Journal of Nuclear Materials 385 (2009) 60–62

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

Effective Hamiltonian for metallic Pu

C.D. Batista *

Los Alamos National Laboratory, Condesed Matter Group (T-11), Los Alamos, New Mexico 87545, United States

A B S T R A C T

We derive a low-energy effective Hamiltonian $\tilde{H}^{Pu}$ for metallic Pu by assuming that intra-atomic Coulomb and spin–orbit interactions are much stronger than the kinetic energy terms. An important property of $\tilde{H}^{Pu}$ is the *exact* cancellation of the effective $f-f$ hopping tensor that places Pu closer to lanthanide systems such as Ce or mixed valent Sm than to the rest of the actinides. The similarity between the low-energy models of Pu and these mixed valent lanthanide systems could be the common root for explaining the large volume expansions observed in all of them.

1. Introduction

Metallic Pu is one of the most complex systems among all the elements of the periodic table. The origin of this complex behavior, that includes six Pu allotropes, lies in the crucial role played by the electron–electron Coulomb interactions. The large values of the specific heat coefficients [1–3] and resisitivity observed in δ and α-Pu are additional indicators of the strongly correlated nature of metallic Pu. As it was pointed out in several works, Pu is located on the border between itinerant and localized electronic behavior [4,5]. While lighter actinides are more itinerant, the kinetic energy term seems to be strongly suppressed in Pu metal.

Strongly correlated behavior is indeed the rule for lanthanide systems. In this case the $f-f$ overlap is usually neglected due to the strong localization of the $4f$-orbitals. The f-electron delocalization occurs mainly due to hybridization with the broad s, p or d conduction bands. In contrast, the $f-f$ overlap gives an important contribution to the electronic delocalization of actinide systems due to the larger extension of the $5f$-orbitals. However, this additional contribution to the electronic delocalization does not seem to be present in Pu metal. In many respects, Pu looks closer to some lanthanide systems than to any of the other actinides. For instance, the huge volume expansion of 26% between α and δ-Pu is similar to the 20% expansion on going from α-Ce to δ-Ce, but has not been observed in any other actinide element. In addition, low temperature susceptibility and high temperature resistivity measurements have been analyzed within a Kondo-like model of localized $5f$ electrons [6].

In a recent paper [7], we derived a low-energy effective model for different actinides by assuming that intra-atomic Coulomb and spin–orbit interactions are much stronger than the kinetic energy terms. In this paper, we will focus on the particular case of metallic Pu and demonstrate that the direct $f-f$ hopping is blocked at low-energies (the effective $f-f$ hopping that results from projecting the original $f-f$ hopping terms into the low-energy subspace is exactly zero). This property of $\tilde{H}^{Pu}$ establishes a clear and formal connection with several mixed valent lanthanide systems. In the derivation of $\tilde{H}^{Pu}$, we let the local $5f$ electronic configurations vary from site to site, but the valences are restricted to be $5f^5$ or $5f^6$ due to our assumption of on-site Coulomb interactions much larger than kinetic energy terms. By also assuming that the spin–orbit interaction is large, we derive the lowest energy multiplet of each configuration ($J=5/2$ for $5f^5$ and $J=0$ $5f^6$) and treat the kinetic energy as a perturbation. The resulting Hamiltonian differs from the one in [8–10] by including $f-d$ hybridization. It is important to note that the lowest energy multiplet of each configuration can be derived for any intermediate coupling scheme between LS and $j-j$. The form of the low-energy Hamiltonian remains the same because the total angular momentum of the lowest energy multiplet does not change with the coupling scheme [11].

Below we will sketch the derivation of the model. Our most striking conclusion will be the cancellation of the $f-f$ hopping at low-energies and the consequent similarity between Pu and Ce or mixed valent Sm at low energies.

Model. We start by considering a multi-band model for $5f$-electrons which includes intra-atomic and inter-atomic (hopping) terms for the f-orbitals plus $d-f$ hybridization: $H=H_d+H_{df}+H_f$, where

$$H_d=\sum_{\mathbf{k},l_z,\sigma}\epsilon_{\mathbf{k},l_z}d^\dagger_{\mathbf{k}l_z\sigma}d_{\mathbf{k}l_z\sigma}$$
$$H_{df}=\sum_{\mathbf{k},l_z,\sigma}V_{\mathbf{k},l_z}d^\dagger_{\mathbf{k}l_z\sigma}f_{\mathbf{k}l_z\sigma}+V^*_{\mathbf{k},l_z}f^\dagger_{\mathbf{k}l_z\sigma}d_{\mathbf{k}l_z\sigma} \quad (1)$$
$$H_f=H_{\mathrm{Coul}}+H_{\mathrm{SO}}+H_{\mathrm{K}}+H_{\mathrm{CEF}}$$

