Accelerating nonequilibrium Green functions simulations: the G1-G2 scheme

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Full two-time NEGF simulations suffer from a cubic scaling of the CPU time with the simulation duration. Recently we have introduced the G1-G2 scheme that exactly reformulates the Hartree-Fock-GKBA into time-local equations, allowing for a dramatic reduction to time-linear scaling [1]. Remarkably, this scaling is achieved quickly, and also for high-level selfenergies, including nonequilibrium GW and T-matrix appro-ximation [2]. Even the dynamically screened ladder approximation is now feasible [3]. I will present applications to nonequilibrium situations including laser excitation of graphene nanoribbons [4] and ion stopping and neutralization by graphene and TMDC monolayers [5].

The scaling advantage of the G1-G2 scheme comes at a price, and I will discuss how these problems can be solved: i) for strong coupling situations and long simulations, the scheme becomes unstable which can be cured using purification schemes [3,4] ii) It is necessary to store the time-diagonal two-particle Green function which rapidly grows with system size. This can be overcome, for the GW approximation, using a recently developed quantum fluctuations approach [6]. Another promising concept to reduce the simulation size is the use of embedding selfenergies. Here, we demonstrate how the embedding concept can be introduced into the G1-G2 scheme, allowing us to drastically accelerate NEGF embedding simulations [7]. A recent review on the G1-G2 scheme can be found here [8].

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