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Basic aspects of the asymmetry of lineshapes in photoemission spectra caused by a cascade of excitations of Fermi-level electrons

The effect of cascade excitations of Fermi-level electrons on the lineshape of photoemission spectra was treated by Doniach and Sunjic (DS) in 1970.1 Their derived lineshape has many issues such as its lack of integrability and failure to closely reproduce experimental data.2 We analyze this problem using a formalism rooted only in the basic quantum mechanics of resonances with a minimalist diagrammatic veneer to categorize the many-body of processes (Tougaard losses, plasmons/hole-shielding, multiplet structure, and perhaps the Shirley background). The accounting for these processes can be done with varying levels of rigor, from simple consideration of energy scales, oscillator strengths, and couplings, through to ab initio calculations of matrix elements. A density-matrix formulation in the many-body space can be applied to remove spurious interferences of states that have ill-defined/incoherent relative phases (differ from shot to shot, due to pulse noise, sample inhomogeneities, temperature, etc.). In our work, we will apply the simplest level of semi-quantitative analysis to propose possible alternatives to the problematic DS lineshape. For example, an incoherent superposition of exponential decays in time yields a lineshape that is asymmetric but integrable.

1 S. Doniach and M. Šunjic, "Many-electron singularity in X-ray photoemission and X-ray line spectra from metals," Journal of Physics C: Solid State Physics 3, 285–291 (1970).

2 A. Herrera-Gomez, D.M. Guzman-Bucio, A.J. Carmona-Carmona, O. Cortazar-Martinez, M. Mayorga-Garay, D. Cabrera-German, C.A. Ospina-Ocampo, B.V. Crist, and J. Raboño-Borbolla, "Double Lorentzian lineshape for asymmetric peaks in photoelectron spectroscopy," Journal of Vacuum Science & Technology A 41(4), (2023).

3 A. Herrera-Gomez, D. Cabrera-German, A. D. Dutoi, M. Vazquez-Lepe, S. Aguirre-Tostado, P. Pianetta, D. Nordlund, O. Cortazar-Martinez, A. Torres-Ochoa, O. Ceballos-Sanchez, and L. Gomez-Muñoz, "Intensity modulation of the Shirley background of the Cr 3p spectra with photon energies around the Cr 2p edge," Surface and Interface Analysis 50, 246–252 (2018).

Keywords

Doniach-Sunjic lineshape, final state effects, multiplets, double-Lorentzian, AAnalyzer

Reference

Double Lorentzian lineshape for asymmetric peaks in photoelectron spectroscopy." Alberto Herrera-Gomez, et. al. Journal of Vacuum Science and Technology A 41, 043208 (2023); doi: 10.1116/6.0002602. ISSN 0734-2101.

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