Coexistent spin-triplet superconducting and ferromagnetic phases induced by the Hund’s rule coupling and electronic correlations II: Effect of applied magnetic field

M. Fidrysiak,1 D. Goc-Jaglo,1 E. Kądzielawa-Major,1 P. Kubiczek,2 and J. Spalek1

1Marian Smoluchowski Institute of Physics, Jagiellonian University, ul. Łojasiewicza 11, 30-348 Kraków, Poland
2I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany

Recently proposed local-correlation-driven pairing mechanism, describing coexisting ferromagnetic phases (FM1 and FM2) and spin-triplet superconductivity (SC) within a single model, based on electronic correlations in an orbitally degenerate Anderson lattice, is extended to situation with an applied magnetic field. The model provides and rationalizes in a semiquantitative manner the principal features of the phase diagram observed for UGe2 in the field absence [cf. Phys. Rev. B 97, 224519 (2018)]. As spin-dependent effects play a crucial role for both ferromagnetic and SC phases, the role of the Zeeman field is to single out different stable spin-triplet SC phases. This analysis should thus be helpful in testing the present real-space pairing mechanism, which can be regarded as complementary to that relevant for the spin-triplet superfluid $^3$He and based on spin-fluctuation theory. Specifically, we demonstrate that the presence of the two phases FM1 and FM2, and associated field-driven metamagnetic transitions between them, induce corresponding metasuperconducting phase transformations of the same type. At the end, we discuss briefly how the spin fluctuations can be incorporated as a next step into the considered here renormalized quasiparticle picture.

I. INTRODUCTION

The discovery of the spin-triplet superconductivity (SC) inside ferromagnetic (FM) phases of uranium compounds UGe$_2$, URhGe, UCoGe, and Ui is directly related to the question of pairing mechanism and the order-parameter symmetry under such circumstances. Due to substantial correlations in the $f$-electron sector, the situation here differs from that for superfluid $^3$He, where a normal (nonmagnetic) Landau-Fermi liquid is unstable against the formation of a pure spin-triplet paired state induced by quantum spin fluctuations in such a weakly correlated quantum fluid below the FM Stoner instability. The uranium compounds may be regarded as those among the first solid state systems with a clear spin-triplet pairing, as the strong effective molecular field acting on spin degrees of freedom in FM phase, at least for UGe$_2$, rules out any spin-singlet SC. Therefore, it is important to see if different phases (A, A$_1$, A$_2$, and B) may still appear in an applied magnetic field, in direct correspondence to those observed in $^3$He. Yet, the SC states in the present situation are intertwined with two FM states, FM1 and FM2, so we would like to single out the different coexisting phases. In brief, the pairing mechanism and order-parameter symmetry for uranium superconductors are yet to be determined in joint theoretical and experimental effort. Here we explicitly identify the possible SC states within the FM and paramagnetic (PM) phases.

Recently, we have proposed that the pairing in UGe$_2$ emerges due to the combined effect of FM exchange interaction (the Hund’s rule coupling) combined with inter-electronic correlations. Ref. [12] is regarded as Part I of our analysis of UGe$_2$ properties. The spin-paired A$_1$ state proved to be the dominant phase there with the pair spins opposite to those of average spin polarization, a natural feature in appearing then half-metallic state. Remarkably, within the approach, the A$_1$ phase emerges in a discontinuous manner at the metamagnetic transition between the two distinct FM phases (FM2 $\rightarrow$ FM1), as is evidenced in the recent specific-heat measurements. Finally, SC practically disappears at the boundary of PM transition, which requires invoking a strongly anisotropic and pressure-dependent form of spin-fluctuation spectrum to explain the character of SC state in terms of pairing by long-wavelength FM excitations. Within our correlation- and exchange-driven pairing scheme all the above features are explained in a unified manner, as both the ferromagnetism and pairing are directly connected and driven by the real-space correlations of the same origin. The changes of applied pressure are theoretically mimicked by us by varying the hybridization magnitude between the localized U 5$f$ and conduction electrons, and regarded as the primary factor inducing the observed evolution.

Studies of the ground state properties as a function of pressure alone are, however, insufficient to discuss fully the relevance of real-space correlation-driven pairing mechanism. This is due to the availability of extensive experimental data covering SC and magnetic properties of UGe$_2$ in the three-dimensional parameter space spanned by pressure, temperature, and applied magnetic field. In particular, any proposed pairing mechanism should minimally be tested against the sequence of metamagnetic and metasuperconducting transitions along the first-order line in the field-pressure plane. In this paper we carry out this program and investigate possible spatially homogeneous phases in the Zeeman magnetic field. The resultant phase diagram agrees well with available data close to the pressure-induced magnetic transitions. We also provide model band structure in the correlated state, as well as other characteristics, such as the $f$-level filling.
in the coexisting phases. The last characteristic points to the almost localized nature of the two of $5f$ electrons out of three of the $U^{3+}$ ions and one itinerant, originating from the suggested by us orbital-selective $5f^3 \rightarrow 5f^2$ ($U^{3+} \rightarrow U^{4+}$) valence transition. As a reference point, we provide the ground-state results within a more general variational scheme in zero applied magnetic field and discuss its subsequent simplification (cf. Appendix A). At the end, we outline possible extensions of our approach to incorporate both the full Gutzwiller-type projection (cf. Appendix A) and the long-wavelength quantum spin fluctuations (cf. Appendix B).

II. MODEL AND METHOD

We start from the four-orbital degenerate Anderson lattice model, formulated in the real-space language, that takes the form

\[
\mathcal{H} - \mu \hat{N}_e = \sum_{ij\sigma} t_{ij} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + V \sum_{i\sigma} \left( \hat{f}^{\dagger}_{i\sigma} \hat{f}_{i\sigma} + \text{H.c.} \right) + \epsilon f_{i} \sum_{i} \hat{n}^{f}_{i} + U \sum_{i} \hat{n}^{f}_{i} \hat{n}^{f}_{i} + U' \sum_{i} \hat{n}^{f,\dagger}_{i} \hat{n}^{f,\dagger}_{i} - 2J \sum_{i} \left( \hat{S}^{f}_{i} \cdot \hat{S}^{f,\dagger}_{i} + \frac{1}{4} \hat{n}^{f,\dagger}_{i} \hat{n}^{f,\dagger}_{i} \right) - \mu \hat{N}_e, \tag{1}
\]

where $\mu$ is the chemical potential for $N_e$-electron $N$-site system, $\hat{f}^{\dagger}_{i\sigma}$ ($\hat{f}^{\dagger}_{i\sigma}$) is the creation (annihilation) operator of $f$ electron on orbital with $l = 1, 2$ on site $i$ and spin $\sigma = \uparrow, \downarrow$, hybridized with two species of conduction electrons characterized by the corresponding operators $\hat{c}^{\dagger}_{i\sigma}$ and $\hat{c}_{i\sigma}$. Additionally, $\hat{n}^{f}_{i} \equiv \hat{f}^{\dagger}_{i\sigma} \hat{f}^{\dagger}_{i\sigma}$ is the particle number operator for $f$ electrons in the original local state $|i\sigma\rangle$ and $\hat{S}^{f} \equiv \left( \hat{S}^{f}_{i\uparrow} + \hat{S}^{f}_{i\downarrow} \right)$ is the spin operator of $f$ electron on orbital $|i\rangle$. In this minimal model the first term represents the $c$-electron hopping, the second an intraatomic hybridization between the subsystems of $f$ and $c$ states; the third is the starting bare atomic $f$-level energy relative to the center of the conduction band. The next two terms express, respectively, the intraorbital and interorbital Coulomb interactions (both of intraatomic nature), whereas the third is ferromagnetic (Hund’s rule) exchange interaction between $f$ electrons. This model has been used by us before to explain the magnetic properties, including classical and quantum criticalities, as well as zero-field SC properties of UGe$_2$.

