

1124-65-205

Jianfeng Lu and **Zhennan Zhou*** (zhennan@math.duke.edu), 120 Science Drive, Durham, NC 27708-0320. *Towards a mathematical understanding of surface hopping methods.*

We develop a surface hopping algorithm based on frozen Gaussian approximation for semiclassical matrix Schrödinger equations. The algorithm is asymptotically derived from the Schrödinger equation with rigorous approximation error analysis. The resulting algorithm can be viewed as a path integral stochastic representation of the semiclassical matrix Schrödinger equations. Our results provide mathematical understanding to and shed new light on the important class of surface hopping methods in theoretical and computational chemistry. Also, I would like to report our recent progress on the improved surface hopping algorithm with various numerical tests. (Received September 08, 2016)