Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

A Comparative Study of Mixed Quantum-Classical and Semiclassical Methods for an Electronic Spectroscopy Benchmark Model PORSCHA MCROBBIE, EITAN GEVA, University of Michigan — We performed a comparative study of the reliability of different mixed quantum-classical and semiclassical approaches to calculating equilibrium one- and two-dimensional electronic spectra. These approaches include the popular second-order Cumulant expansion approximation, the Mixed Quantum-Classical Liouville method, and the Forward-Backward Semiclassical method. The comparison was performed within the framework of a benchmark system that can distinguish between these methods and for which the exact quantum results can be obtained [1]. More recently, this work has been extended to cases where the system is initially prepared in a non-equilibrium state, in order to study electronic pump-vibrational probe type spectroscopies.

Porscha McRobbie
University of Michigan

Date submitted: 27 Nov 2009 Electronic form version 1.4