UNIVERSITÀ DI TRENTO
Dipartimento di Fisica

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Thursday, 25 January 2024: 2:00 p.m.
Aula seminari grande - Palazzina B – via alla Cascata 56 C

BEC seminar
Finite-Temperature electron-vibrational problems: Tensor-Train methodologies in closed and open system approaches

Abstract

Non-Equilibrium Thermo-Field Dynamics (NETFD) is as alternative formulation of quantum statistical mechanics, completely equivalent to the commonly used density matrix approach, that enables the development of finite-temperature of quantum dynamical electron-vibrational models. In this talk I will present NETFD concepts, and show how they can be extended and integrated with Tensor-Train (TT) based numerical tools leading to a novel and powerful theoretical and computational framework for the study of complex quantum dynamical problems. Furthermore, NETFD techniques can be extended to treat truly dissipative open systems via the Hierarchical Equations of Motion (HEOM) approach using TT methodologies. The combination of the TFD machinery with computational advantages of TTs results in a powerful theoretical and computational framework for scrutinizing dynamics of complex multidimensional electron- vibrational systems. The validity and the computational advantages of the developed methodologies is illustrated by applying them to the study of quantum coherence effects in the energy-transfer processes, to the analysis of fingerprints of vibrational modes in electron-transfer and charge- transfer processes in various model and realistic multidimensional molecular systems, as well as to simulation of other fundamental models of physical chemistry.

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