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TITLE POSSIBLE FERMI LIQUID BEHAVIOR OF 5f ELECTRONS IN UPt_3 AT $T >> T_K$

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SUMMARY

The energy of localized electrons should be independent of crystal momentum. Thus the energy of 5f electrons in heavy Fermion systems far above T_K is expected to show no E vs. k dispersion. We have used angle-resolved photoemission spectroscopy on the [10$\bar{1}$0] surface of UPt_3, cleaned by repeated sputter and anneal, to study any possible dispersion of the 5f bands at T = 300 $K >> T_K \approx 50$ K. The measurements were performed at the Synchrotron Radiation Center in Stoughton, WI, at a photon energy hv = 40 eV. At this energy the 5f cross-section is already sufficiently large to yield a significant 5f spectral weight, but not yet large enough to lose all k-dependence. Data were taken at various angle settings of a VG ADES 400 spectrometer along the Γ-M direction in the hexagonal zone. The overall instrument resolution was 250 meV while the acceptance cone of the analyzer was $\pm 2^0$, or about 20% of the Γ-M direction.

Although no dispersion was observed at normal emission by varying the photon energy, substantial energy dispresion, primarily in the d-bands, was evident with k_{11} (i.e., by changing the angle θ while keeping hv constant). From resonant photoemission experiments we established that the primary peak associated with 5f intensity is the peak within 200 meV of E_F. Although our resolution was insufficient to observe any energy shifts, the peak disappeared at several angles near the M-point in the zone. We interpret this as dispersion above E_F. While further measurements are necessary, this raises questions regarding the accepted models for the electronic structure.

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Abstract

The very likely existence of dispersion in the 5f spectra obtained in angle-resolved photoemission at 300K raises questions about the localized nature of 5f electrons at room temperature.

The consensus of opinnion[1-5] regarding heavy fermions is that the f-electrons above T_K are localized with a well-defined moment, and have little or no hybridization with the ligand d-electrons. As the temperature is lowered, a Kondo-like spin compensation occurs, obeying Bose statistics, which suppresses magnetism and allows eventual formation of a Fermi liquid within the Kondo lattice. Thus, below T_K we obtain well-defined heavy electron f-bands which, because of Luttingers theorem, have the same Fermi surface[6,7] as bands obtained from an LDA calculation. The difference is only that they are narrower, thus yielding a much larger effective mass than that obtained from an LDA calculation.

The effect of uncompensated spins at elevated temperatures is rather dramatic on these Kondo lattice bands. Even before T_K is reached, it is expected that the strong magnetic scattering from the small number of uncompensated spins will strongly suppress the hybridization. Indeed, the suppression is exponential in T. Thus the Kondo resonance, and any dispersion associated with the Kondo lattice f-bands, is non-existent at $T>T_K$. This magnetic scattering is responsible for the rapid rise in $\rho(T)$ near T_K.

We have used angle-resolved photoemission spectroscopy[8] on the [1010] surface of UPt_3 to study any possible disprsion of the 5f bands at $T = 300$ K$>>T_K \sim 50$ K[5]. The measurements were performed at a photon energy $h\nu$ = 40 eV where the 5f cross-secton is already sufficiently large to yield a significant 5f spectral weight, but not yet large enough to lose all k-dependence. Data were taken at various angle settings of a VG ADES 400 spectrometer along the Γ-M direction in the hexagonal zone. The overall instrument resolution was 250 meV while the acceptance cone of the analyzer was $\pm 2^0$, or about 20% of the Γ-M direction. Thus this represent a relatively low relsoution experiment with respect to the information we are seeking, but it is nonetheless sufficient to give us an indication of possible dispersion.

