Unified character of correlation effects in unconventional Pu-based superconductors and $\delta$-Pu

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Electronic structure calculations combining the local-density approximation with an exact diagonalization of the Anderson impurity model show an intermediate $5f^5-5f^6$-valence ground state and delocalization of the $5f^5$ multiplet of the Pu atom $5f$-shell in PuCoIn$_5$, PuCoGa$_5$, and $\delta$-Pu. The $5f$-local magnetic moment is compensated by a moment formed in the surrounding cloud of conduction electrons. For PuCoGa$_5$ and $\delta$-Pu the compensation is complete and the Anderson impurity ground state is a singlet. For PuCoIn$_5$ the compensation is partial and the Pu ground state is magnetic. We suggest that the unconventional $d$-wave superconductivity is likely mediated by the $5f$-states antiferromagnetic fluctuations in PuCoIn$_5$, and by valence fluctuations in PuCoGa$_5$.

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Providing a consistent description of correlation effects in the electronic structure of element actinides and their compounds is a complex problem due to the interplay between the localized and the itinerant nature of the 5f electrons. It is commonly accepted that 5f-electrons in light actinides form rather broad conduction bands whereas for the heavy actinides the 5f states are atomic-like. Johansson [1] described this situation as a “Mott transition in the 5f-electron subsystem” taking place between Pu and Am when moving along the Periodic Table. Katsnelson et al. [2] linked the broadening of the 5f band to the “atomic collapse” characterizing the transformation from the high-temperature expanded and the low-temperature compressed phases of Pu.

A quantitative description of the Mott transition in actinides [3] was obtained by the dynamical mean-field theory (DMFT) [4] more than 20 years after the concept was formulated. Further DMFT studies suggested an intermediate-valence nature of the Pu-atom 5f shell [5] and provided justification for the experimentally proved absence of magnetism in $\delta$-Pu [6].

The intermediate-valence and nonmagnetic character of the 5f shell can play an important role in stabilizing the superconducting state exhibited by PuCoGa$_5$ below a critical temperature $T_c$ of 18.5 K. [6,7,8]. The unconventional character of superconductivity in this compound is now generally accepted but the microscopic mechanism responsible for electron pairing remains unknown. The $d$-wave symmetry of the superconducting gap in PuCoGa$_5$ has been proven by point-contact spectroscopy experiments [9] that also provided the first spectroscopic measurements of the gap amplitude and its temperature dependence.

Recently, superconductivity has been discovered also in PuCoIn$_5$ [11], with $T_c = 2.5$ K. The experimental studies of this compound were immediately followed by conventional density functional theory (DFT) calculations in the local-density generalized-gradient approximation (LDA/GGA) [12,13]. Keeping in mind a well known failure of DFT in the case of $\delta$-Pu [14], it can be expected that LDA/GGA does not provide an accurate description of the electronic structure for this strongly correlated material. A few static mean-field correlated band theory calculations were also performed [14,15], making use of different flavors of the LDA/GGA plus Coulomb’s $U$ (LDA+$U$) method. While being an improvement over the conventional band theory, the LDA($GGA$)+$U$ falls short in describing the itinerant-to-localized crossover of the $5f$ manifold in $\delta$-Pu [16] and PuCoGa$_5$ [10].

Here, we report electronic structure calculations of PuCoIn$_5$, PuCoGa$_5$ and $\delta$-Pu performed by combining LDA with the exact diagonalization (ED) [17,18] of a discretized single-impurity Anderson model [19]. In this approach, the band structure obtained by the relativistic version of the full-potential linearized augmented plane wave method (FP-LAPW) [17] is consistently extended to account for the full structure of the 5f-orbital atomic multiplets and their hybridization with the conduction bands [18].

The starting point of our approach is the multiband Hubbard Hamiltonian [19] $H = H^0 + H^{\text{int}}$, $H^0 = \sum_{i,j,\gamma} H^{\gamma}_{i\gamma,j\gamma} c_{i\gamma}^\dagger c_{j\gamma}$, where $i,j$ label lattice sites and $\gamma = (lm\sigma)$ mark spinorbitals $\{\phi_\gamma\}$, is the
one-particle Hamiltonian found from ab initio electronic structure calculations of a periodic crystal; $H^{\text{int}}$ is the on-site Coulomb interaction describing the f-electron correlation. We assume that electron interactions in the $s$, $p$, and $d$ shells are well approximated in DFT.

