PHYSICAL REVIEW B VOLUME 44, NUMBER 19 15 NOVEMBER 1991-I

High-energy spectroscopy in uranium-based systems

J. M. Imer, D. Malterre, M. Grioni, P. Weibel, B. Dardel, and Y. Baer
Institut de Physique, Université de Neuchâtel, CH2000 Neuchâtel, Switzerland

(Received 18 June 1991)

We have carried out high-energy spectroscopy measurements (x-ray photoemission on the $4f$ core level, ultraviolet spectroscopy on the valence band, and bremsstrahlung isochromat spectroscopy) on UPd_3, UPt_3, and URh_3 compounds. A progressive localization of the $5f$ states is expected throughout this series: the $5f$ electrons are usually considered to be itinerant in URh_3, localized in UPd_3, and UPt_3 is a heavy-fermion compound. We show that the different spectroscopic measurements cannot be explained with one-electron band-structure calculations and are best analyzed in terms of the Anderson-impurity model. Many-body effects dominate the spectral functions, suggesting that the correlations between the $5f$ electrons play an essential role in the uranium compounds.

I. INTRODUCTION

Electronic correlations are known to play an important role in transition-metal, lanthanide, or actinide compounds. In fact, the physical properties depend on the competition between correlation (the intra-atomic Coulomb interaction U) and effective bandwidth W which results from the direct overlap of the d or f orbitals on different sites and the hybridization of these orbitals with the other bands.[1] In transition metals, the d states are delocalized, so that their mutual overlaps are important and the bandwidth is larger than the Coulomb interaction. Therefore, it is a good approximation to treat the many-body problem by a one-electron Hamiltonian with a local potential containing exchange-correlation terms [for example, the local-density approximation (LDA)]. In the opposite extreme, the electrons are very localized and the band picture is no longer valid ($W \ll U$). This is the situation encountered in rare-earth systems for which the correlations select a $4f^n$ configuration so that many-body atomiclike models are more appropriate. Between these two asymptotical behaviors, a description of the electronic properties is much more complicated, which is the case for transition-metal oxides and many cerium-uranium compounds. Lanthanides and actinides exhibit unusual physical properties such as valence fluctuations, heavy-fermion behavior, and superconductivity which are due to the high correlation of their f states.[2] The localization and itinerancy of the f electrons and their hybridization with the ligand states in compounds are then fundamental points in the understanding of the physical properties of such systems.

High-energy spectroscopies, such as photoelectron spectroscopy (PES), bremsstrahlung isochromat spectroscopy (BIS), and x-ray absorption spectroscopy, are powerful techniques to get information on these different questions,[3-6] but sophisticated many-body models are needed to interpret the experimental spectra. For example, in $4f$ systems, the anomalous physical properties associated with the f states and encountered in many cerium or ytterbium compounds have been satisfactorily described in the framework of the degenerate Anderson model.[7,8] In this model, the strongly correlated atomiclike f orbitals are hybridized with the conduction electrons leading to a singlet ground state separated from the f excited states by the Kondo energy ($k_B T_K$) which governs the thermodynamic properties. The different phenomenological parameters of the model can be obtained by fitting theoretical spectra to the experimental results. Indeed, the $4f$ Coulomb interaction can be estimated from the energy separation of the different structures appearing in the PES/BIS and core-level x-ray photoemission spectra (XPS). A many-body resonance, whose position with respect to the Fermi level determines the low-energy excitations (Kondo energy) and thus the low-temperature properties, has been observed in high-resolution ultraviolet photoemission spectroscopy (UPS).[9,10] Moreover, these spectroscopic results are consistent with thermodynamic measurements like magnetic susceptibility and specific heat.[11] On the contrary, densities of states obtained from LDA calculations give neither a good description of the PES/BIS spectra nor a satisfactory value of the linear coefficient of the specific heat.[2]

