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Exploring the Design Space of Quantum Heat Engines

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EXPLORING THE DESIGN SPACE OF QUANTUM HEAT ENGINES

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    Quantum heat engines produce a stochastic output due to thermal and quantum fluctuations. We will characterize and optimize the probabilistic output of nanoengines as a function of (i) the feedback of the load on engines, (ii) disorder, (iii) the geometry of the system and (iv) the interactions between its constituents. These are fundamental and pervasive aspects for any quantum heat engine.
    Our theoretical work relied on intense numerical computations using, and developing further, state of the art numerical algorithms for complex and interacting quantum systems.
    Our characterization and optimization of the nanoengines will allow to discern principles and guidelines for the design of future quantum energy technologies.

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1.0 SUMMARY

As devices are miniaturized, it is extremely important to be able to control and convert energy flows effectively. However, at small scale the physics of the system is dominated by quantum effects, and hence, a quantum mechanical description of the system and its excitation is required. A thermodynamic analysis of the work processes or of the energy conversion also needs to take into account of quantum mechanical effects. With this project we have investigated the design space of quantum heat engines, focusing in particular on the effects of coupling of engine and load, interactions within the working fluid and of disorder. We also had the opportunity to work on the control of quantum systems which could help to produce a large variety of heat engines.

Thanks to this project,

- 4 papers have been published (2 in Phys. Rev. E (Rapid), 1 in Phys. Rev. E and 1 in EPJ ST),
- 2 are with referees and
- 1 is being written.

Moreover, I have presented the results from this project at 4 occasions in Singapore and Germany.

2.0 INTRODUCTION

Miniaturization of devices requires a better control of heat flows, cooling and conversion of heat into useful work [1]. It would be important to understand which good guiding principles in the design of such devices are. Currently experiments with nano-engines are done in various setups and with different working substances that include trapped ions [2], nitrogen vacancies [3], single particle or colloidal systems [4–6], piezoresistive devices [7], a micro-meter sized piston [8], ultracold gases [9], quantum dots [10] and even a single spin [11].

The design space that we explore is given by: strength of coupling of engine and load, role of interactions and role of disorder.

- The strength of the coupling of the engine to the load can induce a non-negligible feedback of the load on the engine. More importantly, in strong coupling it is not possible anymore to describe the energy exchange between engine and load as only work. The engine and the load become correlated and this implies a transfer of entropy between the two, and hence of heat.

- The magnitude of the interactions within the engine can change significantly the properties of the working fluid, making it more susceptible in absorbing or releasing heat. Hence this is a key tool to design quantum heat engines, and it is particularly important at a quantum scale in which such coherent effects can take place.

- Disorder is often considered a nuisance, as it tends to increase the amount of friction and hence of entropy generated. This results in less work produced and lower efficiencies. In this project we have investigated how general this picture is and whether, and under which conditions, strong disorder can help reduce entropy generated and increase the work.

3.0 METHODS

Heat engines are systems in contact with an out-of-equilibrium environment. The environment induces a heat current in the engine, while the engine is able to convert some of the heat current into useful work. It is thus necessary to have an appropriate understanding and methodology to address open quantum systems. For these, the most widely used approach is that of master equations, i.e. equations which only evolve the density operator of the system and are valid in weak coupling regimes. In our work we use two different types of master equation: the Lindblad (or Lindblad-Kossakowski-Gorini-Sudarshan) master equation [12, 13], or the Redfield master equation [14]. The former uses more approximations, but ultimately it gives the evolution of a physical density matrix (although maybe not accurate). The latter uses less approximations, but it could return density operator which are unphysical (i.e. some small negative eigenvalues).

Engines are also systems which can be periodically driven. We thus need to consider the effects of periodic driving on an open system. To do so we used a Floquet-dissipative map which allows to compute the time-periodic steady state of the system by computing the null vector of an appropriately constructed matrix. The time dependent properties of the system are then computed by evolving in time the periodic steady state [15].

