Excitons in solids with time-dependent density-functional theory: the bootstrap kernel and beyond

Young-Moo Byun and Carsten A. Ullrich

Department of Physics and Astronomy, University of Missouri
Columbia, Missouri 65211, USA

Time-dependent density-functional theory (TDDFT) is an efficient method to describe the optical properties of solids.\textsuperscript{1} Lately, a series of bootstrap-type exchange-correlation (xc) kernels\textsuperscript{2} have been reported to produce accurate excitons in solids, but different bootstrap-type kernels exist in the literature, with mixed results.\textsuperscript{3} In this presentation, we review and clarify the status of the bootstrap kernels and present a new empirical TDDFT xc kernel to compute excitonic properties of semiconductors and insulators efficiently and accurately. We also discuss the recently proposed nonempirical screened exact-exchange (SXX) approach for excitonic properties,\textsuperscript{4} which can be viewed as a first step towards an excitonic hybrid TDDFT functional. SXX performs well for bound excitons and continuum spectra in both small-gap semiconductors and large-gap insulators, with a computational cost much lower than that of solving the Bethe-Salpeter equation.

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