Abstract Submitted
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Time-dependent second Born calculations for model atoms and molecules in external fields[1] KARSTEN BALZER, SEBASTIAN BAUCH, MICHAEL BONITZ — 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 Kadanoff-Baym equation imposes strong challenges on the numerics—especially when applied to finite systems. Here, we extend previous work [2] to nonequilibrium and propagate the NEGF in the two-time domain. To render calculations possible, an efficient distributed memory algorithm has been developed enabling parallel and well-scalable computation of the NEGF. Also, the use of the finite element discrete variable representation greatly simplifies summations over parts of Feynman diagrams. By comparing to TDHF and full TDSE results, we demonstrate that the second Born approximation carries valuable information about correlation effects in atoms and molecules exposed to external fields [3]. As examples, we present results for He, H_2 and the LiH modeled in one spatial dimension. In addition, we report on spectral and excited state properties.

[1] S. Bauch, K. Balzer, and M. Bonitz, EPL **91**, 53001 (2010);
[2,3] K. Balzer, S. Bauch, and M. Bonitz, PRA **81**, 022510 (2010), PRA **82**, 033427 (2010).

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