Effect of electronic correlations on the quasiparticle dispersion of USb$_2$.

Xiaodong Yang$^1$, Peter S. Riseborough$^1$, Tomasz Durakiewicz$^2$, P.M. Oppeneer$^3$, S. Elgazzar$^3$.

$^1$Physics Dept. Temple University, Philadelphia PA 19122, USA.
$^2$Los Alamos National Labs, Los Alamos New Mexico 87545, USA.
$^3$Department of Physics, Uppsala University, Box 530, Sweden.

E-mail: prisebor@temple.edu

Abstract. Angle resolved photoemission experiments have been performed on USb$_2$, and very narrow quasiparticle peaks have been observed in a band which LSDA predicts to osculate the Fermi-energy. The observed band is found to be depressed by 17 meV below the Fermi-energy, furthermore, the inferred quasiparticle dispersion relation for this band exhibits a kink at an energy of about 23 meV below the Fermi-energy. The kink is not found in LSDA calculations and, therefore, is attributable to a change in the quasiparticle mass renormalization by a factor of approximately 2. The existence of a kink in the quasiparticle dispersion relation of a band which does not cross the Fermi-energy is unprecedented. The origin of the observed depression of the band, its quasi-particle mass enhancement, and the characteristic energy are discussed on the basis of a theoretical model.

1. Introduction

The dispersion relations of quasiparticles that are subjected to large mass enhancements are expected to exhibit kinks in the vicinity of the Fermi energy. These kinks occur at a characteristic energy below which the quasi-particles are renormalized by the electronic correlations and above which they are unrenormalized. The kinks in the dispersion relations were first observed by ARPES experiments [1] almost four decades after they were first predicted [2]. Since enhanced quasi-particles are usually described Landau Fermi-liquid theory, the kinks are expected to be confined to the vicinity of the Fermi surface. Hence, the experimental discovery of kinks in USb$_2$ in a band that does not cross the surface is unexpected [3]. In this paper, we present the experimental results and explain theoretically the origin of the observed quasiparticle mass enhancements.

2. Experimental Results

USb$_2$ is a tetragonal material that orders antiferromagnetically with a relatively low Neel temperature of 209K and a relatively large ordered magnetic moments of 1.88 $\mu_B$ [4, 5]. The material has a quasi-two-dimensional character, presumably due to the presence of uranium planes in the structure. The high-quality flux grown single crystals used in the experiment were cleaved in situ under ultra-high vacuum conditions. Our measurements have determined that the bands show minimal dispersion along the c-direction [3], thereby attesting to the quasi-two-dimensional nature of the bands. We have observed that there is a large discrepancy between
the observed low-energy bands near the Γ point and the LSDA bands. The LSDA calculations show a 5f band that osculates the Fermi-energy at the Γ point and disperses quadratically as $k_x$ is increased. The experimentally determined valence band spectra are shown in fig(1) for $k$ values along the Γ-X direction. The data were taken with a photon energy of 34 eV. It is seen that at the Γ point the observed quasi-particle band is depressed to about 17 meV below the Fermi energy, in contrast to the predictions of LSDA. The red markers indicate the quasi-particle energy, and detailed analysis shows that the curvature of the dispersion relation increases by a factor of 2 at $k_x a \approx 0.18 \pi$, indicating a change in the quasiparticle mass. Close to the Γ point, the intrinsic peak width is estimated to be about 3 meV, however, the peak width increases abruptly for $k_x a > 0.18 \pi$. The abrupt change in the curvature and the rapid change in the width of the peak signifies a change in regime from highly renormalized quasi-particles for excitation energies of $\hbar \omega < 21 meV$ to a regime of modest renormalizations for $\hbar \omega > 21 meV$.

**Figure 1.** The electronic spectral density for USb$_2$ measured along the Γ-X direction.

**Figure 2.** The calculated dimensionless electronic spectral density for various values of $ka/\pi$. The spectral density is plotted in units of $\omega_D$ against the dimensionless frequency $\omega/\omega_D$, where $\omega_D$ is the Debye frequency.

3. Theory
The electronic structure is modeled by two bands taken from the LSDA. One band osculates the Fermi energy at the Γ point and the other has a maximum at the Γ point of about 110 meV and cuts the Fermi energy at the wave vector $k_F a \approx 0.55 \pi$.

