Toward fast and efficient propagators for path integral simulations of hydrogen, water and more complex clusters

G. Guillon[1,2], T. Zeng[2,3], P.-N. Roy[2]

[1] Lab. ICB, Université de Bourgogne Franche-Comté, 21078 Dijon, France
[2] University of Waterloo, Waterloo Ontario N2L 3G1, Canada
[3] Cornell University, Ithaca, New York 14853, United States

More and more demanding applications of the path integral Monte Carlo method are needed to understand structural properties of clusters made of somehow complex molecules.They are also needed to study thespectra of trapped and embedded species, like organic molecules, in cryogenic environment (helium or hydrogen clusters or droplets), as well as the response properties of quantum fluid clusters to various kinds of probes. To meet this demand, different methods have been proposed. Some are dedicated to reduce the number of degrees of freedom and concentrate on those appropriate for the time scale of the problem, giving rise to curved manifold dynamics [1,2,3]. Others are designed to accelerate the convergence rate with respect to the time step by efficient numerical schemes [4]. During this talk, we will present new approximate propagators and energy estimators [5,6] that are accurate, requiring low memory during the computation, and practical for implementation.

[1] E. G. Noya, C. Vega, C. McBride *J. Chem. Phys.***134**, 054117 (2011)
[2] E. Curotto, M. Mella*J. Chem. Phys.***142**, 114110 (2015)
[3] E. Curotto, M. Mella*J. Chem. Phys.***142**, 114111 (2015)
[4] R. E. Zillich, J. M. Mayrhofer, S. A. Chin *J. Chem. Phys.***132**, 0441303 (2010)
[5]G. Guillon, T. Zeng, P.-N. Roy *J. Chem. Phys.***138**, 184101 (2013)
[6] G. Guillon, T. Zeng, P.-N. Roy *J. Chem. Phys.***139**, 184115 (2013)