Abstract Submitted
for the DAMOP18 Meeting of
The American Physical Society

Semiclassical initial value representation for multimode calculation of dissociative electron attachment processes[1] HARINDRANATH AMBALAMPITIYA, ILYA FABRIKANT, University of Nebraska-Lincoln — Dissociative electron attachment (DEA) to polyatomic molecules plays an important role in a vast variety of chemical processes that happen in nature and in industrial world. DEA calculations performed so far [1] were done either in approximation of one vibrational mode or in the local approximation which describes the nuclear motion in the intermediate resonance state by an effective Schroedinger equation with a local complex potential. In the present paper we develop a multimode theory which goes beyond the local approximation by employing the semiclassical initial value representation [2] for calculation of matrix elements of the Green operator for the nuclear motion. We apply this method to calculation of DEA to the CF_3Cl molecule with inclusion of the C-Cl symmetric stretch mode and the CF_3 umbrella mode. [1] I. I. Fabrikant *et al.*, Adv. At., Mol.,Opt. Phys **66**, 545 (2017). [2] W. H. Miller, J. Phys. Chem. A **105**, 2942 (2001).

[1]Supported by the National Science Foundation

Ilya Fabrikant
University of Nebraska-Lincoln

Date submitted: 22 Jan 2018 Electronic form version 1.4