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Calculating Auger Lifetimes Directly from Time Propagation using the Multiconfiguration Time-Dependent Hartree-Fock Method[1]
BRANT ABELN, C. WILLIAM MCCURDY, Department of Chemistry, University of California, Davis, DANIEL HAXTON, Chemical Sciences Division, Lawrence Berkeley National Laboratory — A recent implementation of the multiconfiguration time-dependent Hartree-Fock (MCTDHF) method using an underlying discrete variable representation for the time dependent orbitals as well exterior complex scaling of all electronic coordinates is used to calculate Auger decay rates for states of Be^+. In this approach all electrons are active and the number of orbitals and thus the size of the configuration space can be increased to give improved descriptions of these metastable states. After first populating the $1s2s^2$ (^2S), and the two $1s2s2p$ (^2P) metastable states, we calculated the autocorrelation function of the initial wave function under field-free propagation. In the simplest approach, the Fourier Transform of the autocorrelation function, $\langle\Psi(0)|\Psi(t)\rangle$, can be fit to a Breit-Wigner profile to extract the lifetime and energy of the Auger decaying states. We discuss this and other methods of using MCTDHF to compute the lifetimes of core excited states of atoms and diatomic molecules using this three-electron system as the test case.

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