Abstract Submitted
for the DAMOP12 Meeting of
The American Physical Society

Electron Dynamics with a Mixed Moving/Fixed Frozen Gaussian Basis Set SHUNGO MIYABE, TODD MARTINEZ, Department of Chemistry and The PULSE Institute, Stanford University, Stanford, CA 94305 and SLAC National Accelerator Laboratory, Menlo Park, CA — In this report we simulate the strong field ionization of He atom using frozen Gaussian functions and demonstrate the importance of accurate bound state wavefunction in such a calculation. We expand the time-dependent electronic wavefunction using both static atom-centered Gaussian basis functions and trajectory-guided Gaussian wavepackets. We show that the ground state can be accurately described with a small basis set and we further show that this leads to an improved description of time-dependent processes such as ionization in strong fields. Our method combines the advantages of moving Gaussian wavepackets in the context of strong field attosecond phenomena with the advantages of traditional quantum chemistry techniques for describing low lying electronic states. We have computed the single ionization yield of He atom following its interaction with a 12 fs, 805 nm pulse, and show that the combination of static and moving basis set gives a highly correlated picture of the ionization event. We also computed the potential energy curves of H_2 to show that our method describes the nuclear-dependence of electronic structure very well. In this work, the nuclei are fixed. However, we show how it is possible to model electronic and nuclear dynamics on the same footing.

Shungo Miyabe
Dept of Chemistry and The PULSE Institute, Stanford University and
SLAC National Accelerator Laboratory, Menlo Park, CA 9402

Date submitted: 21 Feb 2012 Electronic form version 1.4