The effects of the interaction Hamiltonian $H^{\text{int}}$ on the electronic structure are described by a $k$-independent one-particle selfenergy $\Sigma(z)$, where $z$ is a (complex) energy. The selfenergy is constructed with the aid of an auxiliary impurity model describing the complete seven-orbital 5f shell. This multi-orbital impurity model includes the full spherically symmetric Coulomb interaction, the spin-orbit coupling (SOC), and the crystal field (CF). The corresponding Hamiltonian can be written as

$$
H_{\text{imp}} = \sum_{\kappa m \sigma'} [\epsilon_{\kappa m} b_{\kappa m \sigma'}^\dagger b_{\kappa m \sigma'} + \sum_{m\sigma} \epsilon_f f_{m\sigma}^\dagger f_{m\sigma}]
+ \sum_{m\sigma} \left[\xi (1 \cdot s + \Delta_{\text{CF}}) b_{m \sigma}^\dagger f_{m \sigma} + h.c.\right]
+ \sum_{\kappa m \sigma'} \left[\epsilon^\prime \sigma \sigma' \sum_{\kappa m} \epsilon_{\kappa m} b_{\kappa m \sigma'}^\dagger f_{m \sigma} + h.c.\right]
+ \frac{1}{2} \sum_{m\sigma m'\sigma'} U_{m\sigma m'\sigma'} f_{m\sigma}^\dagger f_{m'\sigma} f_{m\sigma}^\dagger f_{m'\sigma},
$$

where $f_{m\sigma}^\dagger$ creates an electron in the 5f shell and $b_{m\sigma}^\dagger$ creates an electron in the “bath” that consists of those host-band states that hybridize with the impurity 5f shell. The energy position $\epsilon_f$ of the impurity level, and the bath energies $\epsilon^\prime$ are measured from the chemical potential $\mu$. The parameter $\xi$ specifies the strength of the SOC and $\Delta_{\text{CF}}$ is the crystal-field potential at the impurity. The parameter matrices $V_k$ describe the hybridization between the 5f states and the bath orbitals at energy $\epsilon^\prime$.

The band Lanczos method is employed to find the lowest-lying eigenstates of the many-body Hamiltonian $H_{\text{imp}}$ and to calculate the one-particle Green’s function $[G_{\text{imp}}(z)]_{\sigma \sigma'}$ in the subspace of the $f$ orbitals at low temperature ($k_B T = 1/500$ eV). The self-energy $\Sigma(z)$ is then obtained from the inverse of the Green’s-function matrix $[G_{\text{imp}}]$.

Once the self-energy is known, the local Green’s function $G(z)$ of the electrons in the solid, is used to construct an effective LDA+U potential $V_U$, which is inserted into Kohn–Sham-like equations:

$$
-\nabla^2 + V_{\text{LDA}}(r) + V_U + \xi (1 \cdot s) \Phi^\dagger(r) = \epsilon^\prime \Phi(r).
$$

These equations are iteratively solved until self-consistency over the charge density is reached. In each iteration, a new Green’s function $G_{\text{LDA}}(z)$ [which corresponds to $G(z)$ from Eq. (2) with the self-energy $\Sigma$ set to zero], and a new value of the 5f-shell occupation are obtained from the solution of Eq. (3). Subsequently, a new self-energy $\Sigma(z)$ corresponding to the updated 5f-shell occupation is constructed. Finally, the next iteration is started by evaluating the new local Green’s function, Eq. (2).

