Interaction-driven dynamics in Graphene flakes

Peter Schmitteckert

HQS Quantum Simulations, Rintheimerstr. 23, 76131 Karlsruhe, Germany

We study interaction-driven ultrafast dynamics in finite graphene flakes following an optical pump quench in an interacting tight-binding model. By comparing exact real-time evolution with simulations restricted to particle-hole excitation subspaces, we assess when relaxation can be captured by low-order many-body processes and when this is not sufficient.

This work is is motivated by the observation, that basically all observables in Graphene are described by a non-interacting tight binding Hamiltonian on a honeycomb lattice. One of the few exceptions is the decay of particle-hole excitations, created by a pump laser and probed by a probe laser. These excitations decay in the order of 30 fs, too fast for any relaxation mechanism like phonons except electronic interaction. However, in a description based on non-interacting fermions, including HF or DFT, these excitations can't decay. The typical simulation techniques therefore includes second order Born approximations for the self-energy. We therefore address the question: if an effect is only driven by electron-electron interaction, can we check whether methods based on restricting the particle-hole excitations are justified?

To this end we study the entropy A of the single-particle density matrix ϱ, S = Tr (- ϱ log(ϱ) - (1- ϱ) log(1- ϱ)). This quantity is time independent for unitary time evolutions governed by free fermion systems, and stays single-particle basis independent for interacting systems. To investigate the role of particle-hole excitations we analysed the influence of the number of particle hole excitations we allow.

Looked like a straight-forward plan. Yet, the results are confusing, on small Graphene flakes, second order excitations, i.e. a system including all one- and two- particle-hole excitations, is sufficient to describe the quench. Increasing the system size suddenly increases the importance of higher order particle-hole excitations. For periodic boundary conditions, less excitations are needed albeit leading to much faster relaxation rates. In contrast, for a square lattice, the difference between hard-wall boundary conditions, and periodic BC are significantly smaller.

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[1] Fabian Eickhoff, Satoshi Ejima, Lukas Windgätter, Florian G. Eich, Hannah Rittich, Sebastian Zanker, Peter Schmitteckert, “Interaction-driven dynamics in graphene flakes as a benchmark for quantum simulation”, arXiv:2606.10548