with

* Tel.: +1 505 667 5611; fax: +1 505 665 4063.
E-mail address: cdb@lanl.gov

0022-3115/$ - see front matter © 2008 Elsevier B.V. All rights reserved.
doi:10.1016/j.jnucmat.2008.10.018

$$
\begin{aligned}
H_{\rm SO} &= \lambda \sum_{\mathbf{i},l_z,l'_z,\sigma,\sigma'} \zeta_{l_z\sigma,l'_z\sigma'} f^\dagger_{\mathbf{i}l_z\sigma} f_{\mathbf{i}l'_z\sigma'} \\
H_{\rm K} &= \sum_{\mathbf{i},\mathbf{r},l_z,l'_z,\sigma} t^{\mathbf{r}}_{l_z,l'_z}\left(f^\dagger_{\mathbf{i}l_z\sigma} f_{\mathbf{i}+\mathbf{r}l'_z\sigma} + f^\dagger_{\mathbf{i}+\mathbf{r}l'_z\sigma} f_{\mathbf{r}l_z\sigma}\right) \\
H_{\rm CEF} &= \sum_{\mathbf{i},l_z,l'_z,\sigma} (\epsilon_f \delta_{l_z,l'_z} + B_{l_z,l'_z}) f^\dagger_{\mathbf{i}l_z\sigma} f_{\mathbf{i}l'_z\sigma}.
\end{aligned}
\tag{2}
$$

The operators $f^\dagger_{\mathbf{k}l_z\sigma} = \frac{1}{\sqrt{N}}\sum_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} f_{\mathbf{r}l_z\sigma}$ and $d^\dagger_{\mathbf{k}l_z\sigma} = \frac{1}{\sqrt{N}}\sum_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} d_{\mathbf{r}l_z\sigma}$ create f and d electrons in momentum space with angular momentum l and projection l_z (N is the number of lattice sites). H_d describes a broad d-band (it can also have s or p-character) that is hybridized with the f-orbitals via H_{df}. In H_f, $H_{\rm Coul}$ (not displayed) contains all the intra and inter-orbital on-site $f-f$ Coulomb interactions. λ is the spin–orbit coupling and the matrix elements $\zeta_{l_z\sigma,l'_z\sigma'}$ are: $\zeta_{l_z\sigma,l_z\sigma} = l_z\sigma/2$, $\zeta_{l_z+1\downarrow,l_z\uparrow} = \sqrt{12 - l_z(l_z+1)}/2$, $\zeta_{l_z-1\uparrow,l_z\downarrow} = \sqrt{12 - l_z(l_z-1)}/2$, and zero for other cases. $H_{\rm K}$ describes the f-electron kinetic energy due to orbital overlap with $t^{\mathbf{r}}_{l_z,l'_z}$ being the hopping integrals between the l_z and l'_z orbitals of two ions separated by a relative vector $\mathbf{r}$. In $H_{\rm CEF}$, the hermitian crystal field matrix B_{l_z,l'_z} is usually expanded in a basis of Stevens operators [10], and ϵ_f is the average energy of the f-orbitals.

2. Effective Hamiltonian for Pu

The Hamiltonian H is very difficult to solve due to the multiple orbitals and interactions that appear in its expression. This is a good motivation for finding a simpler low-energy effective Hamiltonian by eliminating high-energy degrees of freedom. For this purpose, we will exploit the fact that the intra-atomic interactions are much bigger than the $f-f$ hopping and hybridization terms $H_{\rm K}$ and H_{df}, i.e., we will consider the strong coupling limit of H. In this limit, we need to diagonalize the intra-atomic terms ($H_{\rm Coul} + H_{\rm SO}$) and treat $H_{\rm K}$ and H_{df} as perturbations. The first consequence of this approach is that no more than two different $5f$ valences, $5f^n$ and $5f^{n+1}$, can appear in the low energy spectrum, $E \ll U$, where U is the characteristic magnitude of $H_{\rm Coul}$. States containing other $5f$ configurations have energies of order U higher than the low-energy states. The lowest energy multiplet of $H_{\rm Coul} + H_{\rm SO}$ has total angular momentum $|L-S|$ (for $n+1<7$), where S is the maximum total spin of the configuration and L is the maximum orbital angular momentum for that value of S. Either n or $n+1$ is an odd number. We will use J (I) for the total angular momentum of the f-configuration that has an odd (even) number of electrons.