Here we extend this approach with a detailed analysis of the coexisting magnetic and SC properties in applied Zeeman field, as well determine the phase boundaries between them. Note that in applied field two terms should be added to Eq. (1):

\[
-g_1 \mu_0 H \sum_i S_i^z \text{ and } -g_2 \mu_0 H \sum_i S_i^z \text{ for } f \text{ and } c \text{ electrons, respectively, where } g_1 \text{ and } g_2 \text{ are gyromagnetic factors, } \mu_0 \text{ denotes material permeability, and } S_i^z \text{ is the z-th spin component for } c \text{ electron. Hereafter, for simplicity, we take } g_f = g_c = g \text{ and introduce reduced field } h = \mu_0 \mu_B H / 2. \text{ Moreover, we include only nearest- and next-nearest neighbor hoppings } t < 0 \text{ and } t' < 0.25|t|, \text{ respectively, and set } U' = U - 2J. \text{ The total electron filling is taken as } n^{\text{tot}} = 3.25. \text{ Such a choice yields, at zero field, the sequence of magnetic and SC states that match the experimental phase diagram of UGe$_2$.

The model (1) is solved within the statistically-consistent Gutzwiller approximation (SGA) that, at zero-temperature, is equivalent to optimization of the energy functional $E_G \equiv \langle \Psi_0 | \mathcal{G} \hat{H} \mathcal{G}^\dagger | \Psi_0 \rangle / \langle \Psi_0 | \mathcal{G}^\dagger \mathcal{G} | \Psi_0 \rangle$ over Slater determinant $|\Psi_0\rangle$ and the set of variables controlling the operator $\hat{P}_G \equiv \prod_{i\alpha} \hat{P}_G_{i\alpha}$ with $\hat{P}_{G\alpha} = \hat{n}_{i\alpha} - n^{(1)}_{i\alpha}$, $n^{(1)}_{i\alpha} = \langle \Psi_0 | \hat{n}_{i\alpha} | \Psi_0 \rangle$. Since the correlations are most prominent in the $f$-electron sector, we take $x^{(f)} = x^{(\uparrow)} = x$ and $x^{(c)} = x^{(\downarrow)} = 0$. In the following we thus skip the orbital indices for the $\lambda$ coefficients as they refer now exclusively to equivalent $f$ orbitals.

Explicitly (for infinite coordination number and non-zero applied Zeeman field), we obtain

\[
E_G = \sum_{ij\sigma} t_{ij} \langle \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} \rangle + V \sum_{i\sigma} g_\sigma \left( \langle \hat{f}^{\dagger}_{i\sigma} \hat{f}_{i\sigma} \rangle + \text{c.c.} \right) + \sum_{i\sigma} \left[ |U' g_\sigma + (U' - J) g_{2\sigma}| \langle \hat{f}^{\dagger}_{i\sigma} \hat{f}^{\dagger}_{i\sigma} \rangle \right]^2 + \sum_{i\sigma} \left[ -2J \langle \hat{S}^{f^{(1)}\dagger}_{i} \rangle \langle \hat{S}^{f^{(2)}\dagger}_{i} \rangle + (U' - \frac{J}{2}) \langle n^{f^{(1)}\dagger}_{i\uparrow} \rangle \langle n^{f^{(2)}\dagger}_{i\uparrow} \rangle + \sum_{i\sigma} \langle \epsilon^{f} - h \hat{S}^{f}_{i\sigma} \rangle \langle \hat{n}^{f}_{i\sigma} \rangle + U \sum_{i\sigma} \hat{A}^{f}_{i\sigma} \langle \hat{n}^{f}_{i\sigma} \rangle \langle \hat{n}^{f}_{i\sigma} \rangle - h \sum_{i\sigma} \sigma \langle \hat{n}^{c}_{i\sigma} \rangle, \tag{2}
\]

where the renormalization factors

\[
\begin{align*}
g_{1\sigma} & = 2(\lambda^{f}_{\uparrow} - \lambda^{f}_{\downarrow}) \cdot (\lambda^{f}_{\sigma} + \lambda^{f}_{\sigma} - \lambda^{f}_{\sigma}) \langle n^{f}_{\sigma} \rangle \langle n^{f}_{\sigma} \rangle, \\
g_{2\sigma} & = (\lambda^{f}_{\uparrow} - \lambda^{f}_{\downarrow})^2 \cdot \langle n^{f}_{\sigma} \rangle^2 + (\lambda^{f}_{\sigma} + \lambda^{f}_{\sigma})^2 \langle n^{f}_{\uparrow} \rangle^2, \\
g_{0\sigma} & = \lambda^{c}_{\sigma} - \lambda^{c}_{\sigma} \cdot \lambda^{c}_{\sigma} \cdot \lambda^{c}_{\sigma} \times \langle n^{c}_{\sigma} \rangle \tag{3}
\end{align*}
\]
appear in response to local electronic correlations \((\bar{\sigma} \equiv -\sigma)\).  

Optimization of \(E_G\) over wave function \(|\Psi_0\rangle\) yields an effective non-linear Schrödinger equation \(\mathcal{H}_{\text{eff}} |\Psi_0\rangle = E |\Psi_0\rangle\) with

\[
\mathcal{H}_{\text{eff}} = \sum_{\mathbf{k}, \sigma} \Psi^\dagger_{\mathbf{k} \sigma} \begin{pmatrix} \epsilon_{\mathbf{k} \sigma} & 0 & q_{\mathbf{\sigma}} V & 0 \\ 0 & -\epsilon_{\mathbf{k} \sigma} & 0 & -q_{\mathbf{\sigma}} V \\ q_{\mathbf{\sigma}} V & 0 & \epsilon^f_{\mathbf{\sigma}} & \Delta_{\sigma, \sigma}^f \\ 0 & -q_{\mathbf{\sigma}} V & \Delta_{\sigma, \sigma}^f & -\epsilon^f_{\mathbf{\sigma}} \end{pmatrix} \Psi_{\mathbf{k} \sigma} + E_0,
\]

expressed in terms of Nambu spinor \(\Psi_{\mathbf{k} \sigma} \equiv \left(\hat{c}_{\mathbf{k} \sigma}^\dagger, \hat{c}_{-\mathbf{k} \sigma}^\dagger, \hat{\bar{f}}_{\mathbf{k} \sigma}^\dagger, \hat{\bar{f}}_{-\mathbf{k} \sigma}^\dagger\right)\). Here

\[
\epsilon_{\mathbf{k} \sigma} = 2t [\cos(k_x) + \cos(k_y)] + 4t' \cos(k_x) \cos(k_y) - \mu - h\sigma
\]

is Zeeman-split tight-binding dispersion relation for bare conduction electrons,

\[
\epsilon^f_{\sigma} = \frac{\partial E_G}{\partial n_i^{(1)}} = \epsilon^f + U \lambda x_i n_i^{(1)} + (U' - J) n_i^{(2)} + U' n_i^{(2)}
\]

\[
+ \left(\frac{\partial g_{\sigma}}{\partial n_i^{(1)}} V \sum_i \langle \hat{f}_{i \sigma}^\dagger \hat{\bar{f}}_{i \sigma} \rangle_0 + \text{c.c.} \right) + \left(\frac{\partial g_{\sigma}}{\partial n_i^{(1)}} U' + \frac{\partial g_{\sigma}}{\partial n_i^{(1)}} (U' - J) \right) |\langle \hat{f}_{i \sigma}^\dagger \hat{\bar{f}}_{i \sigma} \rangle_0|^2
\]

\[- \mu - h\sigma
\]

denotes renormalized \(f\)-electron level, and \(E_0\) is an energy shift (that does not influence expectation values but contributes to the ground state energy). The effective gap parameter, \(\Delta_{\sigma, \sigma}^f\), is obtained from the relation

\[
\Delta_{\sigma, \sigma}^f = \frac{\partial E_G}{\partial \langle \hat{f}_{i \sigma}^\dagger \hat{\bar{f}}_{i \sigma} \rangle_0} = -[g_{\sigma} U' + g_{2\sigma} (U' - J)] \times \langle \hat{f}_{i \sigma}^\dagger \hat{\bar{f}}_{i \sigma} \rangle_0.
\]

The resulting integral Schrödinger-type equation is solved numerically in the loop with minimization of the energy functional [Eq. (2)] over the correlator parameter \(x\). In order to avoid finite-size effects that become severe for weak SC order considered here (in accordance with Anderson criterion), we performed the calculations directly in the thermodynamic limit using adaptive integration.

