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Bldg. 49, Seminar room 108

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Many-particle systems out of equilibrium. A Kadanoff-Baym approach to finite systems including electron correlations

Based on second quantization and quantum statistics, the method of nonequilibrium Green functions (NEGF) [1] provides a very general framework to describe interacting many-particle systems far from equilibrium. Thereby, correlations [2], i.e. beyond-Hartree-Fock-level contributions to the interaction, enter through retardation (memory) effects in the dynamical evolution which is self-consistently determined by the two-time Kadanoff-Baym equations.

In this talk, I will review the NEGF method in respect of applications to spatially inhomogeneous quantum systems such as atoms, molecules or electrons in quantum dots. Thereby, computational advances have been achieved by using specially tailored representations of the NEGF and time-propagation schemes that are adapted for high-performance computing [3,4].

Numerical benchmarks comprise one-dimensional, non-lattice models that describe real and artificial atoms and molecules exposed to external (non-)perturbative fields [4]. Throughout, electron correlations are identified as crucial and are treated in the second(-order) Born approximation.

[1] L.P. Kadanoff and G. Baym, Quantum Statistical Mechanics (Benjamin, New York, 1962).
[2] S. Bauch, K. Balzer and M. Bonitz, EPL 91, 53001 (2010).
[3] K. Balzer, Solving the two-time Kadanoff-Baym equations. Application to model atoms and molecules (PhD thesis, CAU Kiel, August 2011).
[4] K. Balzer, S. Bauch and M. Bonitz, Phys. Rev. A 81, 022510 (2010); ibid. 82, 033427 (2010).

Host: Martin Eckstein, CFEL Condensed Matter Division