We will assume that the two stable configurations of metallic Pu are $5f^5(J=5/2)$ and $5f^6(I=0)$. Since the $5f^6(I=0)$ state corresponds to a closed shell configuration, it can be represented by an empty site (zero holes) while the constrained fermion operator $c^\dagger_{\mathbf{i}J_z}$ ($c^\dagger_{\mathbf{i}J_z} c^\dagger_{\mathbf{i}J'_z} = 0$) creates a hole with angular momentum $J=5/2$ and projection J_z. $\tilde{H}^{\rm Pu}$ takes the following form in this representation:

$$
\begin{aligned}
\tilde{H}^{\rm Pu} = &\sum_{\mathbf{i},\mathbf{r},J_z,J'_z} \tau^{\mathbf{r}}_{J_zJ'_z}(c^\dagger_{\mathbf{i}J_z} c_{\mathbf{i}+\mathbf{r}J_z} + \text{H.c.}) + \sum_{\mathbf{i},J_z,J'_z} C_{J_zJ'_z} c^\dagger_{\mathbf{i}J'_z} c_{\mathbf{i}J_z} \\
&+ \sum_{\mathbf{k},J_z} \tilde{\epsilon}_{\mathbf{k}J_z} \tilde{d}^\dagger_{\mathbf{k}J_z} \tilde{d}_{\mathbf{k}J_z} + (\tilde{V}_{\mathbf{k}J_z} \tilde{d}^\dagger_{\mathbf{k}J_z} c_{\mathbf{k}J_z} + \text{H.c.}),
\end{aligned}
\tag{3}
$$

that is an extended version of the infinite U Periodic Anderson model (PAM) since it includes the $f-f$ hopping term that is significant in general for $5f$ systems. The angular momentum of each fermion is J and the hopping amplitude $\tau^{\mathbf{r}}_{J_zJ'_z}$ depends on the initial and final values of J_z and on the bond orientation. The lattice anisotropy is encoded in $\tau^{\mathbf{r}}_{J_zJ'_z}$, which produces a ligand field splitting of the f-quasiparticle bands, and in the crystal field term.

The matrix elements of the effective hopping $\tau^{\mathbf{r}}_{J_zJ'_z}$ and crystal field matrices are

$$
\tau^{\mathbf{r}}_{J_zJ'_z} = \langle \mathbf{i}, J'_z | \langle \mathbf{i}+\mathbf{r}, 0 | H_{\rm K} | \mathbf{i}, 0 \rangle | \mathbf{i}+\mathbf{r}, J_z \rangle,
\tag{4}
$$

$$
C_{J_zJ'_z} = \langle i, J'_z | H_{CEF} | \mathbf{i}, J_z \rangle,
\tag{5}
$$

where $|\mathbf{i}, J_z\rangle$ denotes the state of the site $\mathbf{i}$ with total angular momentum $J=5/2$ ($5f^5$ configuration) and projection J_z. $|\mathbf{i},0\rangle$ denotes the non-magnetic state ($I=0$) of the site $\mathbf{i}$ ($5f^6$ configuration). These single atom states are computed using the intermediate coupling scheme that is adequate for Pu [12].

Self-evident from the form of $\tilde{H}^{\rm Pu}$ is the existence of only one *effective fermion* (one hole) propagating across the lattice despite there being 5 and 6 electrons in each of the stable valence configurations of Pu. This simplification is a natural consequence of the strong Coulomb intra-atomic interactions [9] and the reason why a "dual" $5f$-electron behavior (some of the $5f$-electrons being partially localized) has to be enforced in band structure calculations [13] to reproduce the properties of actinide systems.

