量子材料科学中心
International Center for Quantum Materials

Seminar

Path Integral Liouville Dynamics

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Peking University

- **Time: 4:00pm, July 1, 2015 (Wednesday)**
- **时间：2015年 7月1日（周三）下午4:00**
- **Venue: Room W563, Physics Building, Peking University**
- **地点：北京大学物理楼　西563**

Abstract

There is currently considerable effort focused on developing ways for including quantum mechanical effects in condensed phase molecular dynamics simulations. No method was able to have the two important properties: conserves the quantum canonical distribution and recovers exact thermal correlation function (of even nonlinear operators, i.e., nonlinear functions of position or momentum operators) in the classical, high temperature, and harmonic limits. We show a novel imaginary time path integral based dynamics method that can accomplish the task and is practical for real molecular systems. Its application to vibrational spectra of a few molecules will be discussed.

About the speaker

Prof. Jian Liu got his bechalor's degree in Polymer Science and Engineering from the University of Science and Technology of China, in 2000. After that, he continued his study for Ph.D in UIUC, under the supervision of Prof. Nancy Makri, and got his degree in 2005. From 2005 to 2012, he did a postdoc and then research associate in UC Berkeley and Stanford with Prof. William Miller and Prof. Todd Martinez respectively. He is a theoretical chemist focussing on quantum dynamics, which is presently one of the hardest topics in molecular simulations. He got several important honors during his study and research, including the Guo Moruo scholorship in 1999, the ACS postdoc research award for the physical chemistry division in 2012, etc.