NSF CENTER FOR RESEARCH ON COMPLEX NETWORKS (CRCN)

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CENTER RESEARCH SEMINAR

Large Scale Exact Quantum Dynamics Calculations:
Massive Parallelization and the Classical Phase Space Picture

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Thursday, October 30, 2014
3:00 p.m. – 4:30 p.m.
Room 150 at Science Building

Biography

Bill Poirier is Chancellor's Council Distinguished Research Professor and also Barnie E. Rushing Jr. Distinguished Faculty Member at Texas Tech University, where he holds appointments in the Department of Chemistry and Biochemistry, the Department of Physics, and also the Center for Chemical Biology. He received his Ph.D. in theoretical physics from the University of California, Berkeley, followed by a chemistry research associateship at the University of Chicago's James Franck Institute. Professor Poirier is a computational chemical physicist, studying the quantum dynamics of molecules. His broad research goal is to understand and to solve the Schroedinger equation, from both foundational and practical perspectives. Within that purview, his interests are quite varied, ranging from evaluating carbon nanomaterials for hydrogen storage, to studying the mass-independent fractionation of sulfur isotopes to understand the atmospheric "oxygen revolution", to developing a new formulation of quantum mechanics without wavefunctions. He currently holds research grants from the National Science Foundation, the NASA Astrobiology Program, the US-Israel Binational Science Foundation, and The Robert A. Welch Foundation.

Abstract

Quantum mechanics is the theory that describes the behavior of matter at the nano scale. Though routinely applied to the electrons in a molecular system, quantum theory is generally not applied to the atomic nuclei (except for very simple molecules), because such “exact quantum dynamics” (EQD) calculations are regarded to be too difficult. This is due to the “curse of dimensionality”: the computational (CPU) cost scales exponentially with system dimensionality. A decade ago, the speaker and this team introduced the first EQD method proven to defeat exponential scaling. Recently, they have developed the much simpler, momentum-symmetrized phase space Gaussian basis that achieves the same goal. A “universal” and remarkably simple code has been written, which is dimensionally independent, and which also exploits massively parallel algorithms. The codes have been used to calculate tens of thousands of exact vibrational quantum states for real molecules such as methyleneimine, acetonitrile, and most recently, benzene. Through these calculations, the speaker will demonstrate how to perform EQD calculations for much larger and more complex systems than ever previously realized.