No dispersion was observed at normal emission by varying the photon energy. This indicates that UPt_3 is in the limit of total non-conservation of $k_\perp$ (i.e., escape depths are very small). On the other hand, substantial energy dispresion of peaks in the photocurrent was evident with $k_{||}$ (i. e., by changing the angle θ while keeping hν constant) since the peaks in the photocurrent should now be due to van Hove singularities in the one-dimensional density of states. This is shown in Fig. 1, where most of these dispersive features below -1 eV can be associated with platinum d-orbitals. Here we display energy distribution curves (EDC 's) at several settings of the analyzer angle with respect to the [1010] direction along the Γ-K-M line in the Brillouin zone. From resonant photoemission experiments we established that the primary peak associated with 5f intensity is the peak within 200 meV of E_F. This is verified by cross-section measurements as well, since no peak is evident for hν < 30 meV. The large, strongly dispeivise peak at -1 ev is primarily uranium d-like in character, as determined from the 6p - 6d resonance at hν =19eV.

Focusing on the 5f peak, we note first of all that it is nearly dispersionless within our resolution of 250 meV. We must point out, however, that LDA calculations would predict a dispe.sion which is smaller than our instrument resolution . However, at polar angles $\theta = 17.5^0$ and 20^0 the peak is absent, reappearing at larger values of θ. The disappearance of the 5f peak can be interpreted as being due to dispersion of a 5f band above E_F near the point M in the Brillouin zone. Its subsequent reappearance reflects the fact that there is mirror symmetry about the M-point as we continue probing along the Γ-M-Γ line in the hexagonal zone. A cross-section argument to explain the disappearance of the peak is less compelling than the dispersion arguement because of the fact that we are in the regime of complete non-conservation of $k_\perp$. All transitions are allowed on the basis of momentum arguements. Moreover, a similar dispersion is actually predicted[9].

The existence of dispersion at 300 K would seem at odds with the expectations of localized electrons. We have already shown previously[10] that there is no temperature dependence of the DOS between 20K and 300K in UPt_3 so that we do not anticipate any temperature dependence in the dispersion. Clearly more work will need to be done, at much higher resolution, to verify the existence of dispersion at 300K. If substantiated, however, it will require some re-thinking regarding the basic underlying assumptions of heavy Fermion phenomena.

1. P.A. Lee, T.M. Rice, J.W. serene, L.J. Sham, J.W. Wilkins, Comments Cond.Mat. Phys. **12,** 99 (1986).

2. C.J. Pethick and D. Pines, Proceedings of the Fifth Int. Conf. on "Recent Progress in Many-Body Theories," Oulu, Finland, Aug. 28, 1987.

