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Autoionizing Resonances in TDDFT[1] HARSHANI WIJEWARDANE, AUGUST KRUEGER, GABRIELLA MULLADY, NEEPA MAITRA, Hunter College of the City University of New York — In an independent particle picture such as the Kohn-Sham system, bound states with an energy above one of the occupied orbital ionizations are truly bound. When interaction is accounted for, configuration coupling turns the bound state into an autoionizing resonance. In exact TDDFT, it is the exchange-correlation kernel that mixes the ionized and bound state, creating a Fano resonance profile. Although autoionization peaks arising from single excitations have been accurately captured with the available functional approximations, resonances arising from double excitations lying in the continuum are missing. By studying a simple model system, we uncover the features of the exact exchange-correlation kernel that are needed to capture the lifetimes and lineshapes of these resonances accurately.

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