Some uranium compounds exhibit behaviors similar to those observed in cerium systems. Nevertheless, their occupied valence-band spectra do not resemble those of cerium. They always present a broad structure near the Fermi level[12] which is sometimes in qualitative agreement with band calculations. In contrast to cerium systems, the importance of correlation in the $5f$ spectral function is not obvious and the fundamental question raised by this situation is the validity of a band formalism for describing the $5f$ electrons. Despite extensive studies in the last few years, this question remains open. The calculated one-electron bands of heavy-fermion systems are too broad to account for the large value of the linear coefficient of the specific heat and still too narrow to account for the measured $5f$ spectral functions.[13] On the other hand, the applicability of the impurity Anderson model to uranium systems is controversial. In this approach, a heavy-fermion behavior is associated with a weak hybridization and a low Kondo temperature

[$\gamma(0)=1.2$ J/mol. K^2 and $T_K=3$ K in CeAl$_3$ (Ref. 14)] giving rise to a narrow f structure at E_F in the spectral function. The observation of large γ in certain uranium compounds [i.e., $\gamma=430$ mJ/mol. K^2 in UPt$_3$ (Ref. 15)] should reflect the strongly localized character of the $5f$ electrons. However, the experimental structure at the Fermi level is too wide to be consistent with a Kondo resonance and the $5f$ electrons are usually considered to be more extended than the $4f$ ones even in heavy-fermion systems. Thus, both approaches, the band picture and the single-impurity Anderson model, seem to miss important aspects of the $5f$ electrons in uranium compounds.

In this paper we would like to investigate the consequence of $5f$ localization on the high-energy spectroscopic results and see how far one model can describe the evolution of the spectroscopic results. We have carried out high-resolution ultraviolet valence-band photoemission, BIS, and core-level x-ray photoemission in the three typical uranium compounds UPd$_3$, UPt$_3$, and URh$_3$, where a progressive delocalization of the $5f$ electrons occurs. The $5f$ states in UPd$_3$ are known to be localized, UPt$_3$ exhibits a heavy-fermion behavior, and URh$_3$ is described in terms of a band picture.

The paper is organized as follows. In Sec. II sample preparation and instrumental techniques are briefly described. Section III is devoted to the presentation of the experimental results: UPS, XPS, and BIS spectra of the different compounds are presented. Finally, in Sec. IV we discuss the results and attempt to investigate if a description in the framework of a many-body model is more appropriate than a comparison with calculated band-structures available in the literature.

II. EXPERIMENTAL DETAILS

Samples were made by arc-melting the constituent materials several times under argon atmosphere. X-ray powder diffraction patterns have confirmed the single-phase nature of each sample. URh$_3$ crystallizes in the cubic AuCu$_3$ structure, whereas UPd$_3$ and UPt$_3$ present a hexagonal phase of the TiNi$_3$ and MgCd$_3$ type, respectively.

The different measurements were performed in an apparatus combining UPS, XPS, and BIS spectroscopies. In all experiments, the sample was cooled below 20 K. In UPS the overall energy resolution estimated from the width of the Fermi step is better than 20 meV. Monochromatized Al $K\alpha$ radiation was used for XPS measurements, yielding an energy resolution of about 0.3 eV. BIS spectra were obtained with a photon energy of 1486.6 eV and a total-energy resolution of 0.5 eV was achieved. The pressure was in the low 10^{-10} Torr range. Clean samples were obtained by scraping the surface with a diamond file.

III. EXPERIMENTAL RESULTS

A. Valence-band spectra

Figure 1 shows the He II ($h\nu=40.8$ eV) spectra of UPd$_3$, UPt$_3$, and URh$_3$. Inelastic backgrounds have been removed by a standard procedure.[16] These spectra are dominated by the transition-metal d states which form a band 6–8 eV wide. In URh$_3$, a narrower structure (0.5 eV wide) at the Fermi level has been attributed to the $5f$ states.[17,18] In UPt$_3$ this structure is strongly reduced and it completely disappears in UPd$_3$. In this latter compound, the spectrum exhibits several features labeled $A-D$ according to the notation of the XPS study by Baer, Ott, and Andres.[19] Comparison with ThPd$_3$ leads these authors to the conclusion that peak A ($E=0.9$ eV) reflects the $5f$ states, whereas the other structures represent the palladium-derived d states. This conclusion has been confirmed by resonant photoemission experiments.[20] The absence of $5f$ intensity at the Fermi level is usually considered as an indication of the localized character of $5f$ states in UPd$_3$. For UPt$_3$ and URh$_3$, the transition-metal-derived density of states prevents a reliable determination of a $5f$ contribution below -1 eV.

