Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Mixed Quantum-Classical Dynamics Methods for Strong-Field Processes: Multiple-trajectory Ehrenfest dynamics + decoherence terms

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— The exact factorization of the electron-nuclear wave function [1, 2, 3] allows to define the time-dependent potential energy surfaces (TDPESs) responsible for the nuclear dynamics and electron dynamics. Recently a novel coupled-trajectory mixed quantum-classical (CT-MQC) approach based on this TDPES has been developed [4], which accurately reproduces both nuclear and electron dynamics. Here we study the TDPES for laser-induced electron localization with a view to developing a MQC method for strong-field processes [5]. We show our recent progress in applying the CT-MQC approach to the systems with many degrees of freedom. [1] A. Abedi, N. T. Maitra, E. K. U. Gross, Phys. Rev. Lett. 105, 123002 (2010). [2] Y. Suzuki, A. Abedi, N. T. Maitra, K. Yamashita, E. K. U. Gross, Phys. Rev. A, 89, 040501(R) (2014). [3] A. Abedi, F. Agostini, Y. Suzuki, E. K. U. Gross, Phys. Rev. Lett. 110, 263001 (2013); F. Agostini, A. Abedi, Y. Suzuki, S. K. Min, N. T. Maitra, E. K. U. Gross, J. Chem. Phys., 142, 084303 (2015). [4] S. K. Min, F. Agostini, E. K. U. Gross, Phys. Rev. Lett.,115, 073001, (2015). [5] Y. Suzuki, A. Abedi, N. T. Maitra, E. K. U. Gross, Phys. Chem. Chem. Phys., 17, 29271 (2015).

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Date submitted: 05 Nov 2015 Electronic form version 1.4