The main purpose of an engine is to do work on a load, and because of this, engines are coupled to it. Such coupling is commonly described, as mentioned above, by a periodic driving. Such description is valid as long as the load is macroscopic and classical. When dealing with small and quantum loads the coupling of the load to the engine cannot be described by a periodic driving. From a “methods” point of view, this implies that one has to study the evolution in the of the engine and of the load, which is numerically much more demanding. It is in fact necessary to keep many tens of levels for a correct description of the load at long times as we do in [16]. Another approach is have a small load and study persistent currents occurring in it, as in our papers [15] and [17, 18]. Having such loads also plays a role in the definitions of work that need to be used. If the load is not a time-dependent driving, using the common definition of work (both quantum mechanically and classically), it would turn out that no work is neither done or received at any point in time. However, the load is lifted, and the engine has gone back to its state after a cycle.

Another tool important to study such systems, in particular when coupled to a load, is exact diagonalization. Here we use symmetries present in the system to describe accurately the overall system, but using less memory.

4.0 RESULTS AND DISCUSSIONS

During this project I have trained 1 postdoctoral fellow, 2 research assistants and 2 undergraduate students. Together we have published 4 papers, 2 more are with referees, and the 7th one is in preparation.

Work supported by this grant has been presented at these conferences or meetings:

1) National University of Defense and Technology, Changsha: Invited Talk, January 2018
2) SMART, Cao Group, Singapore: Invited Talk, July 2017
3) LMU, Schollwock Group, Munich: Invited Talk, April 2017
4) QuEST, Singapore: Invited Talk, November 2016

As for now, we have published 3 papers supported by this grant, submitted 2 papers and preparing at least 2 more papers. We give more details here below.

In the following I summarize the findings from the different studies that we have pursued within this project.

1) Role of interaction between the engine and the load

One critical step in understanding how to design nano-engine is to study the interaction and interplay between the engine and the load. Here we go beyond current semiclassical approximations and consider exactly the interaction between them. We observe motion of the load which would not occur in the semiclassical approximation (Fig.1, top two panels). We also uncover that there is not only work transfer between engine and load, but also entropy transfer, and hence heat (middle two panels show the position of the load on an up-hill slope (left) and the entropy of the load (bottom line in right panel) or of the engine plus the load). Last, we notice the presence of possible resonances depending on the natural frequencies of the engine and of the load [16].

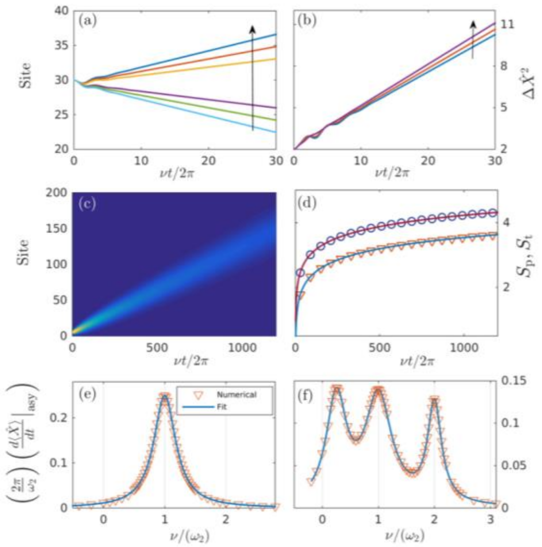

Fig.1: (a) Position and (b) variance vs time for different bath parameters. (c) Density plot of position of the load at different times. (d) Entropy of system plus load, and only of the load versus time, with a logarithmic increase. (e-f) velocity vs energy scales in the load and in the engine, with presence of resonances depending on the number of spins in the engine.

A critical step to understand fundamental design principles for heat engines is to use ideal minimal models. Here we study two spins coupled to two baths which induce a spin current. We then couple the smallest circuit possible to them and try to understand under which conditions the particles in the circuit set into motion and can do work. We realize that certain types of interactions impose symmetries on the system which make doing work impossible [15]. In Fig.2 we show the schematic description of the minimal model studied.