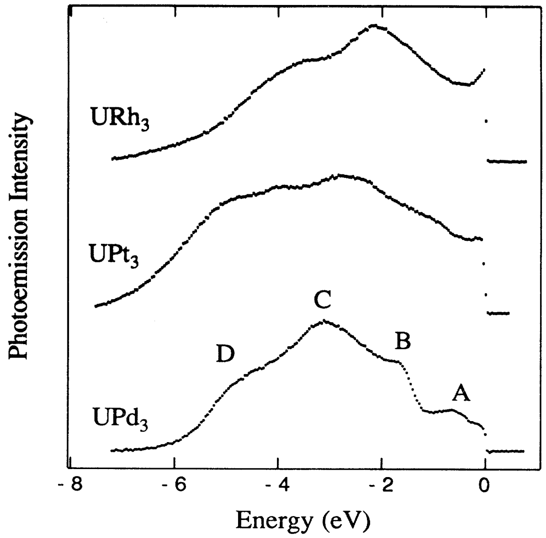

FIG. 1. UPS He II ($h\nu=40.8$ eV) spectra of URh$_3$, UPt$_3$, and UPd$_3$.

The spectra of Fig. 1 show that the $5f$ weight at the Fermi level (E_F) increases with increasing itinerant character of the $5f$ states. Nevertheless, the origin of this intensity remains an open question: does it represent the formation of a $5f$ band as claimed by band-calculation specialists[21,22] or does it reflect the tail of a Kondo resonance as observed in cerium systems? The calculated one-electron $5f$ widths are usually too small to account for the measured PES/BIS spectra[23] and the predictions for the linear coefficient of the specific heat are one order or even several orders of magnitude smaller than the experimental results in heavy-fermion compounds.[2] On the other hand, the interpretation of the PES structure at E_F in terms of a Kondo resonance is not straightforward. In the single-impurity model, the weaker the weight of the Kondo resonance, the larger the mass enhancement. Such a behavior is actually observed in cerium heavy-fermion systems.[11] In uranium systems like UPt$_3$, the weight and the width of the structure at E_F are too strong to be compatible with the large value of the specific heat. However, we showed recently that the introduction of multiplets in an Anderson impurity calculation qualitatively modifies the spectral function[17] so that the spectral weight near E_F not only reflects the Kondo resonance but also a manifold of multiplets excited in the final states of uranium. Therefore, the valence-band experimental spectra could be compatible with an Anderson model even for uranium systems.

B. BIS spectra

In Fig. 2 we have plotted the BIS spectra of the three compounds. As the *p* and *d* states only give a broad structureless feature, these spectra essentially reflect the unoccupied part of the $5f$ spectral function. A spectacular evolution is observed with increasing localization of the $5f$ orbitals. In URh_3, the BIS spectrum exhibits a relatively narrow structure (2–3-eV width) located at about 1 eV above the Fermi level. In UPt_3, a second contribution appears at 3 eV and in UPd_3 both contributions have similar weight and give a broad structure 5–6 eV wide.

Although the width of the URh_3 BIS spectrum (2–3 eV) is compatible with calculated one-electron density of states,[23–25] the spectra of UPd_3 and UPt_3 are again too broad to be described by a band calculation.[26,27] Such a behavior is usually observed in heavy-fermion compounds. The large width of the BIS spectra has been interpreted in terms of different final states: a well-screened peak near the Fermi level corresponding to the $5f$ band and a poorly screened peak at higher energy resulting from the screening by nonlocalized valence electrons or from $5f^{n+1}$ final states.[28,29] Therefore an increase in the relative intensity of the poorly screened peak would reflect a decrease in $5f$ hybridization and then an increase in the $5f$ localization.

We think that this description in terms of well and poorly screened final states or in terms of pure $5f$ configurations is not suitable for uranium compounds. The hybridization between $5f$ and the conduction states is larger and the $5f$ Coulomb interaction smaller than in the case of cerium compounds, so that the final states are strongly mixed. We will discuss this point in the next section.

