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Widths of Autoionizing Resonances from TDDFT[1] SHARMA GOLDSON, CHRIS CANAHUI, Hunter College, City University of New York , NEEPA MAITRA, City University of New York and Hunter College — Autoionizing resonances arising from a bound single excitation lying in the continuum can be captured with the usual adiabatic approximations for the exchange-correlation kernel of time-dependent density functional theory, but those arising from a double excitation cannot. We test a recently derived frequency-dependent kernel [Phys. Chem. Chem. Phys. 11, 4655 (2009)] for the width of the He atom $2s^2$ resonance, and explore the sensitivity on the ground-state approximation used.

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