phys.* **15** 073050
[23] Griffith J S 1971 *The Theory of Transition-Metal Ions* (New York: Cambridge University Press)
[24] Kohn W and Luttinger J M 1965 *Phys. Rev. Lett.* **15** 524
[25] Cherng R W, Refael G and Demler E 2007 *Phys. Rev. Lett.* **99** 130406
[26] Gorshkov A V, Hermele M, Gurarie V, Xu C, Julienne P S, Ye J, Zoller P, Demler E, Lukin M D and Rey A M 2010 *Nat. Phys.* **6** 289
[27] Wu C, Hu J and Zhang S-C 2009 *Int. J. Mod. Phys.* B **24** 311
[28] Kaczmarczyk J, Spałek J, Schickling T and Bünemann J 2013 *Phys. Rev.* B **88** 115127
[29] Scalpino D 2012 *Rev. Mod. Phys.* **84** 1383
[30] Lee P A, Nagaosa N and Wen X-G 2006 *Rev. Mod. Phys.* **78** 17
[31] Dirac P A M 1958 *The Principles of Quantum Mechanics* 4th edn (Oxford: Clarendon)
[32] Klejnberg A and Spałek J 1998 *Phys. Rev.* B **57** 12041
[33] Bünemann J, Weber W and Gebhard F 1998 *Phys. Rev.* B **57** 6896
[34] Jędrak J and Spałek J 2011 *Phys. Rev.* B **83** 104512
[35] Jędrak J and Spałek J 2010 *Phys. Rev.* B **81** 073108

[36] Kaczmarczyk J and Spałek J 2011 *Phys. Rev.* B **84** 125140
[37] Jędrak J, Kaczmarczyk J and Spałek J 2010 arXiv:1008.0021
[38] Spałek J and Zegrodnik M 2013 *J.Phys.: Condens. Matter* **25** 435601
[39] Bünemann J, Gebhard F, Ohm T, Weiser S and Weber W 2005 *Frontiers in Magnetic Materials* (Berlin: Springer)