3. H. Razafimandimby, P. Julde, and J. Keller, Z. Phys. B **54,** 111 (1984).

4. N. d'Ambrumenil and P. Fulde, J. Magn. Magn. Mater. **47-48,** 1 (1985).

5. G.R. Stewart, Rev. Mod. Phys. **56,** 755 (1984).

6. L. Taillefer, R. Newburg, G.G. Lonzarich, Z. Fisk, J.L. Smith, J. Magn. Magn. Mater. **63-64,** 372 (1987).

7. P.H.P. Reinders, M. Springford, P.T. Coleridge, R. Boulet and D. Ravot, Phys. Rev. Lett. 57, 1631 (1986).

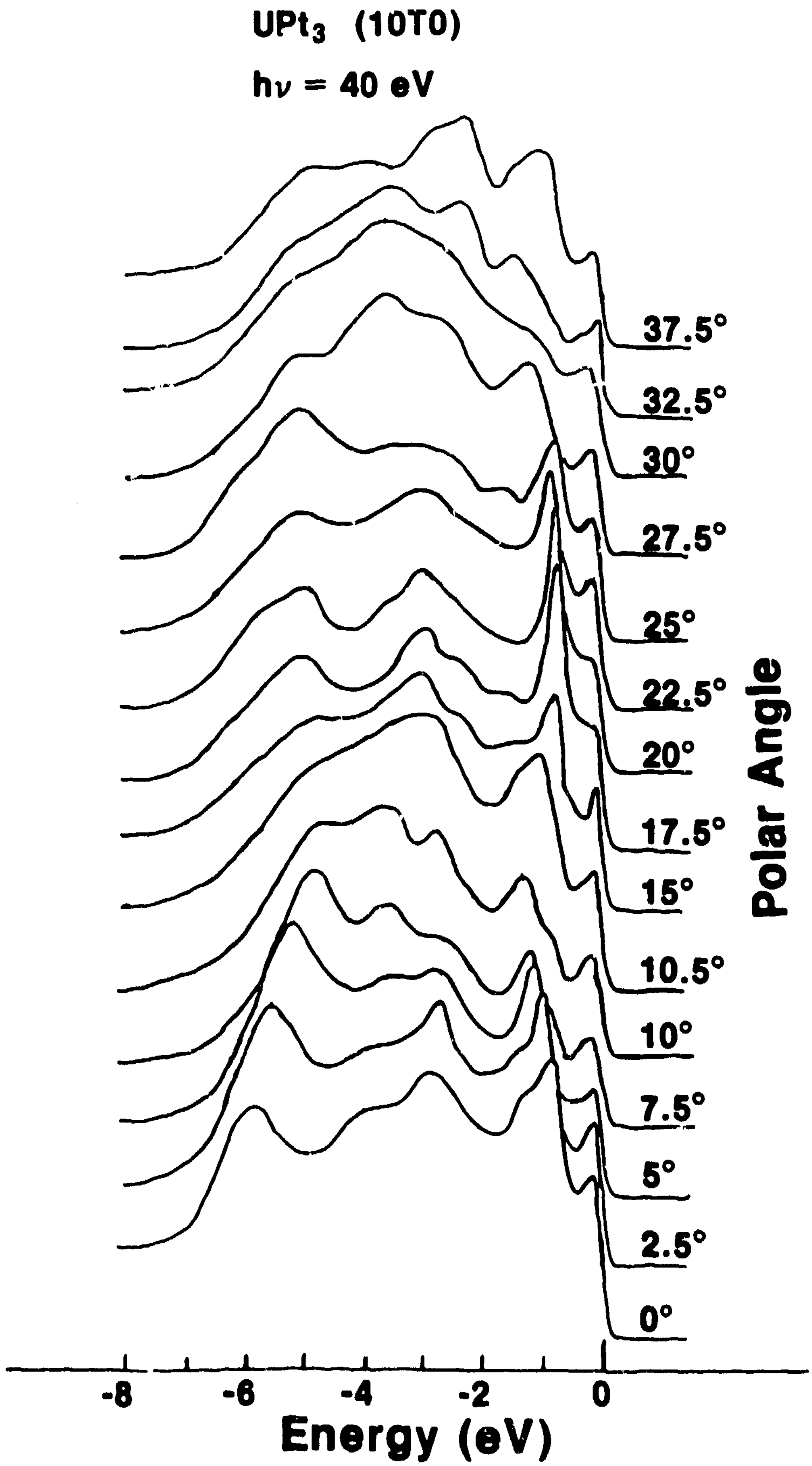
8. A. J. Arko, D. D. Koelling, B. D. Dunlap, C. Capasso, and M. Del Giudice, J. Less Com.Met., **48,** 133 (1989).

9. C.S. Wang, M.R. Norman, R.C. Albers, A.M. Boring, W.E. Pickett, H. Krakauer, N.E. Christensen, Phys. Rev. B 35, 7260 (1987).

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

Figure Caption

Fig. 1 EDC's from a [1010] surface of UPt_3 at $h\nu = 40$ eV, and at various polar angles with respect to the [1010] direction. The feature nearest E_F is due to 5f electrons, and indicates energy dispersion at the M-point in the zone.


UPt$_3$ (10T0)
hν = 40 eV
37.5°
32.5°
30°
27.5°
25°
22.5°
20°
17.5°
15°
10.5°
10°
7.5°
5°
2.5°
0°
Polar Angle
-8
-6
-4
-2
0
Energy (eV)