Improving the scaling in many-electron dynamics simulations

Michael Bonitz, Jan-Philip Joost, Niclas Schlüzen

Institute for Theoretical Physics and Astrophysics, Kiel University

The exponential scaling of quantum dynamics simulations within the Schrödinger equation has led to many theoretical developments and novel concepts in many fields. Our group developed time-dependent restricted active space (TD-RASCI) simulations that allowed to accurately simulate small atoms [1,2]. At the same time, the main focus of our group, in recent years, was on developing methods to propagate the one-particle nonequilibrium Green function (NEGF), instead of the N-body wave function, e.g. [3]. This has been applied to small atoms and molecules [4]. While we could improve the scaling with the basis size, NEGF simulations are hampered by an unfavorable cubic scaling with the propagation duration T, whereas the accuracy is governed by accessible choices for the selfenergy.
Here I report on our recent progress in implementing and testing improved selfenergies [5]. Finally, I present recent results that have allowed us to reduce the scaling with T to linear scaling [6,7] and discuss prospects of applications to atoms and molecules.

[1] D. Hochstuhl and M. Bonitz, Phys. Rev. A 86, 053424 (2012)
[2] D. Hochstuhl, C. Hinz, and M. Bonitz, EPJ-ST 223, 177 (2014)
[3] K. Balzer and M. Bonitz, "Nonequilibrium Green's Functions Approach to Inhomogeneous Systems", Lecture Notes in Physics 867 (2013)
[4] K. Balzer, S. Bauch, and M. Bonitz, Phys. Rev. A 82, 033427 (2010)
[5] N. Schlünzen, S. Hermanns, M. Scharnke, and M. Bonitz, J. Phys. Cond. Matt. 32, 103001 (2020)
[6] N.Schlünzen, J.-P. Joost, and M. Bonitz, Phys. Rev. Lett. 124, 076601 (2020)
[7] J.-P. Joost, N.Schlünzen, and M. Bonitz, Phys. Rev. B 101, 245101 (2020)