

Reduced Hierarchy equations of motion approach to multidimensional spectroscopies of biological systems

Yoshitaka Tanimura

Department of Chemistry, Kyoto University

In complex media such as molecular liquids and biological systems, multidimensional spectroscopy has been shown to be variable tools due to the sensitivity of nonlinear response functions. In this talk, we first give an overview of reduced hierarchy equations of motion approach focusing on its theoretical background and applications to multidimensional spectroscopies. We then apply this methodology to see a possibility to explore a role of dissipation and fluctuation on quantum dynamics of biochemical systems. As the observables of linear and two-dimensional (2D) spectroscopies, the first- and third-order response functions of polarization are calculated for different physical conditions. The profiles of the 2D spectra reflect variety of heat-bath effects including dissipation, fluctuation, dephasing and inhomogeneous broadening.

[1] Y. Tanimura and A. Ishizaki, *Acc. Chem. Res.* 42, 1270 (2009).

<http://pubs.acs.org/doi/abs/10.1021/ar9000444>

[2] Y. Tanimura: *J. Phys. Soc. Jpn.* 75 (2006) 082001.

<http://jpsj.ipap.jp/link?JPSJ/75/082001/>