PROBING EXCITED STATES BY PHOTOELECTRON IMAGING: DYSON ORBITALS WITHIN EQUATION OF MOTION COUPLED-CLUSTER FORMALISM

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Angular distribution of photoelectrons (PAD) contains information about electronic wave functions and thus can be used to determine the nature of the state, as well as monitor its changes in the course of reactions. However, the interpretation of PADs in terms of molecular orbital composition of the ionized state is not straightforward. PADs are related to the so called Dyson orbitals, which can be as states of the leaving electron. Calculation of Dyson orbitals for the ground and excited states within equation-of-motion formalism is described and demonstrated by examples.