Theories of X-ray spectra in Extreme conditions: Real time and Finite-temperature

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Recently there has been considerable interest in x-ray spectra in extreme conditions. Here we discuss several theoretical developments to treat such spectra, including both real time (RT) and finite-temperature (FT) methods. The RT approach is illustrated with calculations of charge-transfer satellites in x-ray photoemission spectroscopy (XPS) using a cumulant Green's function approach with RT-TDDFT calculations of the cumulant [1]. A second example is the development of a real-time, velocity-gauge TDDFT for both core- and valence spectra from intense sources [2]. Next we discuss the development of a finite temperature extension of TDDFT that includes explicit calculations of exchange and correlation effects in the TDDFT kernel $f_{xc}(T,n)$ [3,4]. Finally we describe an extension the theory for FT calculations of x-ray spectra over a broad range of temperatures and densities, including the warm dense matter regime. As an example, the method is applied to a two-temperature model for the analysis of pump-probe XAS experiments.

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