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Nonequilibrium Green function approach to model atoms and molecules

Nonequilibrium Green function (NEGF) techniques attract more and more attention when correlated quantum many-particle dynamics [1] is under investigation. Thereby, the solution of the Kadano-Baym equation (KBE) imposes strong challenges on the numericsespecially when applied to nite systems. This mainly aects the direct propagation of the KBE whereas obtaining equilibrium properties is conceptually relatively simple.
Here, we extend previous work [2] to nonequilibrium situations and propagate the NEGF in the two-time domain. To render calculations possible, an ecient distributed memory algorithm has been developed enabling parallel and well-scalable computation of the NEGF. Also, the use of nite elements in combination with the discrete variable representation [3] greatly simplies summations over parts of Feynman diagrams. By comparing the one-electron density and the dipole moment to time-dependent Hartree-Fock results on one hand and the full solution of the time-dependent Schrödinger equation on the other hand, we demonstrate that the time-dependent second Born approximation carries valuable information about electron-electron correlation eects in atoms and molecules exposed to external elds [4]. As examples, we present results for helium, beryllium, hydrogen and the heteronuclear molecule lithium hydride modelled in one spatial dimension. In addition, we briey report on the spectral and excited state properties as obtained from the NEGF within dierent many-body approximations.

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