



Seminar

Surface hopping algorithms in quantum dynamics and thermal equilibrium sampling

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Time: 10:00am, Oct. 24, 2017 (Tuesday)

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Venue: Room W563, Physics building, Peking University

地点: 北京大学物理楼, 西563会议室

Abstract

We develop a surface hopping algorithm based on frozen Gaussian approximation for semiclassical matrix Schrodinger equations. The algorithm is asymptotically derived from the Schrodinger equation with rigorous approximation error analysis. The resulting algorithm can be viewed as a path integral stochastic representation of the semiclassical matrix Schrodinger 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 path integral molecular dynamics with surface hopping (PIMD-SH) for thermal equilibrium sampling of nonadiabatic systems, where a novel ring polymer representation for multi-level quantum system is proposed for thermal average calculations.

About the speaker

Dr. Zhennan Zhou graduated from Jilin University in 2009 with B.S. and received Ph.D. in Applied Mathematics from University of Wisconsin - Madison in 2014. Before he joined Beijing International Center for Mathematical Research at Peking University, he was William W. Elliott assistant research professor at Duke University.

His primary research interests are in the applied analysis of PDE and stochastic models, and numerical approximation of scientific problems arising from quantum mechanics, theoretical chemistry, solid state physics, materials science, biology, etc.