A methodological remark is in place at this point. The above scheme employs correlator \(\bar{P}_T\) that acts separately on each orbital. In a multi-band system, such as the one considered here, one could expect that the correlator should allow for more general many-body states involving multiple orbitals at once. Such an extension makes it difficult to achieve numerical accuracy required to study SC order emerging on the scale of the order of one Kelvin in uranium materials. We have, nonetheless, performed such an extended analysis for zero field and limited range of model parameters with the results very close to those obtained from the simplified scheme. The discussion of those formal issues is deferred to Appendix [A].

III. RESULTS AND DISCUSSION

A. Zero-field results as a reference point

The SC pairing discussed here is of local interorbital nature, i.e., of odd parity in the orbital and even in the spin indices, as was discussed before. In Fig. 1(a) we draw schematically the sequence of phases obtained for zero applied field. The three SC phases are labeled in a similar manner as those for the case of superfluid \(^3\)He, with \(A_1\) being the polarized phase with the parallel spins (\(\uparrow\uparrow\) only), \(A_2\) phase is that with unequal order parameter amplitudes \((\uparrow\uparrow)\) and \(\downarrow\downarrow\), which finally equalize in the coexistent PM and \(A\) phase. Formally, the above SC states are characterized by non-vanishing anomalous amplitudes detailed in Table I. The coexistent phase \(FM_1 + A_1\) is the most recent, followed by the \(A_2\) phase. At a very minor, if not negligible role in the field ab-
sence. We emulate varying external pressure by the corresponding change in hybridization magnitude (for a detailed discussion of this particular point see Part I and Ref.\textsuperscript{19}). As we show below, the role of the field is to enhance the presence of $A_2$ phase.

For the sake of completeness, we provide in Table I\textsuperscript{11} selected numerical values of the effective SC gap parameters for $H = 0$ in the $A_1$, $A_2$, and $A$ phases. They are defined as partial derivatives of the variational functional with respect to anomalous amplitudes [cf. Eqs.\textsuperscript{7}, \textsuperscript{A17}, and \textsuperscript{A18}] and physically determine the spectrum of projected quasiparticle excitations.\textsuperscript{23} As the SC transition sequence $A_2 \to A_1 \to A$ takes place simultaneously with the corresponding discontinuous magnetic transitions (FM2$\to$FM1 and FM1$\to$PM), they are also discontinuous, but probably too weak to be detected experimentally (note that the maximal value of the SC transition temperature does not exceed 1 K in all uranium systems).\textsuperscript{11,12} However, we obtain a clear sign of metastable $\text{metasupercconducting}$ transition accompanying the corresponding metamagnetic jumps. This issue is discussed next.

### B. Discontinuous phase transition in an applied magnetic field

In Fig. 2(a) we have drawn schematically the sequence of appearing phases with the increasing applied field, starting from the most prominent FM1$\to$A$_1$ coexistent phase. In the present case ($H \neq 0$), the terminal state is always pure high-moment FM2. To illustrate the situation quantitatively, we have plotted in Fig. 2(a)-(c) the total magnetic moment $m^{\text{tot}} = m^i + m^c$ (a) and superconducting gap components (b) and (c)] as a function of hybridization magnitude. Solid lines correspond to applied field $h/|t| = 0.002$, whereas the dashed lines represent the zero-field situation. Shifts of the phase transition points in non-zero magnetic field can be clearly seen. The set of microscopic parameters is: $U/|t| = 3.5$, $J/|t| = 1.1$, $T = 0$ K, $t/|t| = 0.25$, $\epsilon^f/|t| = -4$, $n^{\text{tot}} \equiv n^i + n^c = 3.25$, and the field $h = \frac{1}{2}g\mu_BHz = 0.002|t|$, which corresponds to $\mu_0H = 6.9$ T in physical units if the nearest-neighbor hopping is taken $|t| = 0.2$ eV.

![FIG. 2. (a) Total magnetization, $m^{\text{tot}} = m^i + m^c$ (a) and superconducting gap components (b) and (c)] as a function of hybridization magnitude. Solid lines correspond to applied field $h/|t| = 0.002$, whereas the dashed lines represent the zero-field situation. Shifts of the phase transition points in non-zero magnetic field can be clearly seen. The set of microscopic parameters is: $U/|t| = 3.5$, $J/|t| = 1.1$, $T = 0$ K, $t/|t| = 0.25$, $\epsilon^f/|t| = -4$, $n^{\text{tot}} \equiv n^i + n^c = 3.25$, and the field $h = \frac{1}{2}g\mu_BHz = 0.002|t|$, which corresponds to $\mu_0H = 6.9$ T in physical units if the nearest-neighbor hopping is taken $|t| = 0.2$ eV.\textsuperscript{23} As the SC transition sequence $A_2 \to A_1 \to A$ takes place simultaneously with the corresponding discontinuous magnetic transitions (FM2$\to$FM1 and FM1$\to$PM), they are also discontinuous, but probably too weak to be detected experimentally (note that the maximal value of the SC transition temperature does not exceed 1 K in all uranium systems).\textsuperscript{11,12} However, we obtain a clear sign of metastable $\text{metasupercconducting}$ transition accompanying the corresponding metamagnetic jumps. This issue is discussed next.

### B. Discontinuous phase transition in an applied magnetic field

In Fig. 2(b) we have drawn schematically the sequence of appearing phases with the increasing applied field, starting from the most prominent FM1$\to$A$_1$ coexistent phase. In the present case ($H \neq 0$), the terminal state is always pure high-moment FM2. To illustrate the situation quantitatively, we have plotted in Fig. 2(a)-(c) the total magnetic moment $m^{\text{tot}} = m^i + m^c$ (a) and superconducting gap components (b) and (c)] as a function of hybridization magnitude. Solid lines correspond to applied field $h/|t| = 0.002$, whereas the dashed lines represent the zero-field situation. Shifts of the phase transition points in non-zero magnetic field can be clearly seen. The set of microscopic parameters is: $U/|t| = 3.5$, $J/|t| = 1.1$, $T = 0$ K, $t/|t| = 0.25$, $\epsilon^f/|t| = -4$, $n^{\text{tot}} \equiv n^i + n^c = 3.25$, and the field $h = \frac{1}{2}g\mu_BHz = 0.002|t|$, which corresponds to $\mu_0H = 6.9$ T in physical units if the nearest-neighbor hopping is taken $|t| = 0.2$ eV.

