Beyond perturbation theory: multi-photon and non-radiative recombination effects in spectroscopies

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The conventional calculation of scattering cross sections relies on a treatment based on time-dependent perturbation theory that provides formulation in terms of Green's functions in the frequency domain. In equilibrium, it boils down to evaluating a simple spectral function equivalent to Fermi's golden rule, which can be solved efficiently by a number of numerical methods. However, away from equilibrium, the resulting expressions require a full knowledge of the excitation spectrum and eigenvectors to account for all the possible allowed transitions and intermediate states, a seemingly unsurmountable complication. We have recently presented a new paradigm to overcome these hurdles[1-4]: we explicitly introduce the scattering particles (neutron, electron, photon, positron) and simulate the full scattering event by solving the time-dependent Schrödinger equation. The spectrum is recovered by measuring the momentum and energy lost by the scattered particles, akin an actual energy-loss experiment. I here show how these ideas can be generalized to study multi-photon processes such as coincidence ARPES, and the interplay between radiative and non-radiative recombination channels in X-ray spectroscopies.

References:

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