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Three- to two-dimensional crossover in time-dependent densityfunctional theory¹ SHAHRZAD KARIMI, CARSTEN ULLRICH, University of Missouri — Quasi-2D systems, such as an electron gas confined in a quantum well, are important model systems for many-body theories. Earlier studies of the crossover from 3D to 2D in ground-state DFT showed that local and semilocal exchangecorrelation functionals which are based on the 3D electron gas are appropriate for wide quantum wells, but eventually break down as the 2D limit is approached. We now consider the dynamical case and study the performance of various linearresponse exchange kernels in TDDFT. We compare approximate local, semilocal and orbital-dependent exchange kernels, and analyze their performance for inter- and intrasubband plasmons as the quantum wells approach the 2D limit. 3D (semi)local exchange functionals are found to fail for quantum well widths comparable to the 2D Wigner-Seitz radius, which implies in practice that 3D local exchange remains valid in the quasi-2D dynamical regime for typical quantum well parameters, except for very low densities.

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Carsten Ullrich University of Missouri

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