Einladung zum Oberseminar Wissenschaftliches Rechnen

Julius-Maximilians-Universität Würzburg
Lehrstuhl für Wissenschaftliches Rechnen IX

Dr. Maxim F. Gelin

Department of Chemistry, Technische Universität München

Thermal Schrödinger Equation: Efficient Tool for Simulation of Many-Body Quantum Dynamics at Finite Temperature

I will give a brief overview of a recently developed wave-function-based method for the simulation of quantum dynamics of systems with many degrees of freedom at finite temperature. The method is inspired by the ideas of Thermo Field Dynamics (TFD). As TFD, the method is based on the doubling of the system's degrees of freedom and thermal Bogoliubov transformation. As distinct from TFD, the method implements the doubling of thermalized degrees of freedom only, and relies upon the explicitly constructed generalized thermal Bogoliubov transformation, which is not restricted to fermionic and bosonic degrees of freedom. The solution of TFD dynamic equations is based on a novel technique for the propagation of Tensor Trains (Matrix Product States). The methodology is illustrated by the simulation of the exciton dynamics in the Fenna-Mathews-Olsen complex using a realistic structured spectral density to model the electron-phonon interaction. The results of the simulations highlight the effect of specific vibrational modes on the exciton dynamics and energy transfer process, as well as call for careful modeling of electron-phonon couplings.

Ort: Raum 30.02.003 (2. Stock) (Mathegeb. 30 West) Zeit: Donnerstag, 23.05.2019, 11:00 Uhr

Zu diesem Vortrag laden wir Sie herzlich ein.

gez. Prof. Dr. Alfio Borzì
gez. Prof. Dr. Bernadette Hahn