Adventures in the wavepacket land: DEA of water

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A time-dependent description of the dissociative attachment of water is presented. The molecule is excited by an impinging electron to a resonance state . Water provides a serious challenge and test for theories of polyatomic resonant vibrational excitation, dissociative attachment and electron impact dissociation, and, not at last, is one of the key molecule to all known life in the Universe. It became clear that some of the most interesting phenomena arise from the interplay of the electronic scattering dynamics with the dynamics of nuclear motion, in particular vibration and dissociation of the molecule. Furthermore, recent developments on the time-dependent formulation of the low-lying theory and novel scattering experiments with low-energy electrons on water, encourage a deeper treatment of the molecular dynamics for the interpretation of the scattering cross section. Our approach breacks up into two parts: electron scattering and nuclear motion dynamics. The fixed-nuclei electron-molecule scattering calculations will be performed inside the framework of the R-matrix approach
[J. D. Gorfinkiel et al., J. Phys. B: At. Mol. Opt. Phys. 35 No 3, 543-555]. Wavepacket methods will be used to treat the nuclear motion. The formation and decay of resonances as modified by the coupling with the nuclear motion inform us that for systems with many degrees of freedom a time-dependent picture is needed. Computational methods and algorithms will also be presented to solve the nuclear problem in order to reduce the computational effort that scales exponentially with the number of vibrational degrees of freedom. The methods are sufficiently general and the subject enough multidisciplinary to be applied to the analysis and interpretation of different physical systems, such as other triatomic molecules and processes of interaction between matter and light.