



Duke Kunshan University Mathematical Research Seminar Series

Path integral molecular dynamics with surface hopping for thermal equilibrium sampling of nonadiabatic systems and its infinite-swap limit

Prof. Zhennan Zhou, Peking University

Venue: DKU Academic Building 1084

Date: 11am-12pm, Thursday, 11 October 2018

About the speaker:

Dr. Zhennan Zhou is currently an assistant professor at Beijing International Center for Mathematical Research (BICMR), Peking University. He obtained his PhD degree in UW-Madison in 2014, and worked as a William W. Elliott assistant research professor at Duke University from 2014 to 2017. His major research interests include applied analysis, numerical analysis and stochastic simulations, and he takes special interests in the mathematical problems from quantum mechanics, computational chemistry and biological transportation. He was selected as a Young Professional of "The Thousand Talents Plan" of China (14th).

<http://bicmr.pku.edu.cn/~zhennan/>

Abstract: In this work, a novel ring polymer representation for multi-level quantum system is proposed for thermal average calculations. The proposed representation keeps the discreteness of the electronic states: besides position and momentum, each bead in the ring polymer is also characterized by a surface index indicating the electronic energy surface. A path integral molecular dynamics with surface hopping (PIMD-SH) method ("DS" method) is also developed to sample the equilibrium distribution of ring polymer configurational space. Besides, The infinite-swap limit of this representation has been investigated, which provides an alternative formulation for thermal average calculations and overcomes the limitations of the "DS" method. We also introduce a multi-scale integrator to efficiently sample the infinite-swap limit. This is joint work with Jianfeng Lu.