In order to determine the bath parameters $V_k$ and $\epsilon^\prime$, we assume that the LDA represents the non-interacting model. We then associate the LDA Green’s function $G_{\text{LDA}}(z)$ with the Hamiltonian of Eq. (1) when the coefficients of the Coulomb interaction matrix are set to zero ($U_{m\sigma m'\sigma'} = 0$). The hybridization function $\Delta(\epsilon)$ is then estimated as $\Delta(\epsilon) = -\frac{i}{\pi} \text{Im} \text{Tr}[G_{\text{LDA}}^{-1}(\epsilon + i\delta)]$. The curve obtained for $\Delta(\epsilon)$ is shown in Fig. 1 together with the $j = 5/2, 7/2$ projected LDA densities of the $f$-states. The results also show that the hybridization matrix is, to a good approximation, diagonal in the $\{j, j_z\}$ representation. Thus, we assume the first and fourth terms in the impurity model, Eq. (1), to be diagonal in $\{j, j_z\}$, so that we only need to specify one bath state (six orbitals) with $\epsilon^\prime = 1 \times 5/2$ and $V_k^\times j = 1/2$, and another bath state (eight orbitals) with $\epsilon^\prime = 1 \times 7/2$ and $V_k^\times j = 1/2$. Assuming that the most important hybridization is the one occurring in the vicinity of $E_F$, the numerical values of the bath parameters $V_k^\times j = 1/2$ are found from the relation

$$
\sum_k |V_k^j|^2 \delta(\epsilon_j - \epsilon) = -\Delta(\epsilon)/N_f \text{ integrated over the}
$$

FIG. 1. (Color online) The Pu atom LDA $j = 5/2, 7/2$ projected DOS, and LDA hybridization function $\Delta(\epsilon) = -\frac{i}{\pi} \text{Im} \text{Tr}[G_{\text{LDA}}^{-1}(\epsilon + i\delta)]$. The inset shows the PuCoIn$_5$ crystal structure.
energy interval, $E_F - 0.5\, eV \leq \epsilon \leq E_F + 0.5\, eV$, with $N_f = 6$ for $j = 5/2$ and $N_f = 8$ for $j = 7/2$. The bath-state energies $\epsilon_{5/2,7/2}^{\pm}$ shown in Table I are adjusted to approximately reproduce the LDA 5f states.

The Slater integrals

\begin{equation}
\begin{array}{c}
\text{Material} \\
PuCoIn_5 \\
PuCoGa_5 \\
\delta-Pu
\end{array}
\begin{array}{c}
n_{5/2}^{f} \\
n_{7/2}^{f} \\
\epsilon_{5/2}^{f} \\
V_{5/2}^{f} \\
\epsilon_{7/2}^{f} \\
V_{7/2}^{f}
\end{array}
\begin{array}{c}
4.78 \\
4.38 \\
4.16 \\
0.39 \\
0.76 \\
0.85
\end{array}
\begin{array}{c}
0.36 \\
0.25 \\
0.33 \\
0.21 \\
0.29 \\
0.32
\end{array}
\begin{array}{c}
0.21 \\
0.29 \\
0.27 \\
-0.25 \\
-0.07 \\
-0.01
\end{array}
\begin{array}{c}
0.25 \\
0.34 \\
0.36
\end{array}
\end{equation}

In the calculations we used an in-house implementation of the FP-LAPW method that includes both scalar-relativistic and spin-orbit coupling effects. The calculations were carried out assuming a paramagnetic state with crystal structure parameters for PuCoIn$_5$, PuCoGa$_5$, and $\delta$-Pu taken from Refs. [11, 23, 24], respectively. The Slater integrals were chosen as $F_0 = 4.0\, eV$, and $F_2 = 7.76\, eV$, $F_4 = 5.05\, eV$, and $F_6 = 3.07\, eV$ [25]. They correspond to commonly accepted values for Coulomb’s $U = 4.0\, eV$ and exchange $J = 0.64\, eV$. The SOC parameters $\xi = 0.28\, eV$ for PuCoIn$_5$ and PuCoGa$_5$ and 0.29 $eV$ for $\delta$-Pu were determined from LDA calculations. CF effects were found to be negligible and $\Delta_{CF}$ was set to zero. For the double-counting term entering the definition of the LDA+U potential, $V_U$, we have adopted the fully-localized (or atomic-like) limit (FLL) $V_{dc} = U(n_f - 1/2) - J(n_f - 1)/2$. Furthermore, we set the radii of the atomic spheres to 3.1 a.u. (Pu), 2.3 a.u. (Co), 2.3 a.u. (Ga), and 2.5 a.u. (In). The parameter $R_{Pu} \times K_{max} = 10.54$ determined the basis set size, and the Brillouin zone (BZ) sampling was performed with 1152 k points. The self-consistent procedure defined by Eqs. [11, 23] was repeated until the convergence of the 5f-manifold occupation $n_f$ was better than 0.01.

