

Speeding up GKBA calculations using initial correlations

Daniel Karlsson

Within the NEGF formalism, the GKBA has stood out as a computationally cheap method to investigate the dynamics of interacting quantum systems driven out of equilibrium. Current implementations, however, suffer from a drawback: real-time simulations require noncorrelated states as initial states. Consequently, initial correlations must be built up through an adiabatic switching of the interaction before turning on any external field, a procedure that can be numerically highly expensive. In this work, we extend the GKBA to allow for initially correlated states which makes it possible to efficiently separate the calculation of the initial state from the real-time simulation. We discuss how to efficiently speed up calculations using the new scheme. [1]

[1] Daniel Karlsson, Robert van Leeuwen, Enrico Perfetto and Gianluca Stefanucci, The Generalized Kadanoff-Baym Ansatz with Initial Correlations, *Phys. Rev. B.* 98, 115148 (2018)