Quantum many-body isothermal processes and thermodynamic cycles with free fermions: a summary

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Summary

It is well known that quasi-static thermodynamic transformations are ideal ones and, when reasoning by means of such processes, typically what is not accounted for is the time needed to achieve them. Usually when considering realistic transformations with a finite time duration, one has to deal with genuine out-of-equilibrium dynamics. Thus, such processes that differ from the idealized ones are very interesting in practice, because they are expected to be realized during real experiments: this is true in particular when dealing with quantities related to small-scale systems. With the emergence of technology for producing nano-scale mechanical systems the interest in quantum analogs of thermal cycles is recently growing up [1][2]. The purpose is to find possible advantages of the nano-scale machines over the macroscopic ones, in particular in terms of their effective efficiencies and operation speeds [3]. Simulations of these systems, to gain technical value, have to consider the finite duration of the quantum cycle, thus relaxing the approximation of quasi-static transformations.

Works about the simulation of not idealized quantum cycles are rare in literature, especially the ones considering systems near to the effective dimensions of the small-scale devices that nanotechnologies can currently handle. The problem has to be approached by numerical simulations and the calculations of the quantum mechanical dynamics become rapidly prohibitive as the dimension of the system increases.

To make such intensive computations possible, the very first approximation is idealizing some parts of the devices, thus identifying heat-baths and a much smaller system of interest that constitutes the working substance. Then, the dynamics of the system of interest connected to an heat-bath are usually treated by means of quantum master equations in the Lindblad form, allowing for the simulation of quantum processes resembling thermalizations [4]. Differently from the concept of a thermalization that has not been completed, the idea of non-ideal isothermal process appears not well defined, moreover an analogous treatment is more difficult when dealing with time-dependent Hamiltonians. This is the reason why it is difficult to find works in the literature treating processes resembling non-ideal isothermal processes. Another explanation may be that because of the difficulties in the experimental realizations, simpler composition of processes seemed more easier to deal with, as an example the quantum Otto cycle, that indeed is one of the most studied in literature [7][5].

This thesis, contrary to previous works, focuses on the treatment of non-ideal isothermal processes and on the simulation of quantum cycles making use of them. Despite being the quantum analog of the Carnot cycle the most obvious candidate, here we prefer to consider a different one, having some properties convenient for easing some aspects of our analysis. The quantum cycle we have in mind is characterized by some free parameters by means of which it can resemble the quantum Otto and Carnot cycles. When the transformations are not perfect and approach the idealized ones but with a finite difference, it is not obvious matter to understand which one performs best. In our work more formal definitions of what we understand for non-ideal process (or "imperfect processes") are given and with these the "imperfect versions" of the cycles we intend to discuss are described. From the definition of imperfect Otto cycle and imperfect Carnot cycle we construct the more general imperfect cycle having the convenient properties of reducing into the two and, in the proper limit conditions, also into their perfect counterparts. Thus the study of such a more general cycle, that we call the "mixed cycle", becomes the purpose of this work.

As we mentioned above, simulating quantum systems is a demanding task, even for Hilbert spaces with finite dimension, because the number of basis elements grows at least exponentially with the number of components of the system. Thus, exactly simulating large finite systems is unfeasible and some kind of approximation is needed.

However, a full simulation of a quantum system is not requested to answer any possible query and only a few quantities may be of interest. Thus, it may be possible to reduce the information representing a system to the only relevant one, so to keep almost exact the calculations and at the same time reducing their complexity. Cases where such an information reduction can be easily obtained are quadratic fermionic systems, where the quantities we are interested in when considering thermal machines, that is the work done and heats exchanged with the heat baths, can be calculated by the knowledge of the dynamics of a two-point correlation matrix alone.

In a previous work [6] a framework to treat the evolution of autonomous quadratic systems

coupled with heat baths was presented: provided that the dynamics of the system could be approximated to be Markovian, a way of rapidly computing a two point correlation matrix at every time was established.

In our work such a framework is elaborated and adapted to treat processes where the system of interest is coupled with its environment and some work is done on it at the same time. This is done at the price of assuming a sufficiently small entanglement between the system and heat-baths. Thus, to study the properties of the mixed cycle we chose a quadratic system as a working substance in such a way to drastically simplify the calculations. In particular, we have considered a quantum Ising chain with open boundary conditions: this can be mapped into a quadratic fermionic Kitaev chain, by means of a Jordan-Wigner transformation. This choice was made in order to match some results of our simulator with the one obtained through a code used in a previous work [7], this for the sake of checking the correctness of our routines.

The mathematical framework we work with is proved to be able of reproducing imperfect thermalizations, however nothing has been demonstrated about its ability of reproducing imperfect isothermal processes. As a very first simulation we are interested to test if the computed dynamics agrees with our definition of imperfect isothermal processes. Assuming such a result as positive we then proceed in the simulation of various behaviors of the imperfect mixed cycle. The results of our calculation suggest that imperfect isothermal processes as we defined them are actually reproduced.

An important quantity related to thermal machines is the mean work extraction efficiency. In a real machine the work extracted may fluctuate from a run to another, being for example high in the first and very low in the rest. This is important depending on the task a thermal machine has to achieve, however in many situations they are thought running for an arbitrary long time, thus making of their mean efficiency a crucial feature. The dissipative terms in the equations for the dynamics suggest the existence of limit cycles, that is limit paths that the correlation matrix would approach as the number of machine runs increases. What we found is that with our assumptions such limit paths are approached, so the mean efficiency coincides with the efficiencies of the limit cycles.

As a final simulation we propose a mean efficiency characterization of the imperfect mixed cycle for different parameters. In particular these parameters can be adjusted in such a way that our general protocol turns into an imperfect Otto cycle, thus enabling us to compare the latter with different imperfect Carnot cycles.

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