We are now ready to discuss the solution of Eq. [11]. For PuCoIn$_5$, the ground state of the cluster formed by the 5f shell and the bath is given by a superposition of a magnetic sextet (23%) and a non-magnetic singlet (77%), with occupation numbers $\langle n_f \rangle = 5.40$ in the $f$ shell and $\langle n_{bath} \rangle = 8.40$ in the bath states. This ground state is not a singlet and carries a non-zero magnetic moment. For the 5f shell alone, the expectation values of the spin ($S_f$), orbital ($L_f$) and total ($J_f$) angular moments can be calculated as $\langle \hat{X}_f^2 \rangle = X_f^2 (X_f + 1)$, $\langle \hat{S}_f^2 \rangle = S_f^2$, $\langle \hat{L}_f \rangle = L_f$, and $\langle \hat{J}_f \rangle = J_f$. The individual components of the moments vanish, $\langle \hat{S}_f \rangle = 0$, unless the symmetry is broken by an external magnetic field.

In the case of PuCoGa$_5$, on the other hand, the hybridized ground state of the impurity is a non-magnetic singlet with all angular moments of the 5f-bath cluster equal to zero ($S = L = J = 0$). It consists of $\langle n_f \rangle = 5.30$ f states and $\langle n_{bath} \rangle = 8.70$ bath states. In a pictorial way, we can imagine that the magnetic moment of the 5f shell (for which we get $S_f = 2.18$, $L_f = 4.05$, $J_f = 2.43$) is completely compensated by the moment carried by the electrons in the conduction band. As the value of the 5f magnetic moment fluctuates in time, because of the intermediate-valence electronic configuration, this compensation must be understood as dynamical in nature. The same situation is realized in $\delta$-Pu ($S_f = 2.11$, $L_f = 4.21$, $J_f = 2.62$), whose ground state is found to be a nonmagnetic singlet with $\langle n_f \rangle = 5.21$ and $\langle n_{bath} \rangle = 8.79$.

The 5f-orbital density of states (DOS) obtained from Eq. [22] for the three investigated compounds is shown in Fig. 2. Below the Fermi energy $E_F$ the DOS exhibits the three-peak structure typical for Pu and for a number of its compounds, and its shape is in good agreement with experimental photoemission spectra. It can be noticed that the multiplets for the atomic $f^6$ configuration ($f^6 \rightarrow f^5$ transition, lying closer to $E_F$) are better resolved than for the $f^5$ part of the spectrum ($f^5 \rightarrow f^4$ transition).

Comparison with previous LDA+Hubbard-I (HIA) calculation for $\delta$-Pu [18], and PuCoGa$_5$ [26] shows that the three-peak manifold lying above 2 $eV$ binding energy has a slight upright shift towards $E_F$. At binding energies around 4 $eV$, the LDA+HIA peaks are substantially modified, and in the LDA+ED calculations they are spread over a $\sim 3\, eV$ energy interval. These changes in the DOS are induced by the hybridization and suggest partial delocalization of the $f^5$ multiplet. This is a situation suggested first by Hanzawa [27] in intermediate-valence rare-earth compounds such as SmS or SmB$_6$, where fluctuations occur between two atomic-like $4f$ configurations. Here, the 5f states remain localized for the $f^6$ configuration but become itinerant for the $f^5$ one.

As the many-body resonances lying closer to the Fermi energy are produced by $f^6 \rightarrow f^5$ multiplet transitions, they are in a way analogous to the Racah peaks, specific transitions between Racah multiplets [28] of $f^n$ and $f^{n \pm 1}$. On the other hand, these structures determine the metallic character of the investigated materials that can therefore be considered as a realization of a Racah metal, situated between the two limiting cases represented by fully localized intermediate-valence rare-earth compounds and metallic systems (e.g., nickel) with a non-integer number of $d$ electrons.

Both PuCoGa$_5$ and $\delta$-Pu display a temperature-independent magnetic susceptibility at low temperatures [4, 29]. Analogous to the intermediate-valence rare-earth compounds [50], the magnetic susceptibil-
FIG. 2. (Color online) \( f\)-electron density of states (DOS, \( j = 5/2, 7/2 \) projected) for the Pu atom in PuCoIn\(_5\) (a), PuCoGa\(_5\) (b) and \( \delta \)-Pu (c).

