Fermi Surface Smearing Studied by 2D-ACAR and CP

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Keywords: 2D-ACAR, Compton Profile, Li, Al, γ-Sn, Correlations

Abstract. A detailed analysis of 2D-ACAR data in Al, Li and γ-Sn suggests the existence of a tail above the Fermi momentum. It is attributed to the electronic correlations. We discuss this new finding and compare it with high-resolution Compton profile measurements.

Large electron-electron correlations have been observed in Li [1] by high-resolution (~0.1 a.u.) Compton profiles (CP) experiments. They lead to an increased smearing of the Fermi break due to a tail located above the Fermi momentum \( p_F \). In the case of 2D-ACAR, it is believed that electron-positron correlations affect mainly the shape of the profile below \( p_F \) [2, 3], inducing an increase of the pair momentum density, called Kahana's enhancement, a trend opposite to the electronic correlations.

Above \( p_F \), Carbonne [4] argued that the partial annihilation rate is essentially zero, due to an effective cancellation of certain terms, as compared with the well-known high-momentum many-body tail of the interacting electron gas. However, his arguments are qualitative. Therefore, a tail above \( p_F \), cannot be excluded in 2D-ACAR. So far, this has never been discussed in the literature, despite the high resolution (up to 0.033 a.u. [5]) of the 2D-ACAR spectrometers.

In this report, we analyse 2D-ACAR (Al, Li and γ-Sn) and CP (γ-Sn) measurements. These simple free-electron-like metals were chosen because a clear Fermi surface break is observed and their core contribution is small. We present fits of the data with simple models. For Al, we also show a comparison with momentum densities obtained from LMTO band structure calculations.

The 2D-ACAR measurements on Al [6], Li [7] and γ-Sn [8] were performed at low temperature using annealed single crystals. In Al, a second measurement was made on the same sample with the 2D-ACAR spectrometer of NIRIM. The agreement is excellent. No significant positron trapping was observed by positron lifetime measurements in the Al and γ-Sn samples.

For a precise analysis of the 2D-ACAR results, it is important to know precisely the experimental resolution function. This has been determined (Fig. 1) by fitting a double gaussian function to the positronium (Ps) peak in quartz, measured at 4.2 K. We obtain an intense \( I_1 = 96.5\% \) narrow component \( \phi(w_1) = 0.035 \text{ a.u.} \) and a weak \( I_2 = 3.5\% \) wider component \( \phi(w_2) = 0.16 \text{ a.u.} \). The result is insensitive to the way the core contribution is fitted; a gaussian provides an excellent fit over all the measured momentum range.

For Al we calculated 2D-ACAR by LMTO, while for Li and γ-Sn we used a model very similar to the one described in [6]. In this model, the 2D-ACAR is constructed from the following three contributions: 1) a spherical component for the valence electrons, 2) an exponentially decaying tail above \( p_F \), and 3) a gaussian for the core contribution. The model, which neglects the
Kahana enhancement, is convoluted with the double gaussian resolution function determined from the Ps peak. For our analysis, we selected lines in the 2D-ACAR which are not affected by high-momentum components.

For Al (Fig. 2) the agreement of the LMTO calculation with the measured 2D-ACAR is very good when we add a tail to the calculated pair-momentum distribution. At large $p_z$, the agreement with the core part is remarkable, as already observed for other materials [9]. In Li (Fig. 3) and $\gamma$-Sn, good agreements are also obtained when a tail is included above $p_F$ in the model.

For the three metals, we can also obtain reasonable fits without including tails if we use a much broader resolution ($fwhm_2 = \sim 0.7$ a.u., $I_2 = 2\%$). But we discard this solution because it is not supported by the measurement of the resolution from the Ps peak.

In the CP measurement from $\gamma$-Sn performed at ESRF, we observe a smearing of the Fermi break larger than the experimental resolution ($fwhm = 0.18$ a.u.) [10]. This difference, as in 2D-ACAR, can be attributed to a tail. We show the fit containing a tail in Fig. 4. Here an inverted parabola has been used to describe the valence electrons and a polynomial of degree 3 for core electrons.

In conclusion, our results suggest the systematic presence of tails above the Fermi momentum in 2D-ACAR and CP measurements. These tails are ascribed to the many-body correlations. We think that they have not been observed in the coincidence Doppler measurements [11] because of the lack of resolution of this technique.

References


Fig. 1. Fit of the Ps peak in quartz with a double gaussian resolution function.
Fig. 2. <110> line from 2D-ACAR in Al projected along [110]. Measurements performed in
Geneva (crosses) and at NIRIM (circles) are shown. Calculated core: dashed line. Total pair
momentum calculated by LMTO: with (solid line) and without (dashdot line) tail above \( p_F \)

Fig. 3. 2D-ACAR lines from Li. Fitted core: dashed line. Many-body tail: lower solid line.
Total (with tail above \( p_F \)), convoluted with the resolution function: solid line.
Fig. 4. CP from \( \gamma \)-Sn. Fitted core: dashed line. Total, with tail: prior convolution (dashdot)
and after convolution (solid line) with the experimental resolution.

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