To compute the effective hopping tensor, we will assume that the hopping amplitudes, $t^{\mathbf{r}}_{l_z,l'_z}$, that appear in H_K depend only on the two atoms connected by the hopping process. This implies that we can forget the other $N-2$ atoms and isolate the bond $(\mathbf{i},\mathbf{i}+\mathbf{r})$ under consideration. If we choose the quantization-axis along the bond direction, the hopping term must conserve the l_z quantum number. Therefore, the term of H_K that involves the bond $(\mathbf{i},\mathbf{i}+\mathbf{r})$ under consideration is

$$
H_K(\mathbf{i},\mathbf{i}+\mathbf{r}) = \sum_{l_z=-l,l;\sigma} t^{\mathbf{r}}_{l_z}(f^\dagger_{\mathbf{i},l_z\sigma} f_{\mathbf{i}+\mathbf{r},l_z\sigma} + f^\dagger_{\mathbf{i}+\mathbf{r},l_z\sigma} f_{\mathbf{i},l_z\sigma}).
\tag{6}
$$

The time-reversal symmetry implies that $t_{l_z} = t_{-l_z}$. In addition, relative amplitudes of t_{l_z} for different l_z are fixed by the angular dependence of the different f_{l_z} orbitals [14]:

$$
t_0 = 20t^{\mathbf{r}}, \quad t_1 = -15t^{\mathbf{r}}, \quad t_2 = 6t^{\mathbf{r}}, \quad t_3 = -t^{\mathbf{r}},
\tag{7}
$$

where $t^{\mathbf{r}} = \frac{525}{2\pi}\frac{\hbar^2 r_f^5}{m|\mathbf{r}|^7}$, r_f is the f-sate radius, and m is the electron mass. The axial symmetry of $H_K(\mathbf{i},\mathbf{i}+\mathbf{r})$ under rotations around the bond-axis implies that $\tau^{\mathbf{r}}(J^z,J'^z)$ is diagonal: $\tau^{\mathbf{r}}(J^z,J'^z) = \tau^{\mathbf{r}}(J^z,J^z)\delta_{J_z,J'_z}$. By replacing the expression for $H_K(\mathbf{i},\mathbf{i}+\mathbf{r})$ in Eq. (4), we obtain the following expression for the matrix elements of $\tau^{\mathbf{r}}(J^z,J^z)$:

$$
\begin{aligned}
\tau^{\mathbf{r}}(J^z,J^z) &= \sum_{l_z=-3,3;\sigma} t^{\mathbf{r}}_{l_z} \langle \mathbf{i}+\mathbf{r},0|f^\dagger_{\mathbf{i}+\mathbf{r},l_z\sigma}|\mathbf{i}+\mathbf{r},J_z\rangle\langle \mathbf{i},J_z|f_{\mathbf{i},l_z\sigma}|\mathbf{i},0\rangle \\
&= \sum_{l_z=-l,l;\sigma} t^{\mathbf{r}}_{l_z} |\langle 0|f^\dagger_{l_z\sigma}|5/2,J^z\rangle|^2.
\end{aligned}
\tag{8}
$$

The last step follows from the fact that the matrix elements $\langle \mathbf{i}+\mathbf{r},0|f^\dagger_{\mathbf{i}+\mathbf{r},l_z\sigma}|\mathbf{i}+\mathbf{r},J_z\rangle = \langle 0|f^\dagger_{l_z\sigma}|5/2,J^z\rangle$ and $\langle \mathbf{i},J_z|f_{\mathbf{i},l_z\sigma}|\mathbf{i},0\rangle = \langle 5/2,J^z|f_{l_z\sigma}|0\rangle$ do not the depend on the site index.

Clearly, there are two contributions to each diagonal component of the effective hopping tensor from hopping processes of an electron with orbital angular momentum $l_z = J_z \pm 1/2$ and spin $s^z = \mp 1/2$. We note that each of these contributions is multiplied by hopping amplitudes $t_{J_z\pm1/2}$ of opposite sign according to Eq. (7). The magnitude of $\tau^{\mathbf{r}}(J^z,J^z)$ is then determined by the ratio between the matrix elements $\langle 0|f^\dagger_{J_z+1/2\downarrow}|5/2,J^z\rangle$ and $\langle 0|f^\dagger_{J_z-1/2\uparrow}|5/2,J^z\rangle$. We will show below that the values of these ratios lead to an *exact cancellation of effective hopping tensor*. This property distinguishes Pu from the other actinides.