![FIG. 2. (a) Total magnetization, $m^{\text{tot}} = m^i + m^c$ (a) and superconducting gap components (b) and (c)] as a function of hybridization magnitude. Solid lines correspond to applied field $h/|t| = 0.002$, whereas the dashed lines represent the zero-field situation. Shifts of the phase transition points in non-zero magnetic field can be clearly seen. The set of microscopic parameters is: $U/|t| = 3.5$, $J/|t| = 1.1$, $T = 0$ K, $t/|t| = 0.25$, $\epsilon^f/|t| = -4$, $n^{\text{tot}} \equiv n^i + n^c = 3.25$, and the field $h = \frac{1}{2}g\mu_BHz = 0.002|t|$, which corresponds to $\mu_0H = 6.9$ T in physical units if the nearest-neighbor hopping is taken $|t| = 0.2$ eV.

| \(V/t\) | $100 \times \Delta_{ff}^{(1)}/|t|$ | $100 \times \Delta_{ff}^{(2)}/|t|$ | $100 \times \Delta_{ff}^{(3)}/|t|$ |
|--------|----------------|----------------|----------------|
| 1.1666667 | 0.0000000 | 0.0000000 | 0.0000000 |
| 1.3000000 | 0.0038378 | 0.0000000 | 0.0000012 |
| 1.3333333 | 0.0225363 | 0.0000000 | 0.0000012 |
| 1.4000000 | 0.5660415 | 0.0001295 | 0.0000013 |
| 1.4500000 | 5.8775861 | 0.0000000 | 0.0000014 |
| 1.5000000 | 5.182010 | 0.0000000 | 0.0000014 |
| 1.5500000 | 4.5934998 | 0.0000000 | 0.0000013 |
| 1.6000000 | 4.0906100 | 0.0000000 | 0.0000013 |
| 2.0000000 | 1.8155386 | 0.0000000 | 0.0000012 |
| 2.5000000 | 0.7775326 | 0.0000000 | 0.0000011 |
| 3.0000000 | 0.3706006 | 0.0000000 | 0.0000011 |
| 3.5000000 | 0.1909743 | 0.0000000 | 0.0000010 |
| 4.0000000 | 0.104818 | 0.0000000 | 0.0000010 |
| 4.1000000 | 0.087245 | 0.0000000 | 0.0000010 |
| 4.2000000 | 0.816905 | 0.0000000 | 0.0000011 |
| 4.2500000 | 0.735644 | 0.0000000 | 0.0000010 |
| 4.4000000 | 0.568509 | 0.0000000 | 0.0000010 |
| 5.0000000 | 0.206255 | 0.206256 | 0.0000010 |
Orbital occupancy

$\text{Orbital occupancy}$

$\text{Orbital occupancy}$

$|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|$ $|t|
The slightly different magnitudes of the characteristic transition field $\mu_0 H_x$ in the vicinity of the FM2-FM1 metamagnetic instability for $H = 0$. The weak discontinuity may be detected by the magnetic susceptibility measurements across the boundary for fixed pressure ($V/t$ ratio).

In summary, the observed SC discontinuities in an applied magnetic field are relatively small. However, with the help of sensitive magnetic measurements of $\chi$ susceptibility, they may be relatively easy to detect. Also, the appearance of the second component of the SC gap at the $A_1 \rightarrow A_2$ transition may become detectable in the pair tunneling spectroscopy.

C. Electronic structure

FM and SC phase transitions have a strong impact on the electronic (renormalized-band) structure. Particularly interesting is the situation near the boundary between FM2-A2 and FM1-A1 states. To elucidate the changes on both sides of the transition, in Figs. 3 and 4 we have drawn an exemplary structure along the high-symmetry lines just below ($V/t = 1.26$) and just above that value ($V/t = 1.262$) for the field value $h = 2 \cdot 10^{-3}|t|$. The slightly different magnitudes of $V$ are selected to vi-
sualize the situation on both sides of the discontinuous FM1→FM2 transition. The spin subbands with domi-
nant $f$ character are drawn in blue. The spin splitting is induced mainly by the Hund’s rule and on-site repulsion $U$ (the effects of applied field and pairing are of minor importance). Remarkably, the $c$ electrons (marked in red in the lower panel) exhibit also a comparable spin splitting. This effect is caused by the circumstances that the $c$ electrons are hybridized with their $f$ electron partners and, therefore, the Hund’s rule interaction is transmuted from $f$- to $c$-system. Note that the occupancy of each of $f$ orbitals is $n_f^+ = 1 \pm \delta$, with $\delta \ll 1$ [cf. Fig. 4(b)], where the small portion $\delta$ comes from the upper spin subband which crosses the Fermi (zero-energy level) near $\Gamma$ point. This is explicitly visualized on the density of states (right panel), where the $f \downarrow$ subband barely touches the Fermi energy and the majority spin subband is practically filled. So, to a good accuracy, the system is a half metal with pre-
dominant spin-minority carriers at the Fermi level. This is the reason why the $A_2$ phase is stable then and with the amplitudes $\Delta_{\uparrow\uparrow} \gg \Delta_{\uparrow\downarrow}$. The situation turns into an extreme case, with only $\Delta_{\uparrow\uparrow} \neq 0$ in the FM1 + $A_1$ phase. The latter result rationalizes nicely the related observation in $H = 0$ situation. Note, however, that the exact half-metallic behavior, obtained in the present model, might be obscured in the real material by other bands that are weakly coupled to the considered $f$-$c$ sub-
system.

D. Effect of spin fluctuations (tentative)

Our present approach, based on first nontrivial order (SGA) of treating the interelectronic correlations on lo-
cal scale, cannot explain enhanced residual specific heat appearing at temperatures well below $T_c$ in UGe$_2^{14}$ as well as the strong effective mass enhancement at the FM1→FM2 transition there $^{14,28}$ Additionally, NQR relaxation with an anomalous temperature dependence takes place at the FM to PM transition at low temperature. $^{29}$ All these features may be explained qualitatively in terms of FM spin fluctuations. Whereas the overall features of a transition from non-unitary to uni-
tary SC are well reproduced by our phase diagram (also for UTe$_2$, cf. Ref. $^{27}$), the long-wavelength fluctuations should be included, particularly for low-moment systems UCoGe and Uf. A general way to extend our work is as follows. We start from the effective Hamiltonian $^{[1]}$, but with renormalized microscopic parameters $U\lambda_{\uparrow\downarrow}^2$ and $Jg_{2\sigma}$ [cf. Eq. $^{[2]}$], and proceed with the Hubbard-Stratonovich transformation, as outlined in Appendix $^{[3]}$ for the case of FM state. To include fluctuations of the SC order parameter, one should include also the bilin-
ear representation of the spin part $\sim Jg_{2\sigma}$, derived in Ref. $^{[28]}$. This type of approach would introduce spin-fluctuations into the picture of electronic states renormal-
ized by local correlations. However, a quantitative im-
plementation of this program is quite cumbersome, as it requires computation of renormalized coupling constants at each stage of the analysis, before and after including the fluctuations in each order. Nonetheless, we believe that such a solution is possible to tackle, as the renor-
malized coupling parameters are reduced in the process already at the level of SGA. It is tempting to suggest that the effective picture should be not far away from that based on $1/N$ expansion with effective parameters $U$ and $J$ (cf. Appendix $^{[4]}$. $^{29}$ We should see the progress along these lines (including SC fluctuations) in near fu-
ture.

IV. OUTLOOK

In the preceding paper $^{12}$ regarded here as Part I, we have constructed a fairly complete zero-magnetic-field phase diagram composed of spin-triplet paired states co-
existing with the ferromagnetic FM1 and FM2 phases. The $A_2$ and $A$ SC states appear in the field absence only with very small amplitudes. In the present work we have shown that the applied magnetic field allows for fine tuning of those phases and is likely to make them observable. In this manner, one can detect the phases analogous to those seen clearly only for the superfluid $^3$He. $^{29}$ However, in distinction to $^3$He, here the pairing is of $s$-wave character, i.e., with intraatomic spin-triplet and the orbital singlet to make the wave function of the local pair antisymmetric. It should be emphasized that this picture holds here for moderately correlated systems, in which the pairing is induced by the Hund’s rule com-
bined with the short-range intraatomic interaction. In the strong-correlation limit, this type of pairing would take the form of the intersite (real-space) character with either spin-triplet or spin-singlet nature, depending on the band filling $^{30,33}$

The principal result of this and the preceding $^{12}$ work is to describe, within a single (orbitally degenerate) Anderson lattice model, coexistent FM and spin-triplet SC phases. In this way, we extend the well established ap-
proaches to correlated normal and magnetic systems $^{23}$ to the description of the SC states coexisting with them. It must be emphasized that such a renormalized mean field theory may be generalized to a more involved systematic diagrammatic expansion, DE-GWF $^{32,33}$ However, such an approach becomes quite involved in the multi-orbital situation, particularly for multiple coexisting phases $^{33,34}$ Inclusion of higher-order correlations introduces then an additional admixture of intersite correlations to the pairing. This will be an objective of a separate study.

