Graduate School Seminar

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Talks in SS 2016

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Semiclassical Wigner Propagation for Including Quantum Effects in Vibrational Spectra

Rapid progress of the laser facilities and measuring techniques has made the vibrational (non-)linear spectroscopy an ubiquitous tool to probe dynamics of complex many-body systems. Measuring precise and detailed spectra can yield accurate information on the dynamics of the system in question, if supplemented by a theoretical simulation, that reveals the underlying microscopic mechanisms. Thus, the demand of theoretical methods that can cope with explaining such spectra for complex many-body systems and thus unravelling intricate phenomena in condensed phase becomes apparent.
Semiclassical techniques constitute an indispensable element in the repertoire of quantum mechanical methods. Their basic achievement is to approximately calculate quantum observables from purely classical dynamical data. This allows one to profit from the robustness of classical molecular dynamics simulations whose range of applicability can be from small molecules up to large biomolecules. A quite elegant pathway to develop semiclassical methods is to utilize the Wigner representation. Here, the entire quantum mechanics is recast in terms of phase-space quasi-probability density distribution, the Wigner function, which constitutes a one-to-one representation of the density operator, including coherences. The main advantage of this representation is that an exact quantum average takes the form of a classical phase space integral with the only difference that the Wigner function is used instead of a classical probability density. This makes the connection between quantum and classical mechanics apparent and thus facilitates the development of approximate semiclassical methods.
In this talk, a basic introduction to semiclassical methods in Wigner representation will be given. First results on Wigner propagation, autocorrelation functions and optical response functions will be shown as well.

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Talk: English
Slides: English

Location: Institute of Physics, Albert-Einstein-Str. 24, HS1