The matrix element under consideration can be rewritten in the following form:

$$
\begin{aligned}
\langle 5/2,j^z|f_{J_z+1/2\downarrow}|0\rangle &= \langle 5/2,j^z|e^{-i\mathbf{J}^2\theta} e^{i\mathbf{J}^2\theta} f_{J_z+1/2\downarrow} e^{-i\mathbf{J}^2\theta} e^{i\mathbf{J}^2\theta}|0\rangle \\
&= e^{-ij(J+1)\theta}\langle 5/2,J^z|e^{i\mathbf{J}^2\theta} f_{J_z+1/2\downarrow} e^{-i\mathbf{J}^2\theta}|0\rangle
\end{aligned}
\tag{9}
$$

where $J=5/2$ and $\mathbf{J}^2$ is the Casimir operator associated to the the total angular momentum $\mathbf{J}$. To obtain the expression for $e^{i\mathbf{J}^2\theta} f_{J_z+1/2\downarrow} e^{-i\mathbf{J}^2\theta}$ it is convenient to write $f_{J_z+1/2\downarrow}$ as a linear combination of annihilation operators f_{j,j_z} with well defined total angular momentum $j = l+s$ and projection j_z:

$$f_{J_z+1/2\downarrow} = \alpha_{j_z} f_{j_1 j_z} - \beta_{j_z} f_{j_2 j_z}$$
$$f_{J_z-1/2\uparrow} = \beta_{j_z} f_{j_1 j_z} + \alpha_{j_z} f_{j_2 j_z}, \tag{10}$$

where $j_1 = 7/2$ and $j_2 = 5/2$. We note that α_{j_z} and β_{j_z} are the Clebsch–Gordan coefficients that result from adding the orbital angular momentum $l = 3$ and the spin $s = 1/2$. By using

$$e^{i\mathbf{J}^2\theta} f_{j j_z} e^{-i\mathbf{J}^2\theta} = e^{ij(j+1)\theta} f_{j j_z}, \tag{11}$$

we obtain

$$e^{i\mathbf{J}^2\theta} f_{J_z+1/2\downarrow} e^{-i\mathbf{J}^2\theta} = e^{ij(j+1)\theta}(\alpha_{j_z}^2 + \beta_{j_z}^2 e^{-i2j}) f_{J_z+1/2\downarrow} + e^{ij(j+1)\theta}\alpha_{j_z}\beta_{j_z}(1 - e^{-i2j}) f_{J_z-1/2\uparrow}. \tag{12}$$

Eqs. (9) and (12) combined with the normalization condition, $\alpha_{j_z}^2 + \beta_{j_z}^2 = 1$, lead to the desired expression for the ratio between matrix elements:

$$\frac{\langle 5/2, j^z | f_{J_z+1/2\downarrow} | 0\rangle}{\langle 5/2, j^z | f_{J_z-1/2\uparrow} | 0\rangle} = \frac{-\beta_{j_z}}{\alpha_{j_z}}. \tag{13}$$

The Clebsch–Gordan coefficients β_{j_z} and α_{j_z} are

$$\alpha_{5/2} = 1/\sqrt{7} \quad \beta_{5/2} = \frac{\sqrt{6}}{\sqrt{7}}$$
$$\alpha_{3/2} = \frac{\sqrt{2}}{\sqrt{7}} \quad \beta_{3/2} = \frac{\sqrt{5}}{\sqrt{7}} \tag{14}$$
$$\alpha_{1/2} = \frac{\sqrt{3}}{\sqrt{7}} \quad \beta_{1/2} = \frac{2}{\sqrt{7}}.$$

Finally, according to Eqs. (7) and (13), we obtain:

$$\tau^{\mathbf{r}}(5/2, 5/2) = t^{\mathbf{r}} |\langle 5/2, 5/2 | f_{3\downarrow} | 0\rangle|^2 \left[-1 + 6\frac{\alpha_{5/2}^2}{\beta_{5/2}^2} \right] = 0$$
$$\tau^{\mathbf{r}}(3/2, 3/2) = t^{\mathbf{r}} |\langle 5/2, 3/2 | f_{2\downarrow} | 0\rangle|^2 \left[6 - 15\frac{\alpha_{3/2}^2}{\beta_{3/2}^2} \right] = 0 \tag{15}$$
$$\tau^{\mathbf{r}}(1/2, 1/2) = t^{\mathbf{r}} |\langle 5/2, 1/2 | f_{1\downarrow} | 0\rangle|^2 \left[-15 + 20\frac{\alpha_{1/2}^2}{\beta_{1/2}^2} \right] = 0.$$

This result is a direct consequence of the cancellation of the single-electron $f - f$ hopping for $j = |l - s| = 5/2$ (single-electron hopping terms $f^\dagger_{\mathbf{i}+\mathbf{r},jj_z} f_{\mathbf{r},jj_z'}$ vanish for $j = |l - s|$ [16]).