C. 4*f* XPS spectra

In Fig. 3 the uranium $4f$ core-level spectra are reported for UPd_3, UPt_3, and URh_3. The spectra show an 11-eV splitting into $4f_{7/2}$ and $4f_{5/2}$ components. In UPt_3 and UPd_3 the main lines are significantly broader and more asymmetric than in URh_3. Small satellites are visible at higher binding energies in all spectra but their intensities are nearly constant in the series. It has been suggested that the intensity of these high-energy satellites reflects the localized character of the *f* states,[30] but our results do not confirm this suggestion. Despite the width variation of the main structure, the three spectra are rather similar and the strong $5f$ localization, which occurs from URh_3 to UPd_3, weakly affects the $4f$ spectral function. This quasi-insensitivity of core-level spectra to localization contrasts with the situation encountered in cerium materials, where the delocalization of $4f$ states induces the formation of satellites in the core-level photoemission spectra. These satellites are associated with mixed final states and their intensities in the framework of the Anderson model allow an estimation of the hybridization strength and $4f$ electronic configuration in the ground state. In the next section we will discuss the

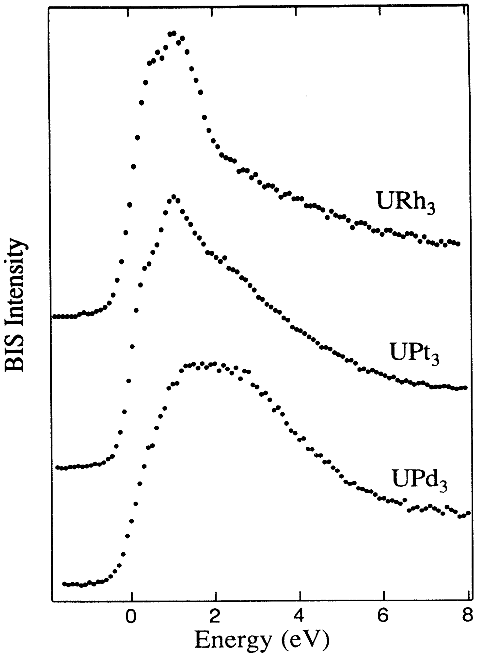

FIG. 2. Inverse photoemission spectra ($h\nu = 1486.6$ eV) of URh_3, UPt_3, and UPd_3.

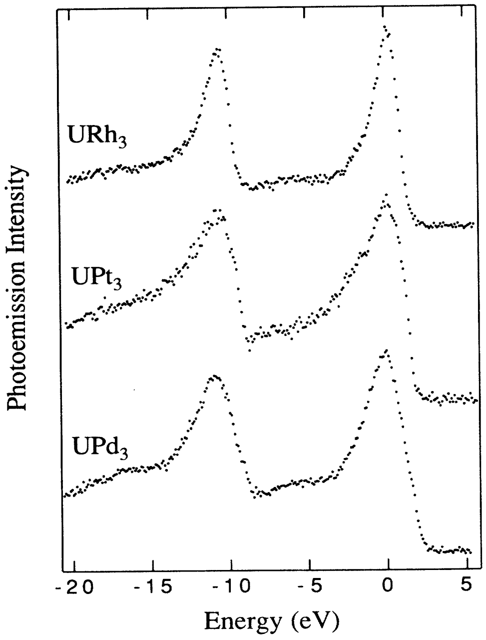

FIG. 3. X-ray photoemission spectra on the uranium $4f$ level of URh_3, UPt_3, and UPd_3.

core-level spectra of uranium compounds in the framework of the Anderson impurity model.

