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Cumulant approach for electronic excitations in x-ray and electron spectra[1]

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A quantitative treatment of electronic excitations and other many-body effects in x-ray and electron spectra has long been challenging. Physically, electronic correlations and atomic vibrations lead to inelastic losses and damping effects that are ignored in ground state methods or approximations such as TDDFT. Quasi-particle (QP) approaches such as the GW approximation yield significant improvements, as demonstrated in real-space Greens function [1] and GW/Bethe-Salpeter equation [2] calculations, but still ignore multi-electron excitations. Recently such excitations have been treated with considerable success using cumulant expansion techniques and the quasi-boson approximation [3,4]. In this beyond QP approach, excitations such as plasmons and electron-hole excitations appear as satellites in the spectral function. The method naturally accounts for multiple-satellites and can be extended to include extrinsic losses and interference effects. Extensions for effects of vibrations and strong correlations including charge-transfer satellites may also be possible [5]. These advances are illustrated with a number of applications.

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