Many-Pole Model Calculations of Inelastic Losses in XPS[1] J.J. KAS, J.J. REHR, University of Washington, M. GUZZO, L. REINING, Ecole Polytechnique — Inelastic losses such as satellites in x-ray photo-emission spectra (XPS) are difficult to treat theoretically due to the importance of many-body effects beyond the quasi-particle approximation. Here we present an approach based on an exponential (i.e., cumulant) representation[2] of the one-particle Green's function, together with[3] a many-pole model of the dielectric function, which incorporates dynamic effects beyond the GW approximation. In this method the photo-electron is treated as in inverted LEED state which couples to the system via neutral, quasi-boson excitations. The approach yields an approximation to the XPS in terms of a convolution of a quasi-particle calculation and a spectral function that includes contributions from both intrinsic and extrinsic excitations,[4] as well as interference between them. The method is illustrated with recent experimental results.[5]

[2]M. Guzzo et al., Phys. Rev. Lett. **107**, 166401 (2011)
[3]J. Kas et al., Phys. Rev. B **76**, 195116 (2007)
[4]L. Hedin et al., Phys. Rev. B **58**, 15565 (1998)
[5]Guzzo, op. cit.

J. J. Kas
University of Washington

Date submitted: 13 Dec 2011   Electronic form version 1.4