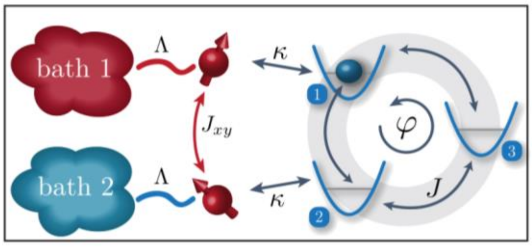

Fig.2: Schematic representation of a minimal engine made of two spins each coupled to a different bath. The load is also minimal, 3 sites, so as to give insight into basic principles and symmetries necessary for the functioning of the engine.

2) Role of interaction in the steady state

Engines are fundamentally open systems (i.e. systems in contact with an environment) which work at steady state. However, the steady state can be significantly different depending on the interaction strength in the system. We explore more this design direction, in systems for which there exist a classical limit [19]. We show the signatures of period doubling in the quantum systems, and also chaotic dynamics. On the left we show a classical bifurcation map (top panel), and two quantum bifurcation maps for intermediate effective Plank constant (medium panel) and smaller one (bottom panel).

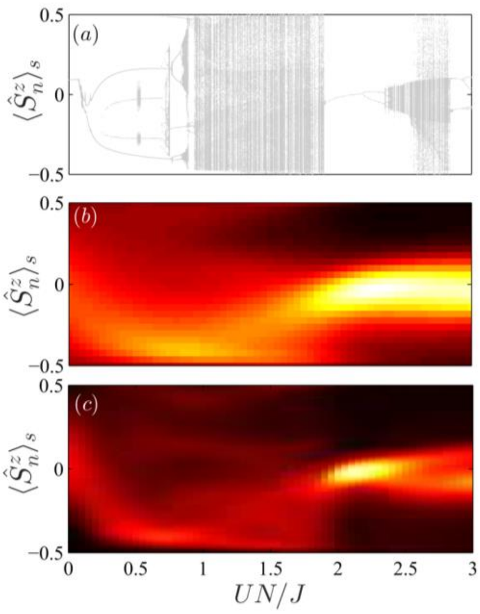

Fig.3: (a) Classical bifurcation map for a two-well potential coupled to a non-equilibrium environment. (b, c) Quantum bifurcation map for the same system respectively for N=25 and N=100.

We also study a circuit in which we impose a current and we study how the current survives the coupling to an external bath, for different values of the interaction [18]. In Fig.4 we observe oscillatory behaviour in the current which depends significantly on the strength of the interaction, on the number of particles, and on the influence of the external bath. This can teach us about the behaviour of currents in quantum engines.

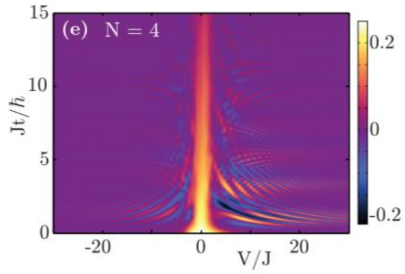

Fig.4: Density plot of current as a function of time and interaction strength.

Similarly to the project discussed in Fig.2, we continue studying a minimal model which we reduce even further and we use it to study the effect of interaction. Here, we uncovered that certain typically used modelization of the quantum systems bring wrong qualitative prediction on the possible existence of currents and their characterization [17]. We consider a circuit directly coupled to two baths (without intermediate spin currents as the one in Fig.2 and we study both the heat and the particle currents. Here we show the particle in yellow (multiplied by 10) and the spin currents in the top and bottom part of the circuit. The x-axis is the strength of the interaction D between the particles, and it shows again how interactions can change significantly the properties of the system in a way that the particle current can be reversed (crosses the zero line).

