Time-linear non-equilibrium Green's function approach to correlated quantum transport

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The non-equilibrium Green's function (NEGF) is a powerful approach for describing correlated quantum systems out of equilibrium [1]. High-order diagrams can be systematically included to achieve high accuracy, and a large variety of observables is directly accessible. Open quantum systems, in contact with reservoirs, can be treated non-perturbatively in the system-reservoir coupling. However, for large-scale (ab-initio) calculations, the computational solution of the NEGF equations, either in Dyson or Kadanoff-Baym form, is extremely demanding, scaling cubically with simulation time. The Generalized Kadanoff-Baym Ansatz (GKBA) reduces the computational scaling from cubic to quadratic with simulation time [2]. Recently, it was shown that the integro-differential GKBA equations can be equivalently recast as a set of time-local first-order ordinary differential equations (ODE) [3]. The computational cost of the ODE scheme is linear instead of quadratic, which means that GKBA time evolutions can be performed with the same scaling as the fastest quantum methods available, such as time-dependent density-functional theory. Here, we extend the time-linear GKBA formulation to a correlated quantum-transport setup. This formulation thus enables treating, on the same footing, inter-particle interactions, external drives and/or perturbations, and coupling to reservoirs with a continuum set of degrees of freedom.

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[2] P. Lipavský, V. Špička, and B. Velický, Phys. Rev. B 34 (1986) 6933.

[3] N. Schlünzen, J.-P. Joost, and M. Bonitz, Phys. Rev. Lett. 124 (2020) 076601.