Even though the present approach provides a semi-
quantitative description of the coexistent phases (cf. Fig. 1 in Ref. $^{12}$ and Fig. 3 here), one important ingredi-
eut of the theoretical picture is still missing. Namely, the incorporation of the quantum spin fluctuations into our correlated-system picture. This is, again, not easy task and most of the recent approaches start by introducing effective paramagnon-electron coupling through dynam-
FIG. 8. Renormalized band structure for $h/|t| = 0.002$ and $V/t = 1.26$ in the FM$_2+A_2$ phase (set of other parameters: $U/|t| = 3.5$, $J'/|t| = 1.1$, $T = 0$ K, $n^{\text{tot}} = 3.25$, $t'/|t| = 0.25$, $e'/|t| = -4$). The eigenenergies are represented by dotted lines. The partial spectral-weight contributions from $f$-electrons [(a) and (b)] are marked in blue, whereas those for $c$-electrons [(c) and (d)] in red. Color intensity represents the spectral-weight magnitude. In panel (e) spin-resolved density of states is presented.

FIG. 9. (a)-(d) Band structure for $h/|t| = 0.002$ and slightly larger hybridization $V/t = 1.262$ in the FM$_1+A_1$ phase (the remaining parameters are same as in Fig. 8). Eigenenergies are represented by dotted lines, partial contributions from $f$-electrons are marked in blue, whereas those for $c$-electrons in red. Color intensity represents the spectral weight. (e) Orbital- and spin-resolved density of states.
icle susceptibility introduced in a purely phenomenological manner. Such a scheme is unable to capture subtle differences in fluctuation spectrum between various FM states. The way to approach the problem with inclusion of the correlations is to start with the microscopic renormalized effective Hamiltonian, coming from our SGA method, outlined briefly in Appendix B and incorporate microscopic $1/N$-type corrections to the uncorrelated wave function $|\Psi_0\rangle$. Such an approach, if completed, should lead to a full theory including both the (short-range) correlations and (long-range) contribution due to the spin fluctuations in $\text{UGe}_2$ system. The procedure is, most likely, even indispensable to describe the compounds with small FM moments, \cite{Sakurai1967,Medici1991,Medici1992} (viz. UCoGe\cite{Sakurai1967} and UH\cite{Medici1991}). The system URhGe can be placed in between the two extreme cases.

At the end, we should mention that the present model neglects spin-orbit coupling and magnetocrystalline anisotropy in the uranium compounds mentioned above, \cite{Sakurai1967,Medici1991,Medici1992} from the fact that the overall phase diagram and the coexistent phases are reproduced correctly we draw the conclusion that the orbital moment may be frozen (we consider only spin-aligned phases) and that the anisotropic character of the system in enforced naturally by the presence of the long-range FM order along the easy axis. Obviously, this may not be that simple if we would like to discuss the situation in the field by changing its orientation.

### ACKNOWLEDGMENTS

This work was supported by the Grant OPUS No. UMO-2018/29/B/ST3/02646 from Narodowe Centrum Nauki (NCN).

#### Appendix A: Statistically Consistent Gutzwiller Approximation (SGA): Simplified vs. full forms

In the preceding paper\cite{Mazurenko2020} (cf. Appendix A there) we have discussed in detail the SGA approximation. Here we provide a more formal background. First, the multi-band trial function for the ground state in our variational approach is selected in the form

$$
|\Psi_G\rangle = \prod_i \hat{P}_i |\Psi_0\rangle,
$$

(A1)

where $|\Psi_0\rangle$ is an antisymmetrized product (Slater determinant) of single-particle wave functions, in general describing non-correlated broken symmetry state, for which the Wick’s theorem hold. $\hat{P}_i$ is the so called Gutzwiller correlator that changes the weights of various many-body configurations in the variational wave function $|\Psi_G\rangle$. The general form of $\hat{P}_i$ is

$$
\hat{P}_i = \sum_{\lambda i, \lambda' i'} \lambda_{i, \lambda' i'} |I, i\rangle\langle I', i'|,
$$

(A2)

where the states $\{|I, i\rangle\}$ span the local Fock space of the correlated orbitals at site $i$ and the variational variables $\lambda_{i, \lambda' i'}$ form a matrix, here taken in the real-valued and symmetric form. Any correlated local spin-orbital state can be represented as

$$
|I, i\rangle = \prod_{\alpha \in I} \hat{f}_{\alpha i}^\dagger |0, i\rangle,
$$

(A3)

where $\alpha = (l, \sigma)$ labels combined spin-orbital indices and the symbol ‘$<$’ indicates a specified selected ascending order of the creation operators. Likewise

$$
\langle I', i | = \prod_{\alpha \in I'} \langle 0, i | \hat{f}_{\alpha i},
$$

(A4)

contains the annihilation operators in the descending order, so that

$$
|I, i\rangle|I', i\rangle = \prod_{\alpha \in I} \hat{f}_{\alpha i}^\dagger \hat{f}_{\alpha i} \prod_{\gamma \in I \cup I'} (1 - \hat{n}_{\gamma i}).
$$

(A5)

The basic task is to evaluate the ground state energy. For that purpose, we should evaluate the averages

$$
\langle \Psi_G | \hat{O}_i | \Psi_G \rangle = \frac{\langle \Psi_0 | (\prod_j \hat{P}_j) \hat{O}_i (\prod_j \hat{P}_j^\dagger) | \Psi_0 \rangle}{\langle \Psi_0 | (\prod_j \hat{P}_j^\dagger) (\prod_j \hat{P}_j) | \Psi_0 \rangle}.
$$

(A6)

The products of local correlators can be rearranged by using the fact that $\hat{P}_i$ and $\hat{P}_j$ commute for $i \neq j$. In effect,

$$
\langle \hat{O}_i \rangle = \frac{\langle \prod_{j \neq i} \hat{P}_j^2 \hat{P}_i \hat{O}_i \hat{P}_i^\dagger \rangle_0}{\langle \prod_j \hat{P}_j^2 \rangle_0},
$$

(A7)

where the averages with the subscript ‘$0$’ are taken in the uncorrelated state, so that when applied the Wick theorem to the averages in the uncorrelated $\langle \ldots \rangle_0$ representation, we obtain

$$
\langle \prod_j \hat{P}_j^2 \rangle_0 \langle \hat{O}_i \rangle = \langle \prod_{j \neq i} \hat{P}_j^2 \rangle_0 \langle \hat{P}_i \hat{O}_i \hat{P}_i^\dagger \rangle_0
$$

$$
+ \sum_{\text{all pairs of n. n. contractions}} \langle \prod_{j \neq i} \hat{P}_j^2 \rangle_0 \langle \hat{P}_i \hat{O}_i \hat{P}_i^\dagger \rangle_0 + \ldots,
$$

(A8)

where the symbol

$$
\sum_{\text{all pairs of n. n. contractions}} \langle \hat{A} \rangle_0 \langle \hat{B} \rangle_0
$$

(A9)
represents all the nonzero pair contractions selected for a given broken-symmetry state. A detailed procedure is quite cumbersome and will not be detailed here.

Under the so-called Gutzwiller condition, the functional \( \langle \Psi_G | H | \Psi_G \rangle \equiv \langle \hat{P}_G \hat{\Sigma} \hat{P}_G \rangle \), which can be used to evaluate \( \langle \Psi_G | H | \Psi_G \rangle \) (note that all the \( f \)-dependent terms are local).

