Greater Boston Area Theoretical Chemistry Lecture Series

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Reduced Hierarchal Equations of Motion Approach to Multi-dimensional Spectroscopies

Quantum coherence and its dephasing or relaxation by coupling to an environment plays an important role in nonadiabatic transition, photoexcitation and tunneling processes as well as ultrafast nonlinear spectroscopies. I first introduce a system-bath model to explain how fluctuation and dissipation arises from the environment, and the concept will be illustrated with some examples from chemistry and biology. Then I derive the quantum hierarchal Fokker-Planck equations (QHFPE) on the basis of the Feynman-Vernon influence functional formalism. The derived QHFPE can deal with strong system-bath coupling and non-Markovian noise. Various applications of the QHFPE approach, including resonant tunneling diode and quantum heat-engine will also be discussed.

By applying hierarchal formalism to multi-electric states, we can investigate laser excitation and photoisomerization process described by multi-electric state numerically rigorously. This approach facilitates the calculation of both linear and nonlinear spectra. As an example, we computed Wigner distributions for excited, ground, and coherent states. We then investigated excited state dynamics involving transitions among these states by analyzing linear absorption and transient absorption processes and multi-dimensional electronic spectra with various values of the heat bath parameters. Our results provide predictions for spectroscopic measurements of photoexcitation and photoisomerization dynamics.

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4:15 pm

MIT Building 4, Room 237

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