IV. DISCUSSION

It seems now well established that the XPS and BIS $5f$ spectral functions exhibit many-body effects which cannot be described by a density-functional calculation: the calculated one-electron $5f$ widths of heavy-fermion materials are usually significantly smaller than the measured valence-band UPS and BIS spectra.[31,32] These discrepancies in highly correlated solids are not surprising. Indeed, in the LDA the ground state of an interacting electron system is described by a one-electron Schrödinger equation (the well-known Kohn-Sham equation) including a correlation and exchange potential.[33] On the other hand, the electronic excitations (valence-band spectra) are determined by one-particle Green functions. It has been shown that although the chemical potential μ and the Fermi surface are correctly described with the LDA formalism, the eigenvalues of the Kohn-Sham equation for $\varepsilon_k \neq \mu$ must not be interpreted as corresponding to elementary excitations.[34] Although in normal metals the band calculations give a qualitative description of the photoemission spectra, the use of LDA calculations to interpret the spectroscopic results in narrow-band systems is questionable. Different attempts to improve the LDA description have been proposed. For example, to account for the different structures of the valence-band spectrum in cerium compounds, a LDA supercell model has been developed.[35] In this approach, one assumes that one cerium site has either one more or one less $4f$ electron in the final state so that LDA calculations, with these constraints, give the position of the atomiclike $4f^2$ and $4f^0$ peaks. Nevertheless, the calculated effective mass is not in agreement with experimental results (linear coefficient of the specific heat).

Recently, a comparison of "exact" Monte Carlo results with a LDA calculation has shown that a one-dimension periodic Anderson lattice model provides a better description of specific heat, BIS/PES spectra, and magnetic properties than the LDA.[36] This was the motivation to analyze our spectroscopic results in the framework of the Anderson impurity model and to simulate the different spectral functions (UPS, XPS, BIS) with the same set of parameters. As shown in the preceding section, the $5f$ signal of UPd_3 and UPt_3 is masked by the transition-metal conduction states so that we will restrict our discussion to the unoccupied part of the $5f$ spectral function (BIS) and to the core-level spectra. Nevertheless, we have shown recently that the occupied part could also be described by an impurity Anderson model modified to include the $5f$ multiplet effects. The calculations we present here are carried out with the Gunnarsson-Schönhammer model[8] initially developed for cerium systems and more recently used for uranium oxide[37] and uranium-based intermetallics.[38] As shown in Ref. 37, this model can be extended to uranium systems by introducing renormalized parameters. We restrict the basis states to the $5f^2$, $5f^3$, and $5f^4$ configurations. As suggested by a renormalized atom calculation,[39] we choose for the Coulomb interaction $U_{ff}=2$ eV and for the energy difference between the $5f^2$ and $5f^3$ configurations $\varepsilon_f=0.8$ eV (this situation contrasts with the case of cerium where $U_{ff}=7$ eV and $\varepsilon_f=1.5-2$ eV) so that the hybridization will more strongly mix the different configurations.

In Fig. 4 we have reported several $4f$ XPS spectra calculated for different hybridization strengths. We also indicate in this figure the population of $5f$ states (n_f) for the different parameters. We notice that n_f is nearly constant when the hybridization strength Δ increases by a factor of 6. This behavior reflects the mixing of the 3 configurations favored by the small values of U_{ff} and ε_f. An increase of Δ simultaneously enhances the weight of the $5f^4$ and $5f^2$ configurations in the ground state so that the resulting changes of the $5f$ population cancel each other. For large hybridization strength ($\Delta=0.3$ eV), the spectrum is dominated by a narrow line and satellites appear at higher binding energies. When the hybridization decreases, a progressive broadening of the main line is observed as well as an increase in the satellite intensities. Comparison with experimental data shows that the satellite intensities are overestimated in the calculation but the narrowing of the main line with increasing Δ is correctly reproduced. Such a description of the core-level photoemission spectra in terms of the Gunnarsson-Schönhammer model has been previously attempted for Th and U compounds,[40,41] and it has been shown that the final states are strongly mixed, leading to a dependence of the spectra on the shape of the conduction band in contrast to the cerium case. Therefore an improved version of the model taking into account a more realistic energy dependence of the hybridization strength and an explicit multiplet splitting describing the coupling of the $4f$ hole with the different $5f$ configurations should be developed

