

MO 22: Theorie: Moleküldynamik

Zeit: Donnerstag 15:15–16:15

Raum: VMP 6 HS-G

MO 22.1 Do 15:15 VMP 6 HS-G

Trajectory based non-Markovian dissipative quantum dynamics — •WERNER KOCH¹, FRANK GROSSMANN¹, and DAVID TANNOR² — ¹Institut fuer Theoretische Physik, Technische Univeris-taet Dresden, 01062 Dresden, Germany — ²Department of Chemical Physics, The Weizmann Institute of Science, Rehovot 76100, Israel

The availability of an exact description of the full non-Markovian influence of a heat bath on a test system without terms explicitly non-local in time allows an efficient evaluation of system dynamics exhibiting effects of decoherence and dissipation[1]. Trajectory based methods have proven to be suitable to numerically evaluate the stochastic integrals which result from the unraveling of the path integrals of the influence functional formalism[2]. We consider oscillator test systems and scattering barriers. The coupling to the environment is bilinear in the pointer variable of the system and those of an ensemble of harmonic oscillators with a fixed temperature. We present effects of the influence of the environment on the test system quantum dynamics and discuss issues arising during such calculations.

[1] Stockburger, J. T. and Grabert, H., Phys. Rev. Lett., 88(17):170407 (2002)

[2] Koch, W. , Grossmann, F., Stockburger, J. T., and Ankerhold, J., Phys. Rev. Lett., 100(23):230402 (2008)

MO 22.2 Do 15:30 VMP 6 HS-G

Treatment of systems coupled to a bath within a semiclassical hybrid approach — •CHRISTOPH-MARIAN GOLETZ and FRANK GROSSMANN — TU Dresden

Semiclassical methods in initial value representation are widely used in molecular and atomic physics since they are suitable to treat systems with several degrees of freedom with an acceptable memory effort in contrast to full quantum mechanical methods.

The semiclassical hybrid method [1] in addition combines the very small computational effort of the single-trajectory Thawed Gaussian method according to Heller and the very good accuracy of the multi-trajectory approach going back to Herman and Kluk. We present a first application of this approach to a molecular system embedded in a bath based on the Caldeira-Leggett model (e.g. [2]). We show that the hybrid method is applicable for the investigation of coherence properties of such a system.

[1] F. Grossmann, J. Chem. Phys., **125**, p. 014111, 2006

[1] H. Wang et. al., J. Chem. Phys., **114**, p. 2562, 2001

MO 22.3 Do 15:45 VMP 6 HS-G

Geometric phase and symmetry effects in dissociation dynamics of H₃ — •ULRICH GALSTER and JAN-MICHAEL ROST — Max-Planck-Institut für Physik komplexer Systeme, Dresden

Distinct structures have been observed in the distribution of breakup-geometries in three-body predissociation of Rydberg states of H₃ [1]. Although a close relation to symmetry properties of the initial vibrational state and the involved non-adiabatic coupling is obvious, a detailed understanding of the formation of these structures is difficult to obtain. New insight in the dissociation process has been gained by means of quasi-classical simulations. They allow a comprehensible view on the formation of specific breakup-patterns under the influence of geometry-dependent non-adiabatic couplings and the evolution of nuclear configurations on the dissociative potential energy surfaces.

[1] Galster, Baumgartner, Müller, Helm, Jungen, Phys.Rev.A **72** 062506 (2005)

MO 22.4 Do 16:00 VMP 6 HS-G

Flourescence quenching in organic donor-acceptor dyads: a first principles study — •THOMAS KÖRZDÖRFER and STEPHAN KÜMMEL — University of Bayreuth

Perylene bisimide is a prototypical organic dye frequently used in organic solar cells and light emitting devices as an hole-transporting material. Recent FRET(Förster-resonant-energy-transfer)-experiments on a bridged organic donor-acceptor dyad of triphenyl diamine and perylene bisimide [1] revealed a strong flourescence quenching on the perylene bisimide. This quenching is absent in a solution of free donors and acceptors and thus originates from the inclusion of the saturated C₁₂H₂₄-bridge [2]. We investigate the cause of the flourescence quenching as well as the special role of the covalently bound bridge by means of time dependent density functional theory and molecular dynamics. We show that the conformational dynamics of the bridged system leads to a charge transfer process between donor and acceptor that causes the acceptor flourescence quenching [3].

[1] P. Bauer et al., Chem. Mater. 19, 88 (2007).

[2] Ch. Scharf et al., Chem. Phys. 328, 403 (2006).

[3] T. Körzdörfer and S. Kümmel, to be published.