

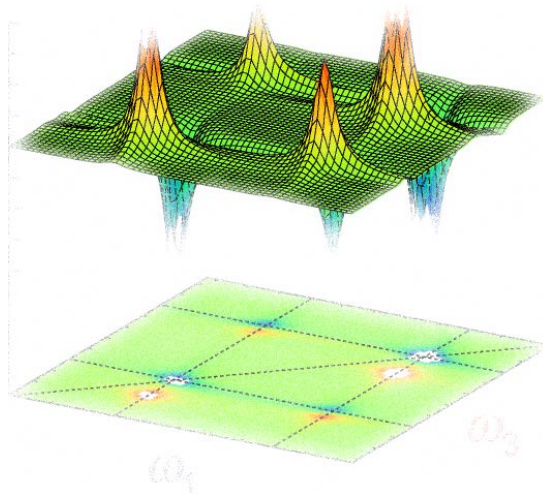


Tuesday, May 15<sup>th</sup> & 22<sup>nd</sup>, 2012  
**Mini Lecture Series**  
**Theory of Multidimensional Spectroscopies**  
**Yoshitaka Tanimura**  
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Spectral line shapes in the condensed phase contain information on various dynamic processes that modulate the transition energy, such as microscopic dynamics, inter- and intramolecular couplings, and solvent dynamics. In this course of lectures, the roles of different physical phenomena that arise from the peculiarities of dissipative dynamics in multidimensional spectra will be described. The methodology will be illustrated by calculating multidimensional signals using optical Liouville path, molecular dynamics (MD) simulations, path-integrals and reduced hierarchy equations of motion approaches. A Brownian oscillator model with the nonlinear system-bath interaction will be employed to explain how fluctuation and dissipation arises from the environment. Using the hierarchy formalism, one can precisely calculate multidimensional spectra for a single and multimode anharmonic system for inter- and intramolecular vibrational modes, and these can be compared with 2D spectra obtained from molecular dynamics simulations.

CONTENTS

1. Introduction
2. Observables in multidimensional spectroscopies
3. Optical Liouville paths and Albrecht diagrams
4. Experiments of 2D Raman & 3DIR
5. Full MD approach
6. Path integral approach
7. Fokker-Planck approach
8. Response function approach
9. Program codes; NonMarkovian2009+2DES



Time: 2 - 6 pm

Location: FRIAS Seminar Room, Albertstr. 19, Freiburg