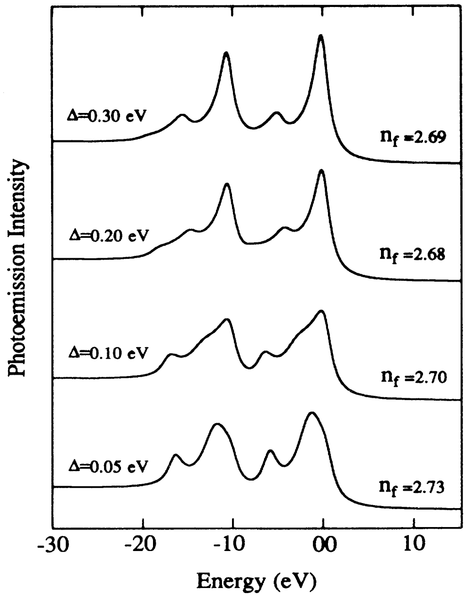

FIG. 4. Calculated uranium $4f$ spectra for different values of the hybridization strength Δ ($\varepsilon_f=0.8$ eV and $U_{ff}=2$ eV).

for uranium systems. The energy dependence of the hybridization strength could be estimated from band calculations but the determination of the multiplet structure is a very complicated problem involving relativistic atomic calculations with two open f shells in intermediate coupling.

The calculated BIS spectra with the same set of parameters are reported in Fig. 5. Two structures are found around 1 and 3 eV showing a strong relative intensity dependence on hybridization: the high-energy peak decreases with increasing hybridization strength. In order to simulate the experimental data, we have convoluted our calculated spectra with a Gaussian [full width at half maximum (FWHM) = 2 eV]. We think that the multiplet splitting of the relevant final-state configurations is responsible for this broadening. An atomic calculation supports this suggestion by showing that the BIS spectra extend up to several eV for the different $5f$ configurations of uranium.[42] We have also added a "background" modeled by an arctan function to describe the transition into the unoccupied p and d states. With this crude calculation, the experimental results (Fig. 2) are roughly reproduced. As discussed above, sophisticated one-electron band calculations cannot explain the width of the BIS structure: two narrow structures of mainly $5f_{7/2}$ and $5f_{5/2}$ character are predicted in the first 2 eV above the Fermi level in these three compounds[24–27] and then the one-electron density of states is significantly narrower than the observed spectra. In spite of its limitations, the description of BIS with the Anderson model seems to be more appropriate than the one given by the LDA, corroborating the one-dimension Anderson lattice approach.[36]

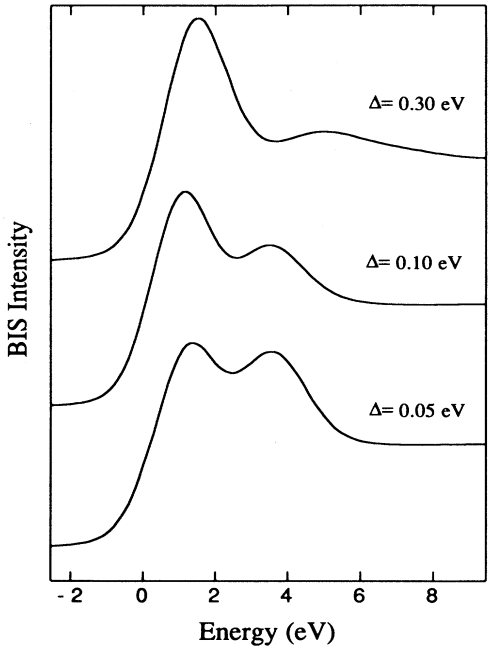

FIG. 5. BIS calculated spectra for different values of the hybridization strength Δ. The calculated spectra were convoluted with a Gaussian function to simulate the broadening due to the multiplet effect. A background was added to account for the transition into the unoccupied p and d states.

