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Quantum Dynamics of Electrons Made Fast: Achieving Linear Time-Scaling for Nonequilibrium Green Functions NICLAS SCHLUENZEN, JAN-PHILIP JOOST, CHRISTOPHER MAKAIT, MICHAEL BONITZ, Univ Kiel
— The accurate description of the nonequilibrium dynamics of correlated electrons is crucial for warm dense matter and dense quantum plasmas. Among others, the nonequilibrium Green functions (NEGF) method has proven to be a powerful tool to reliably predict the quantum dynamics. However, NEGF simulations are computationally expensive due to their T^3 scaling with the simulation duration T . With the introduction of the generalized Kadanoff–Baym ansatz (GKBA)[1], T^2 scaling could be achieved for second-order Born (SOA) selfenergies[2] which has substantially extended the scope of NEGF simulations. Recently[3], we could show that GKBA-NEGF simulations can be performed with order T^1 scaling for SOA, GW, and T-matrix selfenergies, and even for the screened ladder approximation[4]. Here, we show numerical results for various many-body approximations and demonstrate that a tremendous computational speed-up can be achieved in practice.

[1]P. Lipavský *et al.*, Phys. Rev. B **34**, 6933 (1986)
[2]S. Hermanns *et al.*, Phys. Scr. **2012** 014036 (2012)
[3]N. Schlünzen *et al.*, *Phys. Rev. Lett.* **124**, 076601 (2020)
[4]J.-P. Joost *et al.*, Phys. Rev. B **101**, 245101 (2020)

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