Ab initio Theory and Computation of Correlated Multiple-Particle Excitations in Materials

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Abstract:
Excited-state phenomena in a material typically give rise to its defining attributes and determine its usefulness. These phenomena are particularly important in processes of energy generation, transport and storage. However, *ab initio* methods for them - especially for correlated multiple-particle (3- or 4-particle) excitations, nonlinear optical processes, and ultra-fast electron dynamics including relevant electron-electron interactions - have been under explored and hence limiting their studies for real materials. In this talk, we report recent progress on the *ab initio* theory and computation of such excited-state phenomena based on the interacting Green's function approach to many-body perturbation theory. We present our new formalism and computational method on 3- and 4-particle Green's functions with applications to trions, biexcitons, and singlet fission. We also present our development of a time-dependent GW approach to the study of time-dependent processes and nonlinear optics, in particular, the phenomenon of shift currents.

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