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Time-dependent optimized effective potential for quantum wells
HARSHANI WIJEWARDANE, CARSTEN A. ULLRICH, Department of Physics and Astronomy, University of Missouri-Columbia — Most present applications in time-dependent density-functional theory employ adiabatic approximations for the exchange- correlation (XC) potential, ignoring all functional dependence on densities at previous times. In this talk, we describe the electron dynamics in quantum wells beyond the adiabatic approximation, using the time-dependent optimized effective potential (TDOEP) method. In TDOEP, the XC potential is a functional of the time-dependent orbitals, and follows from an integral equation over space and time. We solve the full TDOEP integral equation for quantum well intersubband dynamics in exact exchange as well as self-interaction corrected ALDA. Various properties of the resulting time-dependent XC potential, such as its asymptotics, memory dependence, and discontinuity upon population of a new subband level are discussed. This work is supported by NSF DMR-0553485 and Research Corporation.

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