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Approaching the quantum limit for plasmonics: linear atomic chains EMILY TOWNSEND, GARNETT BRYANT, National Institute of Standards and Technology — Linear atomic chains, such as atom chains on surfaces, linear arrays of dopants in semiconductors, or linear molecules, provide ideal testbeds for studying quantum plasmonics in nanosystems. We study the many-body excitations of finite (10-25) linear atomic chains. We use both time-dependent density functional theory (TDDFT) and exact diagonalization to analyze the excitations. TDDFT reveals optically driven excitations that can be single-particle-like, plasmon-like or mixed states. Such states can have very different dependencies on the electron-electron interaction strength, which can be used to help identify the states. TDDFT can identify plasmonic resonances, but it does not reveal how to quantize them. Exact diagonalization is used to get the full quantum description. However, exact diagonalization results can be very different from TDDFT results. Highly correlated, multi-excitonic states, also strongly dependent on the electron-electron interaction strength, appear in the exact response but not in TDDFT excitation spectra. These excitonic many-body states make it hard to identify plasmonic excitations. Exact results are also strongly dependent on the strength of the exchange interaction. We present these results to show how quantum plasmons appear in linear atomic chains.

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