In effect, we obtain Landau-type functional \( L \) which, at \( T = 0 \), is composed of \( \langle H \rangle_G \) and incorporates the condition for the chemical potential, the enforced normalization \( \langle \Psi_G | \Psi_G \rangle = 1 \), as well as the requirement of having the same number of particles in the initial \( | \Psi_0 \rangle \) and correlated \( | \Psi_G \rangle \) states (before and after the projection with \( \hat{P}_G \)), namely

\[
L \equiv \left[ \langle \hat{H} \rangle_G - \mu \sum_i \left( \sum_{\alpha} \langle \hat{p}_{i\alpha}^f \rangle + \sum_{\beta} \langle \hat{p}_{i\beta}^c \rangle - n_{i}^{\text{tot}} \right) \right] + \sum_i \eta_i \left( \langle \hat{P}_G^2 \rangle \right)_0 - 1 + \sum_{i\alpha\beta} \eta_{i\alpha\beta} \left( \langle \hat{P}_G^2 \hat{f}_{i\alpha}^f \hat{f}_{i\beta}^c \rangle - \langle \hat{f}_{i\alpha}^f \hat{f}_{i\beta}^c \rangle \right).
\]

The functional \( L \) needs to be optimized with respect to all \( \lambda \) and \( \eta \) parameters, representing additional constraints in SGA approximation, as well as \( \mu \) and \( | \Psi_0 \rangle \). Minimization with respect to \( | \Psi_0 \rangle \) leads to an effective (renormalized) quasiparticle Hamiltonian in an applied magnetic field with the renormalized parameters defined as

\[
\begin{align*}
\hat{c}_{k\sigma} & = \frac{1}{2} \frac{\partial L}{\partial \eta^0_{k\sigma}}, \\
\tilde{\nu} & = \frac{1}{4} \frac{\partial L}{\partial \eta^0}, \\
\tilde{\Delta} & = \frac{1}{2} \frac{\partial L}{\partial A^0_{f\sigma}}, \\
\tilde{A} & = \frac{1}{4} \frac{\partial L}{\partial A^0_{f\sigma}},
\end{align*}
\]

and \( \epsilon_{k\sigma} \) given by Eq. (5). The bare (renormalized) parameters read

\[
\begin{align*}
n^0_{f\sigma} & = \left\langle \hat{f}_{i\alpha}^f \hat{f}_{i\beta}^c \right\rangle_0, \\
n^0_{c\sigma} & = \left\langle \hat{c}_{i\alpha} \hat{c}_{i\beta} \right\rangle_0, \\
\tilde{\nu}^0 & = \left\langle \hat{f}_{i\alpha}^f \hat{f}_{i\beta}^c \right\rangle_0, \\
A^0_{f\sigma} & = \left\langle \hat{f}_{i\alpha}^f \hat{f}_{i\beta}^c \right\rangle_0, \\
A^0_{f\sigma} & = \left\langle \hat{f}_{i\alpha}^f \hat{f}_{i\beta}^c \right\rangle_0.
\end{align*}
\]

Note that the averages \( A^{(1)} \) define the uncorrelated broken-symmetry state, whereas Eqs. \( A^{(5)} \) define the physical state. Also, the Hamiltonian \( A^{(14)} \) is self-consistent in which the quantities defining the physical state are \( \mu, \Delta_{f\sigma}, \Delta_{f\sigma}, \tilde{\nu}, \tilde{\epsilon}_{f\sigma}, \) and the band dispersion relation of \( \epsilon_{k\sigma} \) for bare \( c \) electrons. They are determined from a system of five self-consistent equations. Note also that in the effective Hamiltonian \( [4] \) the anomalous averages \( \tilde{\nu} \) are set to zero, which means that the direct hybrid \( (c-f) \) pairing is regarded as negligible. This is not the case for the singlet-paired systems.

In Fig. (10) we display the selected properties of SC state on the basis of full solution of the self-consistent equations obtained with the help of Hamiltonian \( A^{(14)} \), for the three selected values of the Hund’s rule exchange integral \( J \). Namely, in (a) we display the total magnetic moment \( m^\text{tot} \). Panel (b) shows the dominant (spin-down) pairing amplitude in FM1+AF and PM + A phases. In panel (c) we draw the ground-state energy, whereas in (d) we plot the condensation energy (the energy difference between the SC state and that corresponding to the appropriate pure FM phase). All these characteristics are quantitatively similar to those obtained earlier within the simplified picture with \( \Delta_{f\sigma} \equiv 0 \). From that we draw the conclusion that the hybrid component of the pairing has a negligible effect on the pairing. Also, the component \( \Delta_{f\sigma} \) of the pairing amplitude of \( f \)-electrons (i.e., the one with zero \( z \) spin-component of the pair) is suppressed in this system with relatively large \( U \). Hence, the simplified solution detailed in Appendix A of Ref. [12] represents to a good accuracy the full solution. The same type of pic-
FIG. 10. Exemplary phase diagram obtained with the multi-orbital correlator in the $f$-electron sector. (a) The total magnetization $m$, (b) pairing amplitude $A_{f,\sigma}$, (c) ground state energy $E_G$ per lattice site, (d) SC condensation energy $\Delta E$, all as a function of hybridization for $n = 3.2$, $\epsilon_f = -3|t|$, $U + J = 5|t|$, square lattice density of $c$ states: $t < 0$, $t' = 0.25|t|$ and for three rations $J/U = 0.5, 0.45, 0.4$. Note that $A_1$ phase is characterized by $A_{f\uparrow} = 0$, whereas in $\Lambda$ phase we have $A_{f\uparrow} = A_{f\downarrow}$. The condensation energy for $J/U = 0.4$ is so low that it is hardly visible on the scale. Note that despite seemingly discontinuous behavior, $\Delta E$ does not exhibit jumps across the joint metamagnetic and metasuperconducting transitions, but it varies extremely rapidly in the narrow parameter range. For the zero-field case this has been detailed in Appendix D of Ref. 43.

Appendix B: Incorporation of quantum spin fluctuations in an orbitally degenerate system: An outline

The atomic part of the Hamiltonian (1) for $f$ electrons located on orbitals $l = 1, 2, \ldots, d$, where $d$ is their degeneracy, can be rewritten in the form

$$\mathcal{H}_I = U \sum_{il} \hat{n}_{il} f(l) \hat{n}_{il} f(l) + \frac{K}{2} \sum_{\sigma \sigma'} \hat{n}_{il} f(l) \hat{n}_{il} f(l) - J \sum_{il} \hat{S}_{il} f(l) \hat{S}_{il} f(l),$$

(B1)

where $K = U' - J/2$ and the primed summation is performed over $l \neq l'$. Note that the interaction parameters $U$, $K$, and $J$ are taken as the same for each pair $(l, l')$ of orthogonalized orbitals. Therefore, we introduce next the global spin- and particle-number operators as

$$\hat{S}_i^f = \sum_{l=1}^d \hat{S}_i^f(l), \quad \hat{n}_{i\sigma} = \sum_{l\sigma} \hat{n}_{il\sigma},$$

(B2)

Expressing the orbital-dependent operators in Eq. (B1) through their global correspondants, we obtain

$$\mathcal{H}_I = \frac{1}{2} K \sum_i \left( \hat{n}_i \right)^2 - J \sum_i \left( \hat{S}_i^f \right)^2 + I \sum_{il} \hat{n}_{il} f(l) \hat{n}_{il} f(l)$$

(B3)

with $I = U - K - \frac{1}{2} J$. Assuming the standard relation for $d$ electrons $U' = U - 2J$ we obtain $K = U - \frac{5}{2} J$, $I = J/2$. We thus have decomposed the intraatomic interaction into the three parts: local charge, spin, and the Hubbard-type correlations, respectively. Now, noticing that the first two terms give contribution of the order of $d^2$, whereas the third one $\sim d$, and disregarding charge fluctuations, we have, to the first approximation,

$$\mathcal{H}_I = - \left( J + \frac{I}{3d} \right) \sum_i \left( \hat{S}_i^f \right)^2,$$

