Real-time cumulant approach for inelastic losses in x-ray spectra
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Intrinsic inelastic losses in core level x-ray absorption (XAS), emission (XES), and
x-ray photo-emission spectra (XPS), arise from excitations of the system due to
the sudden creation or annihilation of a deep core hole. Additional extrinsic losses
arise during the propagation of the photoelectron, and interference processes are also
important. These excitations are reflected in the satellite peaks observed in XPS.
Formally the distribution of these excitations are described in terms of the core-hole
spectral function, which can be calculated in terms of the core-hole Green’s function
represented in exponential form. Here we discuss an approach for calculating the
exponent, or cumulant in terms of local density fluctuations via real-space, real-time
time-dependent density functional theory. The role of extrinsic and interference
terms is also discussed. Our method is illustrated in calculations of XAS and XPS
for number of systems, including weakly correlated as well as d- and f-electron
materials.

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