



# UNIVERSITÀ DEGLI STUDI DI MILANO

## SEMINARI ERC



Data

*Venerdì 2 Febbraio 2018, ore 11:00*  
*Aula Montanari, Dipartimento di Chimica*

Oratore

**Prof. Frank Grossmann**  
Institut fuer Theoretische Physik  
Technische Universitaet Dresden

Titolo

**"Semiclassical initial value representations: Basics and applications to quantum dissipation"**

Coordinatore

**Michele Ceotto**  
*Dipartimento di Chimica*

**Abstract:**

The semiclassical initial value formalism to solve the time-dependent Schroedinger equation will be reviewed. Special focus will be laid on Heller's thawed and frozen Gaussians [1], as well as on the Herman-Kluk propagator [2]. A combination of the frozen and thawed Gaussian methods for many degree of freedom systems, the semiclassical hybrid dynamics [3], will then be introduced.

After a brief digression to the semiclassical description of the scattering of two identical particles [4], we present results for the quantum-classical transition of a nonlinear oscillator coupled to an Ohmic heat bath [5], as well as for the thermalization of the expectation values of such an oscillator [6]. We contrast two different approaches to open system dynamics: the explicit treatment of the bath degrees of freedom and the reduced density matrix method, respectively.

[1] E. J. Heller, J. Chem. Phys. **62**, 1544 (1975), J. Chem. Phys. **75**, 2923 (1981)

[2] M. Herman and E. Kluk, Chem. Phys. **91**, 27 (1984)

[3] F. Grossmann, J. Chem. Phys. **125**, 014111 (2006)

[4] F. Grossmann, M. Buchholz, E. Pollak and M. Nest, Phys. Rev. A **89**, 032104 (2014)

[5] C.-M. Goletz and F. Grossmann, J. Chem. Phys. **130**, 244107 (2009)

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