V. CONCLUSION

In this paper, we have presented and discussed the spectroscopic properties of several uranium compounds. We have studied the influence of the progressive localization of $5f$ electrons on different spectral functions (U $4f$ XPS, BIS, PES). In PES the $5f$ weight is partially masked by the transition-metal d states. Nevertheless, a systematic behavior is observed: the $5f$ contribution at the Fermi level decreases with increasing localization. The $4f$ core-level spectra appear to be less sensitive to the $5f$ localization: only a broadening of the main line is observed. On the contrary, BIS spectra exhibit a spectacular evolution: a structure at 3 eV above E_F seems to be correlated with the localization; it strongly increases from URh_3 to UPd_3. This modification of the $5f$ BIS spectra cannot be interpreted on the basis of LDA band-structure calculations. On the other hand, we show that an impurity Anderson model correctly simulates the evolution of the BIS but difficulties are found in the description of the XPS $4f$ spectra with the same set of parameters. These results indicate that the impurity Anderson model gives a qualitative description of the spectra of uranium systems. However, this approach should certainly be improved by including the multiplet structure or the energy dependence of the hybridization strength. On the other hand, for light actinide compounds band calculations fail to reproduce the $5f$ excitation spectra, especially in heavy-fermion compounds, but they provide a good description of ground-state properties such as cohesion energy, lattice parameters, etc.[43] This situation clearly demonstrates that correlation plays an important role in the properties of uranium systems. At the present time, the predictions of the LDA formalism seem not to be reliable beyond the ground-state properties, whereas many-body calculations based on the single-impurity model show encouraging agreement with the excitation spectra. This description with two complementary approaches underlines their respective limitations and is not very satisfactory. Further decisive progress in the elucidation of these uranium compounds awaits the development of a broader formalism yielding a unified interpretation of their different properties.

ACKNOWLEDGMENT

This work has been supported by the Fonds National Suisse de la Recherche Scientifique.

---

[1] L. Hedin and S. Lundqvist, in *Solid State Physics*, edited by F. Seitz, D. Turnbull, and H. Ehrenreich (Academic, New York, 1969), Vol. 1, p. 1.

[2] P. A. Lee, T. M. Rice, J. W. Serene, L. S. Sham, and J. W. Wilkins, Comments Condens. Matter Phys. **12**, 99 (1986).

[3] J. C. Fuggle, F. . Hillebrecht, Z. Zolnierek, R. Lässer, Ch. Freiburg, O. Gunnarsson, and K. Schönhammer, Phys. Rev. B **27**, 7330 (1983).

[4]J. W. Allen, S. J. Oh, O. Gunnarsson, K. Schönhammer, M. B. Maple, and M. S. Torikachvili, Adv. Phys. **35**, 275 (1986).

[5]J. W. Allen, J. Magn. Magn. Mater. **76-77**, 324 (1988).

[6]Y. Baer and W. D. Schneider, *Handbook on the Physics and Chemistry of Rare-Earths,* edited by K. A. Gschneidner, L. Eyring, and S. Hüfner (Elsevier, Amsterdam, 1987), Vol. 10, p. 1.

[7]P. W. Anderson, Phys. Rev. **124**, 41 (1961).

[8]O. Gunnarsson and K. Schönhammer, Phys. Rev. B **28**, 4315 (1983).

[9]F. Patthey, B. Delley, W.-D. Schneider, and Y. Baer, Phys. Rev. Lett. **55**, 1528 (1985).

[10]F. Patthey, B. Delley, W.-D. Schneider, and Y. Baer, Phys. Rev. Lett. **58**, 1283 (1987).

[11]F. Patthey, J.-M. Imer, W.-D. Schneider, H. Beck, Y. Baer, and B. Delley, Phys. Rev. B **42**, 8864 (1990).

[12]J. M. Imer, Ph.D. thesis, Université de Neuchâtel, 1990.

[13]J. W. Allen, S. J. Oh, L. E. Cox, W. P. Ellis, M. S. Wire, Z. Fisk, J. L. Smith, B. B. Pate, I. Lindau, and A. J. Arko, Phys. Rev. Lett. **54**, 2635 (1985).

[14]K. Andres, J. E. Graebner, and H. R. Ott, Phys. Rev. Lett. **35**, 1779 (1975).

[15]G. R. Stewart, A. L. Giorgi, B. L. Brandt, S. Foner, and A. J. Arko, Phys. Rev. B **28**, 1524 (1983).

[16]S. Tougaard, Phys. Rev. B **34**, 6779 (1986).