(B4)

i.e., the total local spin fluctuations provide the leading contribution. In the FM state one can take $\hat{S}_i^f = \langle \hat{S}_i^f \rangle \hat{e}_z + \hat{s}_i^f$, where the static part of magnetization introduces a natural anisotropy axis for spin fluctuations expressed by $\hat{s}_i^f = \hat{s}_i^f(\tau)$, where $\tau$ is the imaginary time. To include the dynamic fluctuations one utilizes the Hubbard-Stratonovich transformation

$$\exp(\hat{a}^2) = \int_{-\infty}^{\infty} dx \exp(-\pi x^2 - 2\hat{a}x\sqrt{\pi})$$

(B5)

for each spin-operator component $\hat{S}_i^f(\tau)$. By including also the single-particle part $\hat{H}_0$, we obtain the following expression for the system density matrix.
\[ \rho = T e^{-\beta \hat{H}_0} \prod_i \int D \xi_i^\alpha (\tau) \exp \left( -\frac{1}{\beta} \int_0^1 d\tau (\xi_i^\alpha)^2 - \int_0^1 d\tau 2i\sqrt{\pi} \beta J \xi_i^\alpha (\tau) A_i^\alpha (\tau) \right), \]  

where \( D \xi_i^\alpha (\tau) \) denotes functional integration over each Gaussian random field \( \xi_i^\alpha (\tau) \), \( \beta \equiv (k_B T)^{-1} \), \( \tau \) is in the units of \( \beta \), and \( A_i^\alpha (\tau) \equiv \hat{S}_i^\alpha (\tau) \). One can see that this form is of the same type as that for the Hubbard with explicitly rotationally invariant interaction term

\[ U \hat{n}_i \hat{n}_i = \frac{1}{4} U (\hat{n}_i + \hat{n}_i)^2 - \frac{1}{3} U \hat{S}_i^2 \]  

and fluctuating field \( \hat{S}_i^\alpha (\tau) \). Therefore, the spin-fluctuation contribution can be calculated in the same manner as in the Hubbard model with the part \( \langle \hat{S}_i^2 \rangle \neq 0 \). However, in order to incorporate the fluctuations starting from the SGA (renormalized mean-field) solution, replacing the Hartree-Fock solution as a saddle-point approximation, our coupling constant must be also renormalized, \( J \to J_{\chi J} \) as contained when solving self-consistent equation for \( \langle \hat{S}_i^2 \rangle_0 \). Implementation of this program is quite involved, both analytically and numerically, so it should be analyzed in detail separately. In any case, the spin-fluctuation contribution will renormalize the SGA characteristics by not just an additive contribution. However, a further generalization of expression \( \langle B_i \rangle \) is required to include also the pairing fluctuations. This can be implemented in the following manner. We start from the binomial representation of the Hund’s rule part which, for the simplest spin \( S = 1 \) case \( (l = 1, 2, \ldots) \), takes the form

\[ \hat{S}_i^{l(1)} \hat{S}_i^{l(2)} + \frac{3}{4} \hat{n}_i^{(1)} \hat{n}_i^{(2)} = \sum_{m=-1}^{1} \hat{A}_{im}^{l} \hat{A}_{im}^{l} \]  

where the pairing amplitude components are defined as

\[ \begin{cases} 
\hat{A}_{11}^{l} = \hat{f}^{(1)\dagger} \hat{f}^{(2)\dagger}, \\
\hat{A}_{10}^{l} = \frac{1}{\sqrt{2}} (\hat{f}^{(1)\dagger} \hat{f}^{(2)\dagger} + \hat{f}^{(1)\dagger} \hat{f}^{(2)\dagger}), \\
\hat{A}_{1-1}^{l} = \hat{f}^{(1)\dagger} \hat{f}^{(2)\dagger}.
\end{cases} \]  

This bilinear form can be transformed to the corresponding representation \( \langle B_i \rangle \) and will involve additional fluctuating fields \( \{ \eta_m^{\alpha}(\tau) \} (m = -1, 0, +1) \) which express three local components of the pairing \( \Delta_{im}^{l} \). In general, one can decompose the Hund’s rule term into two components, diagonal (magnetic moment) and off-diagonal (pairing gap) according to the prescription provided in Ref. \[ \[36\].

