

Abstract Submitted
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Performance of the exact adiabatic density functional to describe Rabi physics JOHANNA ILDEMAR FUKS, Nano-Bio Spectroscopy group and ETSF Center, Dpto. Física de Materiales, Universidad del País Vasco, Av. Tolosa 72, E-20018 San Sebastian, Spain, NICOLE HELBIG, Forschungszentrum Jülich D-52425 Jülich Germany, HEIKO APPEL, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany, ILYA TOKATLY¹, ANGEL RUBIO², Nano-Bio Spectroscopy group and ETSF Center, Dpto. Física de Materiales, Universidad del País Vasco, Av. Tolosa 72, E-20018 San Sebastian, Spain — Through the exact solution of few-electron systems interacting with a monochromatic laser we study the performance of adiabatic density functionals within time-dependent density-functional theory (TDDFT) to reproduce Rabi oscillations. The non-linear dynamics of the Kohn-Sham (KS) system shows the characteristic features of detuned Rabi oscillations even if the exact resonant frequency is used. We illustrate this effect by comparing the exact time-dependent many-body solution of a He-atom in one dimension and a few-site Hubbard model with the solution of TDDFT-KS equations for different adiabatic exchange-correlation functionals. Preventing the detuning introduces a new strong condition to be satisfied by approximate new xc-functionals.

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