[17]J. M. Imer, D. Malterre, M. Grioni, P. Weibel, B. Dardel, Y. Baer, and B. Delley, Phys. Rev. B **43**, 1338 (1991).

[18]A. J. Arko, C. G. Olson, D. M. Wieliczka, Z. Fisk, and J. L. Smith, Phys. Rev. Lett. **53**, 2050 (1984).

[19]Y. Baer, H. R. Ott, and K. Andres, Solid State Commun. **36**, 3680 (1980).

[20]B. Reihl, N. Mårtensson, D. E. Eastman, A. J. Arko, and O. Vogt, Phys. Rev. B **26**, 1842 (1982).

[21]P. Marksteiner, P. Weinberger, R. C. Albers, A. M. Boring, and G. Schadler, Phys. Rev. B **34**, 6730 (1986).

[22]B. D. Dunlap, G. W. Crabtree, J. D. Jorgensen, H. A. Kierstead, D. D. Koelling, W. K. Kwok, D. J. Lam, S. K. Malik, A. W. Mitchell, and S. C. Strite, Phys. Rev. B **39**, 5640 (1989).

[23]O. Eriksson, B. Johansson, M. S. S. Brooks, and H. L. Skriver, Phys. Rev. B **40**, 9508 (1989).

[24]T. Oguchi and A. J. Freeman, J. Magn. Magn. Mater. **61**, 233 (1986).

[25]A. J. Arko, B. W. Yates, B. D. Dunlap, D. D. Koelling, A. W. Mitchell, C. G. Olson, M. Del Guidice, Z. Fisk, and J. L. Smith, in *Theoretical and Experimental Aspects of Valence Fluctuations,* edited by L. C. Gupta and S. K. Malik (Plenum, New York, 1987), p. 39.

[26]R. C. Albers, A. M. Boring, and N. E. Christensen, Phys. Rev. B **33**, 8116 (1986).

[27]R. C. Albers, Phys. Rev. B **32**, 7646 (1985).

[28]C. Laubschat, W. Grentz, and G. Kaindl, Phys. Rev. B **37**, 8082 (1988).

[29]F. U. Hillebrecht, D. D. Sarma, and N. Mårtensson, Phys. Rev. B **33**, 4376 (1986).

[30]W. D. Schneider and C. Laubschat, Phys. Rev. Lett. **46**, 1023 (1981).

[31]A. J. Arko, B. W. Yates, B. D. Dunlap, D. D. Koelling, A. W. Mitchell, D. J. Lam, Z. Zolnierek, C. G. Olson, Z. Kisk, J. L. Smith, and M. del Guidice, J. Less-Common Met. **133**, 87 (1987).

[32]J. W. Allen, J. Magn. Magn. Mater. **76-77**, 324 (1988).

[33]P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).

[34]L. J. Sham and W. Kohn, Phys. Rev. **145**, B561 (1966).

[35]N. R. Norman, D. D. Koelling, and A. J. Freeman, J. Magn. Magn. Mater. **47-48**, 255 (1985).

[36]M. M. Steiner, R. C. Albers, D. J. Scalapino, and L. J. Sham, Phys. Rev. B **43**, 1637 (1991).

[37]O. Gunnarsson, D. D. Sarma, F. U. Hillebrecht, and K. Schönhammer, J. Appl. Phys. **63**, 3676 (1988).

[38]A. Grassmann, Physica B **163**, 547 (1990).

[39]J. F. Herbst and R. E. Watson, Phys. Rev. Lett. **34**, 1395 (1975).

[40]D. D. Sarma, F. U. Hillebrecht, O. Gunnarsson, and K. Schönhammer, Z. Phys. B **63**, 305 (1986).

[41]J. W. Allen, J. S. Kang, Y. Lassailly, M. B. Maple, M. S. Torikachvili, W. Ellis, B. Pate, and I. Lindau, Solid State Commun. **61**, 183 (1987).

[42]F. U. Hillebrecht, H. J. Trodahl, V. Sechovsky, and B. T. Thole, Z. Phys. B **77**, 373 (1989).

[43]B. Johansson, O. Eriksson, M. S. S. Brooks, and H. L. Skriver, Phys. Scr. **T13**, 65 (1986).