Figure 3 shows the band structure and the corresponding Fermi surfaces obtained from LDA+ED calculations. The shade of colors encodes the size of the energy gradient.

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The electronic specific-heat coefficient can be estimated as 
\[
\gamma = \frac{\pi^2 k_B^2}{3} \frac{m}{2 \hbar^2} \left( \frac{\partial F}{\partial \mu} \right)_{\mu=0} \left( \frac{\partial F}{\partial \mu} \right)_{\mu=0}
\]
for \( \delta \)-Pu, we get \( \gamma \approx 44 \text{ mJ K}^{-2} \text{ mol}^{-1} \), in very good agreement with experimental data. For PuCoGa\(_5\), we get \( \gamma \approx 43 \text{ mJ K}^{-2} \text{ mol}^{-1} \) which is smaller than the experimental value of 80–100 mJ K\(^{-2} \) mol\(^{-1} \). For PuCoIn\(_5\), the estimated \( \gamma \) value of \( \approx 52 \text{ mJ K}^{-2} \text{ mol}^{-1} \) is even further away from the experimental value of \( \approx 180 \text{ mJ K}^{-2} \text{ mol}^{-1} \). In this case, it is difficult to obtain an accurate value for \( \gamma \) due to the sharp DOS peak in the vicinity of \( E_F \) (see Fig. 2). When taken right at the DOS peak position, the \( \gamma \) value of 95 mJ K\(^{-2} \) mol\(^{-1} \) is obtained. Also, note that a possible enhancement of \( \gamma \) due to the electron-phonon interaction is not taken into account.
sponding Fermi Surface (FS) for PuCoIn$_5$, calculated from the solutions of Eq. 5, which represents an extended LDA+$U$ static-mean-field band structure with the 5f-states occupation matrix obtained from the local impurity Greens function Eq. 2. For comparison, Fig. 5 shows also the FS for PuCoGa$_5$ (Fig. S2 of Ref. 10). Close similarities in the band structure of the two compounds are immediately apparent. Both are compensated multiband metals, as the Fe-based superconductors, and for both materials the $f$ bands move away from the Fermi level when the Coulomb-U is included, as can be seen by examining the $f$-weighted fatbands. The Fermi surfaces are composed by four sheets (1–4), one that is hole-like (FS-1) and three that are electron-like (FS-2,3,4). The Fermi velocities ratio $\langle v_{\pi,\pi}^2 \rangle/\langle v_{\pi,\pi}^2 \rangle$ of 1.54 for PuCoIn$_5$, and 1.55 for PuCoGa$_5$ are calculated in reasonable agreement with the experimental anisotropy ratio of the critical field $H_{c2}$, 2 – 2.3 for PuCoIn$_5$, and indicate a two-dimensional character of the electronic structure.

DFT electronic structure calculations for Pu-based 115 material have recently been reported by Ronning et al. 13 and Zhu et al. 12 Their analysis of the DFT band structure and FS (see, e.g., Figs. 3 and 4 of Ref. 12) indicated two possible superconducting gap symmetries, the so-called $s\pm$ and $d_{x^2-y^2}$, which correspond to a pairing potential peaked at the $(\pi, \pi, 0)$ reciprocal lattice position. The conclusion was drawn that for Pu-based "115" superconductors, the $s\pm$ order parameter is more likely that the $d_{x^2-y^2}$ one. This is in contradiction with point-contact spectroscopy results 10 showing a zero-bias conductance anomaly that is not expected for $s\pm$ gap symmetry 32.

The presence of a 5f local moment dynamically compensated by the surrounding conduction electrons together with the $f^5$-,$f^6$ intermediate-valence ground state in PuCoGa$_5$ and PuCoIn$_5$ opens various possibilities for unconventional superconductivity. In PuCoIn$_5$ the Pu f-shell local moment is not fully compensated and superconductivity could be related to an antiferromagnetic quantum critical point 11,33. On the other hand, in PuCoGa$_5$ the ground state is a singlet and it seems more plausible that superconductivity results from a valence instability, as in heavy-fermion superconductors 34.

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