MS09.04.05 SOME NEW INELASTIC SCATTERING RESULTS CONCERNING ELECTRON CORRELATION IN Li METAL. W. Schuelke, G. Stutz, A. Kaprolat and K. Hoeppner, Institute of Physics, University of Dortmund, D-44221 Dortmund, Germany

The standard correction of LDA(local-density approximation)-calculated Compton profiles with respect to correlation, the so-called Lam-Platzman (LP) correction is isotropic and makes use of the occupation number density n(k) of a correlated free electron system. High resolution directional Compton profile measurements on Li metal, which we have performed at DESY/ HASYLAB, have shown the following deviations from LDA-calculated and LP-corrected profiles where we shall interpret these deviations in terms of additional correlation effects: (i) The orientation dependence of these deviations, seen in the directional Compton profile differences, can be explained as a consequence of a coupled mode of a hole and a plasmon, so-called *plasmaron*, in the spectral density function, which determines the hole-creation in the Compton scattering process. (ii) The strong smearing of the Fermi-discontinuity in the experimental data, seen in the derivatives of the Compton profiles, as well as the lower maximum value of the absolute profiles, when compared with the LDA-calculations, can partly be traced back to the life-time broadening of the spectral density function of the recoil electrons. (iii) The occupation number density n(k), that we have reconstructed by utilizing theorems about Fourier-transformed Compton profiles does not fit, within the limits of current theories, calculated n(k)'s of correlated free electron systems. It is believed that this discrepancy between theory and experiment should urge calculations of n(k) for lattice-bound electron systems, which should take into account both additional collective modes of electrons in an ion-lattices, the so-called zone boundary collective states, seen by the author in measurements of the dynamical structure factor of Li, which can also couple to the holes, and the hole-phonon coupling. The findings concerning n(k) have found strong support by a semi- empirical determination of the local-field-correction function G(q) of electrons in Li metal, which we have performed using measurents of the dynamical structure factor. The much stronger increase of G(q) for q>2kF (kF=Fermi-momentum), than predicted by current theories, can be interpreted, according to Farid et al. (1993), as being due to the same behaviour of n(k), which we have found for the reconstructed n(k).

Farid B., Heine V., Engel G.E. & Robertson I.J. (1993). Phys. Rev. B 48, 11602