

数学与系统科学研究院

计算数学所学术报告

报告人：周珍楠 助理教授

(北京国际数学研究中心)

报告题目：

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

邀请人：刘歆副研究员

报告时间：2017 年 11 月 9 日 (周四)

上午 10:30-11:30

报告地点：数学院科技综合

301 报告厅

报告摘要:

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.

欢迎大家参加！