---

1. S. S. Saxena, P. Agarwal, K. Ahilan, F. M. Grosche, R. K. W. Haselwimmer, M. J. Steiner, E. Pugh, I. R. Walker, S. R. Julian, P. Monthoux, G. G. Lonzarich, A. Huxley, I. Sheikin, D. Braithwaite, and J. Flouquet, “Superconductivity on the border of itinerant-electron ferromagnetism in UGe\(_2\),” Nature \[406\], 587 (2000)
2. N. Tateiwa, T. C. Kobayashi, K. Hanazono, K. Amaya, Y. Haga, R. Settai, and Y. Onuki, “Pressure-induced superconductivity in a ferromagnet UGe\(_2\),” J. Phys.: Condens. Matter \[13\], L17 (2001)
3. C. Pfeilderer and A. D. Huxley, “Pressure dependence of the magnetization in the ferromagnetic superconductor UGe\(_2\),” Phys. Rev. Lett. \[89\], 147005 (2002)
4. A. Huxley, I. Sheikin, E. Ressouche, N. Kernava, N. Braithwaite, R. Calemczuk, and J. Flouquet, “UGe\(_2\): A ferromagnetic spin-triplet superconductor,” Phys. Rev. B \[63\], 144519 (2001)
5. D. Aoki, A. Huxley, E. Ressouche, D. Braithwaite, J. Flouquet, J.-P. Brison, E. Lhotel, and C. Paulsen, “Coexistence of superconductivity and ferromagnetism in URhGe,” Nature \[413\], 613 (2001)
6. N. T. Huy, A. Gasparini, D. E. de Nijs, Y. Huang, J. C. P. Klaasse, T. Gertenmulder, A. de Visser, A. Hamann, T. Görlich, and H. v. Löhneysen, “Superconductivity on the border of weak itinerant ferromagnetism in UGe\(_2\),” Phys. Rev. Lett. \[99\], 067006 (2007)
7. T. C. Kobayashi, S. Fukushima, H. Hidaka, H. Kotegawa, T. Akazawa, E. Yamamoto, Y. Haga, R. Settai, and Y. Onuki, “Pressure-induced superconductivity in ferromagnet UIr without inversion symmetry,” Physica B \[378\], 355 (2006)
8. P. W. Anderson and W. F. Brinkman, “Theory of Anisotropic Superfluidity in 3He,” in Physics of Liquid and Solid Helium, Vol. Part II, edited by K. H. Bennemann and J. B. Ketterson (J. Wiley & Sons, New York, 1978) pp. 177–286.
9. D. Vollhardt and P. Wölfle, The Superfluid Phases of Helium 3 (Taylor & Francis, 1990).
10. M. M. Wysokiński and J. Spałek, “Properties of an almost localized Fermi liquid in an applied magnetic field revisited: a statistically consistent Gutzwiller approach,” J. Phys.: Condens. Matter \[26\], 055601 (2014)
11. D. Aoki, K. Ishida, and J. Flouquet, “Review of U-
based Ferromagnetic Superconductors: Comparison between UGe$_2$, URhGe, and UCoGe,” J. Phys. Soc. Japan 88, 022001 (2019)
12 E. Kądziela-Major, M. Fidyrsiaik, P. Kubiczek, and J. Spałek, “Spin-triplet paired phases inside a ferromagnet induced by Hund’s rule coupling and electronic correlations: Application to UGe$_2$,” Phys. Rev. B 97, 224519 (2018)
13 A. Harada, S. Kawasaki, H. Mukuda, Y. Kitaoka, Y. Haga, E. Yamamoto, Y. Onuki, K. M. Itoh, E. E. Haller, and H. Harima, “Experimental evidence for ferromagnetic spin-pairing superconductivity emerging in UGe$_2$: A 57-Ge-nuclear-quadrupole-resonance study under pressure,” Phys. Rev. B 75, 140502 (2007)
14 N. Tateiwa, T. C. Kobayashi, K. Amaya, Y. Haga, R. Settai, and Y. Onuki, “Heat-capacity anomalies at $T_c$ and $T^*$ in the ferromagnetic superconductor UGe$_2$,” Phys. Rev. B 69, 180513 (2004)
15 K. G. Sandeman, G. G. Lonzarich, and A. J. Schofield, “Ferromagnetic superconductivity driven by changing Fermi surface topology,” Phys. Rev. Lett. 90, 167005 (2003)
16 M. M. Wysokiński, M. Abram, and J. Spałek, “Ferromagnetism in UGe$_2$: A microscopic model,” Phys. Rev. B 90, 081114 (2014)
17 M. M. Wysokiński, M. Abram, and J. Spałek, “Criticalities in the itinerant ferromagnet UGe$_2$,” Phys. Rev. B 91, 081108 (2015)
18 M. M. Wysokiński, J. Kaczmarczyk, and J. Spałek, “Correlation-driven d-wave superconductivity in Anderson lattice model: Two gaps,” Phys. Rev. B 94, 024517 (2016)
19 M. Abram, M. M. Wysokiński, and J. Spałek, “Tetracritical wings in UGe$_2$: A microscopic interpretation,” J. Magn. Magn. Mat. 400, 27 (2016)
20 P. Kubiczek, “Spin-triplet pairing in orbitally degenerate Anderson lattice model,” (2016), MSc. Thesis, Jagiellonian University, Kraków, Poland.
21 J. Bünnemann, T. Schickling, and F. Gebhard, “Variational study of Fermi surface deformations in Hubbard models,” Europhys. Lett. 98, 27006 (2012)
22 P. W. Anderson, “Theory of dirty superconductors,” J. Phys. Chem. Solids 11, 26 (1959)
23 J. Spałek, A. Datta, and J. M. Honig, “Discontinuous metal-insulator transitions and Fermi-liquid behavior of correlated electrons,” Phys. Rev. Lett. 59, 728 (1987)
24 M. Fidyrsiaik, M. Zegrodnik, and J. Spałek, “Realistic estimates of superconducting properties for the cuprates: reciprocal-space diagrammatic expansion combined with variational approach,” J. Phys.: Condens. Matter 30, 475602 (2018)
25 T. Terashima, T. Matsumoto, C. Terakura, S. Uji, N. Kinura, M. Endo, T. Komatsubara, and H. Aoki, “Evolution of Quasiparticle Properties in UGe$_2$ with Hydrostatic Pressure Studied via the de Haas-van Alphen Effect,” Phys. Rev. Lett. 87, 166401 (2001)
26 M. Manago, S. Kitagawa, K. Ishida, K. Deguchi, N. K. Sato, and T. Yamamura, “Enhancement of superconductivity by pressure-induced critical ferromagnetic fluctuations in UCoGe,” Phys. Rev. B 99, 020506 (2019)
27 S. Ran, C. Eckberg, Q.-P. Ding, Y. Furukawa, T. Metz, S. R. Saha, I.-L. Liu, M. Zic, H. Kim, J. Paglione, and N. P. Butch, “Spontaneously polarized half-gapped superconductivity,” (2018), arXiv:1811.11808
28 J. Spałek, “Spin-triplet superconducting pairing due to local Hund’s rule and Dirac exchange,” Phys. Rev. B 63, 104513 (2001)
29 Y. Takahashi, Spin Fluctuation Theory of Itinerant Electron Magnetism (Springer Berlin Heidelberg, 2013)
30 A. Klejnberg and J. Spałek, “Hund’s rule coupling as the microscopic origin of the spin-triplet pairing in a correlated and degenerate band system,” J. Phys.: Condens. Matter 11, 6553 (1999)
31 A. Klejnberg and J. Spałek, “Metal-insulator transition, gap opening due to the combined orbital-spin ordering, and spin-triplet superconductivity,” Phys. Rev. B 61, 15542 (2000)
32 J. Bünnemann, W. Weber, and F. Gebhard, “Multiband gutzwiller wave functions for general on-site interactions,” Phys. Rev. B 57, 6896 (1998)
33 J. Spałek and M. Zegrodnik, “Spin-triplet paired state induced by Hund’s rule coupling and correlations: a fully statistically consistent Gutzwiller approach,” J. Phys.: Condens. Matter 25, 435601 (2013)
34 M. Zegrodnik, J. Spałek, and J. Bünnemann, “Coexistence of spin-triplet superconductivity with magnetism within a single mechanism for orbically degenerate correlated electrons: statistically consistent Gutzwiller approximation,” New J. Phys. 15, 073050 (2013)
35 M. Zegrodnik, J. Bünnemann, and J. Spałek, “Even-parity spin-triplet pairing by purely repulsive interactions for orbitally degenerate correlated fermions,” New J. Phys. 16, 033001 (2014)
36 T. Hattori, Y. Ihara, Y. Nakai, K. Ishida, Y. Tada, S. Fujimoto, N. Kawakami, E. Osaki, K. Deguchi, N. K. Sato, and I. Satoh, “Superconductivity Induced by Longitudinal Ferromagnetic Fluctuations in UCoGe,” Phys. Rev. Lett. 108, 066403 (2012)
37 Y. Tada, S. Fujimoto, N. Kawakami, T. Hattori, Y. Ihara, K. Ishida, K. Deguchi, N. K. Sato, and I. Satoh, “Spin-Triplet Superconductivity Induced by Longitudinal Ferromagnetic Fluctuations in UCoGe: Theoretical Aspect,” J. Phys.: Conf. Series 449, 012029 (2013)
38 B. Wu, G. Bastien, M. Taupin, C. Paulsen, L. Howald, D. Aoki, and J.-P. Brison, “Pairing mechanism in the ferromagnetic superconductor UCoGe,” Nat. Commun. 8, 14480 (2017)
39 A. B. Shick and W. E. Pickett, “Magnetism, Spin-Orbit Coupling, and Superconducting Pairing in UGe$_2$,” Phys. Rev. Lett. 86, 300 (2001)
40 A. B. Shick, V. Janiš, V. Drchal, and W. E. Pickett, “Spin and orbital magnetic state of UGe$_2$ under pressure,” Phys. Rev. B 70, 134506 (2004)
41 J. Karbowski and J. Spałek, “Interorbital pairing for heavy fermions and universal scaling of their basic characteristics,” Phys. Rev. B 49, 1454 (1994)
42 O. Howczak, J. Kaczmarczyk, and J. Spałek, “Pairing by Kondo interaction and magnetic phases in the Anderson-Kondo lattice model: Statistically consistent renormalized mean-field theory,” Phys. Stat. Sol. (b) 250, 609 (2013)
43 E. Kądziela-Major, “Exchange Interactions, Electronic States, and Pairing of Electrons in Correlated and Hybridized Systems,” (2018), PhD. Thesis, Jagiellonian University, Krakow, Poland.
44 A. Klejnberg and J. Spałek, “Simple treatment of the metal-insulator transition: Effects of degeneracy, temperature, and applied magnetic field,” Phys. Rev. B 57, 12041 (1998)
45 W. E. Evenson, J. R. Schrieffer, and S. Q. Wang, “New
Approach to the Theory of Itinerant Electron Ferromagnets with Local-Moment Characteristics,” *J. Appl. Phys.* **41**, 1199 (1970).

* U. Lindner, “A generalized Ginzburg-Landau functional for systems with correlation,” *J. Phys.: Condens. Matter* **3**, 347 (1991).