Spoke 2, WP1, Research topics, Topic b6 [Condensed Matter and Low-dimensional Systems]

Nonequilibrium steady states and time evolution of low-dimensional open quantum systems

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Use case definition

Given the basic assumption of a Markovian dynamics (on very general grounds) an open quantum system is typically described within the Lindblad Master Equation (LBE) approach

A few examples:

- Ultracold atoms, condensed matter systems (spin chains/networks, electronic systems, topological insulators/superconductors, et cetera) [phase diagram, relaxation dynamics];
- Quantum biology and quantum chemistry [molecule engineering, molecular electronic devices];
- Implementing quantum algorithms and experimentally realizing Markovian dynamics;
- Application to high-energy physics;
- Application to «classical» problems via the mapping of classical, correlated systems onto quantum models (e.g., traffic flows in complex networks).
- .....

Use case definition

Status of the art

<u>To summarize the present status of the art:</u>

-The coupled system-bath dynamics is encoded in a set of differential equations for the time evolution of the elements of the density matrix;

-The difficulty in solving the equations is determined by their (large) number and by the need for tailgaiting the relaxation dynamics of the system over time scales that can be pretty long;

-The evolution in time of the density matrix is typically loaded over the dynamics of correlation functions;

-Solving for a steady state allows for trading the differential equations for algebraic equations: this is a simplification, but the number can still be prohibitively large, especially for interacting systems;

-The typical scales over which the system must be monitored when following its relaxative dynamics can be also prohibitively large, also due to the presence of quasisteady states, corresponding to local minima of the free energy.

Use case definition

Expected improvements within our activity

<u>The main improvements we expect to achieve within our activity should primarely concern</u>:

- The possibility of investigating the nonequilibrium steady states and the relaxation dynamics of systems defined over complex networks («junctions»): this would allow for a more realistic description of, e.g., complex molecules, quantum devices, et cetera, but also of «classical» problems, such as a traffic jam at a tournabout: this requires modifying «standard» codes to account for the nontrivial topology of the system;
- The possibility of implementing large computation/storage resources to study the time evolution over large time scales: this would allow for ruling out the risk of finding spurious solutions. This would require improving standard numerical methods by letting the code perform an educated sampling of the steady states it detects. This would also imply complementing the standard numerical methods of solutions of the MLE with Monte Carlo methods, possibly better suited for some specific purposes;
- A systematic inclusion of the interaction, which is required in order to faithfully describe realistic systems and which should again require a combination of standard numerical methods of solutions of the MLE with Monte Carlo, as well as density matrix renormalization group, methods.

Use case definition

References

- G. Benenti et al., PRB 80, 035110 (2009)
- A. Nava et al., PRB 103, 115139 (2021)
- A. Nava et al., SciPost Phys. Core 5, 022 (2022)
- A. Nava et al., J. Phys. Conf. Ser. 2164, 012051 (2022)
- A. Nava et al., PRB 107, 035113 (2023)
- A. Nava et al., Int. Jour. Theor. Phys. 62, 37 (2023).

Use case expected activities

Tentative table of expected activities

- First period [Month 0-3]: Writing and implementing the LME over complex networks, coding the equations, doing preliminary checks over simple systems.
[KPI.1: increasing the connectivity (number of branches) of studied junctions/networks, having nonzero interactions over more than a single-a few sites. AT: factor 10]

- Second period [Moth 3-18]: Looking for the NESS in complex, large low-dimensional lattice systems/networks. Finding the expected values of physically relevant observables, adding disorder (LME approach)
[KPI.2: Increasing the number of sites with a nonzero interaction, averaging the disorder over a large number of system's replica, further increasing the system size. AT: factor 10-100 for the interaction and the disorder, extra factor of 100 for the system size, so to cover at least two decades]

- Third period [Month 19-36]: System dynamics, time evolution toward the NESS, getting rid of «false» steady states, combining the LME with Quantum Monte Carlo and DMRG methods, studying the effects of the temperature
[KPI.3: Increasing the typical time scales of the time evolutions, realizing efficient combinations of different numerical methods, adding the temperature. AT: factor of 10-100 in the time scales, suppression of the probability of incorrectly finding the steady state].

Computing resources

Tentative table of expected activities

- Computation: (Approximatively) 50.000 core hour/year (over three years)

- Storage: (Approximatively) 0.5 Terabyte