In this way, we have demonstrated that the effective hopping tensor of Pu is identically zero no matter what is the value of the hopping amplitudes $t^{\mathbf{r}}$ or what is the coupling scheme (*LS*, intermediate or $j - j$) used to obtain the states of the lowest energy multiplets ($|\mathbf{i}, J_z\rangle$ and $|\mathbf{i}, 0\rangle$). We note that the cancellation of the effective $f - f$ hopping tensor results from a destructive interference between two different low-energy processes. In other words, the dominant Coulomb and spin–orbit interactions frustrate the $f - f$ kinetic energy and increase the tendency towards localization. Therefore, the effective Hamiltonian H^{Pu} becomes a simple periodic Anderson model:

$$\tilde{H}^{\mathrm{Pu}} = \sum_{\mathbf{i} J_z J_z'} C_{J_z J_z'} c^\dagger_{\mathbf{i} J_z'} c_{\mathbf{i} J_z} + \sum_{\mathbf{k} J_z} \tilde{\epsilon}_{\mathbf{k} J_z} \tilde{d}^\dagger_{\mathbf{k} J_z} \tilde{d}_{\mathbf{k} J_z} + (\tilde{V}_{\mathbf{k} J_z} \tilde{d}^\dagger_{\mathbf{k} J_z} c_{\mathbf{k} J_z} + \mathrm{H.c.}), \tag{16}$$

like the one used to describe mixed valent lanthanide systems that fluctuate between a closed shell and a magnetic configuration. Examples of these systems are Ce and mixed valence Sm and Yb compounds. From the point of view of the low-energy effective model that describes the electronic degrees of freedom, Pu is much closer to the $4f$-electron (lanthanide) systems than to the $5f$'s or actinides.

The cancellation of the $f - f$ hopping tensor at low-energies is a unique characteristic of the Pu metal (this is not true for Pu compounds) that makes its low-energy model qualitatively similar to the one used for Ce or mixed valent Sm [15]. This similarity could be the common root for explaining the huge volume expansions observed in both elements. There are several implications of immediate relevance: Magnetism is strongly suppressed in $\tilde{H}^{\mathrm{Pu}}$ when the concentration of f-electrons differs significantly from an integer value, and our results presented in Ref.[7] place both α and δ-Pu in the mixed valence regime in agreement with the observed lack of magnetic ordering [1,18]. In contrast, a serious limitation of band structure calculations is that the *ad hoc* hypothesis of partial localization leads to magnetic ordering in δ-Pu [17].

References

[1] J.C. Lashley et al., Phys. Rev. B 72 (2005) 054416.
[2] P. Javorsky et al., Phys. Rev. Lett. 96 (2006) 156404.
[3] J.C. Lashley et al., Phys. Rev. Lett. 91 (2003) 205901.
[4] B. Johansson, J. Magn. Magn. Mater. 47 (1985) 231.
[5] J.G. Tobin, K.T. Moore, B.W. Chung, M.A. Wall, A.J. Schwartz, G. van der Laan, A.L. Kutepov, Phys. Rev. B 72 (2005) 085109.
[6] S. Méot-Reymond, J.M. Fournier, J. Alloys Compd. 232 (1996) 119.
[7] C.D. Batista, J.E. Gubernatis, T. Durakiewicz, J. Joyce, Phys. Rev. Lett. 101 (2008) 016403.
[8] G. Zwicknagl, A.N. Yaresko, P. Fulde, Phys. Rev. B 65 (2002) 081103(R).
[9] D.V. Efremov et al., Phys. Rev. B 69 (2004) 115114.
[10] T. Hotta, Rep. Prog. Phys. 69 (2006) 261.
[11] The overlap between single-ion eigenstates of the *LS* and $j - j$ coupling schemes is large [10].
[12] G. van del Laan et al., Phys. Rev. Lett. 93 (2004) 097401.
[13] J.M. Wills et al., J. Electron Spectrosc. Rel. Phenom. 135 (2004) 163.
[14] W.A. Harrison, Phys. Rev. B 28 (1983) 550;
J.M. Wills, W.A. Harrison, Phys. Rev. B 28 (1983) 4363.
[15] A. Chainani et al., Phys. Rev. B 65 (2002) 155201.
[16] P. Fulde, J. Keller, G. Zwicknagl, Solid State Phys. 41 (1988) 1.
[17] P. Söderlind, B. Sadigh, Phys. Rev. Lett. 92 (2004) 185702.
[18] R.H. Heffner et al., Phys. Rev. B 73 (2006) 094453.