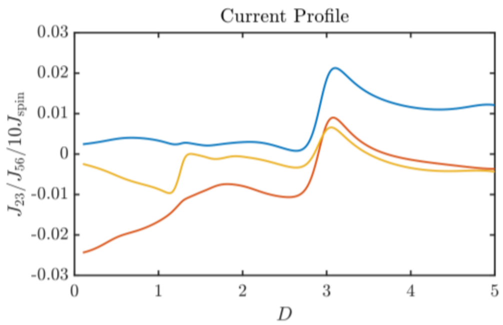

Fig.5: Particle and energy current in the load as a function of the interaction strength D.

Along these lines, we realized that we could improve how to do control in quantum systems which, can then be used as a new tool for the design of quantum heat engines. We presented a protocol which allows to do this with great precision with the use of a large constant and a small time-dependent magnetic field [20]. In this work we focused on a diamond with nitrogen vacancies, something that has already been used to realize heat engines, but it can be extended to many dipolar systems.

3) Role of disorder in work processes

The presence of disorder is an important dimension of the parameter space because 1) it is present in materials, devices and systems and 2) it can significantly alter the properties of the system.

In Fig.7 we are studying the work dissipated versus the inverse temperature β=1/kT, for different amount of disorder, drawn from different disorder distributions (Gamma distribution, blue, and normal distribution, green) in presence of different interaction strength (weak, top panel, intermediate, medium panel, strong, bottom panel).

We notice that the results from the Gamma distribution are non-monotonous, as if the disorder can help to produce less dissipated work. The results from the Gamma distribution can be qualitatively predicted from a strong disorder approximate described by the red-dashed line [21].

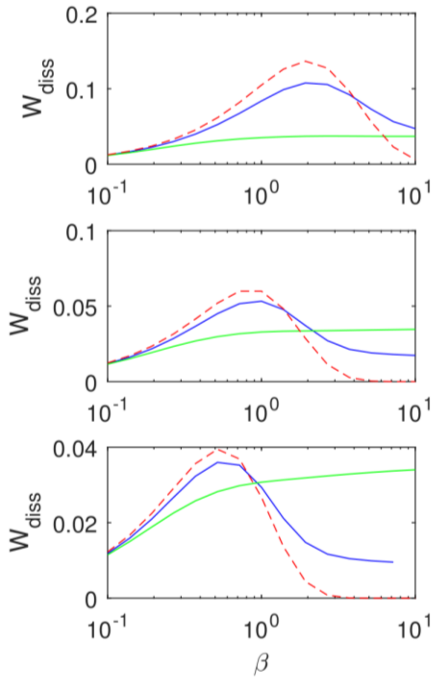

Fig.6: Work dissipated as a function of temperature for weak, intermediate and strong disorder respectively in the top, intermediate and bottom panel. The blue line corresponds to disorder drawn from a Gamma distribution while the green line is for disorder from a Normal distribution (we use the same variance for both distributions). The red line represents a simple analytical model which, as we predicted, is in agreement with the Gamma distribution.

CONCLUSIONS

We have significantly extended the understanding of different important parameters for the design of quantum engines.

We have shown that disorder can have a “lubricating” effect and help in reaching better performance. This is due to the fact that disorder would favour one component of the Hamiltonian which does not commute with another one which, in its turn, is disfavoured by disorder. This work has been submitted and under review [21].

The role of interaction of the engine with the load has been explore in a series of works [15-18]. We have clearly shown that there is entropy transfer between the engine and the load even when the overall set-up is not connected to any bath. This is due to the correlations that build between the engine and the load which, at small scales, cannot be neglected. We have also shown minimal models in which the type of interaction between the engine and the load is the key to get the engine to function or not [15]. It is thus important to ensure that the type of interaction between the engine and the load, and its magnitude, are well designed.

The role of interactions within the engine also affect the overall functioning of the engine [17-19]. They can change the relaxation time scales of the coupling of the system to the bath [18]. They can also induce a reversal of the current of the particle current, hence changing completely the thermoelectric-like properties of the system itself [17]. Last interaction can also induce a dynamics which, in the classical limit, can be chaotic. This opens new opportunities in completely changing the evolutions dynamics, even inducing Floquet time crystals [19].

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