The spectral density was obtained by treating the electron-phonon interaction as a perturbation via Green’s function techniques. The unperturbed single-electron Green’s functions are denoted by $G_0^{\sigma,\tau}(k, \omega)$ and are given by

$$G_0^{\sigma,\tau}(k, \omega) = \frac{\delta^{\sigma,\tau}}{\hbar \omega + \mu - \epsilon_k^{\sigma} + i \eta_k}$$

(1)

where $\sigma$ and $\tau$ are band indices. The Green’s functions $G^{\sigma,\tau}(k, \omega)$ for the interacting electrons are given in terms of the bare Green’s function and the self-energies $\Sigma^{\sigma,\rho}(k, \omega)$ via the matrix
Dyson’s equations

\[ G^{\sigma,\tau}(k, \omega) = G_0^{\sigma,\tau}(k, \omega) + \sum_{\rho,\lambda} G_0^{\sigma,\rho}(k, \omega) \Sigma^{\rho,\lambda}(k, \omega) G^{\lambda,\tau}(k, \omega) \]  \hspace{1cm} (2)

Using the structure of the unperturbed Green’s functions, Dyson’s equations can be re-written as a pair of matrix equations. The matrix of electronic self-energies is calculated from the phonon-emission and absorption processes \[2\] and is given by

\[ \Sigma^{\sigma,\rho}(k, \omega) = \frac{1}{N} \sum_{\tau,q,\alpha} \lambda_{q,\alpha}^{\sigma,\tau} \lambda_{q,\alpha}^{\tau,\rho,\ast} \left[ \frac{1 - f_{k-q} + N_q}{\hbar \omega + \mu - \epsilon_{k-q}^{\tau} - \hbar \omega_{q,\alpha}} + \frac{f_{k-q} + N_q}{\hbar \omega + \mu - \epsilon_{k-q}^{\sigma} + \hbar \omega_{q,\alpha}} \right] \]  \hspace{1cm} (3)

where \( \lambda_{q,\alpha} \) are the electron-phonon coupling constants. The vertex corrections have been neglected in accordance with Migdal’s theorem \[6\]. For the intraband scattering processes, the electron-phonon coupling constant will be assumed to be independent of the band indices \( \sigma \) and \( \tau \).

The self-energy which is off-diagonal in the band indices is quite unremarkable but does have the effect of repelling the two branches of the electronic dispersion relation, and contributes to the depression of the observed band below the Fermi energy. The intra-band processes for the osculating band does has an imaginary part which gradually falls to zero as the Fermi energy is approached. From a Kramers-Kronig analysis, one finds that this has the consequence that the real part of the intra-band self-energy has a maximum near this energy and, therefore, does not result in a renormalization of the quasi-particle mass. On the other hand, the inter-band self-energy describes the scattering of an electron involving a momentum change of \( qa \approx 0.54\pi \), with either the emission or absorption of a virtual phonon. This produces a narrow gap in the imaginary part of the inter-band self-energy of the order of \( 2 \hbar \omega_q \) where the imaginary part falls rapidly to zero. The abrupt drop of the imaginary part of the inter-band self-energy results in a rapidly varying real part which produces the quasi-particle mass enhancement. The spectral density calculated from the imaginary parts of the Green’s function is shown in fig(2). It is seen that in addition to the quasi-particle peak the spectra shows the presence of an incoherent structure at energies near \( \omega_D/2 \).

4. Discussion

For small values of \( k \), the calculated spectral density shows a narrow quasiparticle width which disperses quadratically, however, the inferred effective mass is increased by a factor of approximately two over the band mass. For larger values of the momentum, the width of the quasi-particle peak rapidly broadens and the peak disperses quadratically but at a rate determined by the unrenormalized band mass, as shown in fig(3). It is seen that the cross-over from the renormalized quasiparticle peak to the unrenormalized peak occurs at an energy given by approximately \( qa/\pi \omega_D \), in contrast to the standard description of electron-phonon mass enhancements where the cross-over occurs at \( \omega_D \). This difference occurs since the interband scattering process is responsible for the quasi-particle mass srenormalization and this involves low-energy excitations of electrons between the bands near which require a finite momentum transfer. This finding is in accordance with the experimental results, since the observed cross-over occurs at an energy which is significantly lower than the reported Debye frequency \[5\].

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Figure 3. The dispersion for the various features in the calculated electronic spectrum (solid lines). The dashed redline represents the rigidly shifted band dispersion relation found from the LSDA calculations, and the dashed blue line represents the shifted dispersion relation with the renormalized quasiparticle mass.

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