



**AFRL-AFOSR-VA-TR-2024-0022**

---

Foundations of Statistical Mechanics and Quantum Correlations

**de oliveira, thiago**  
**UNIVERSITY FEDERAL FLUMINENSE**  
**RUA MIGUEL DE FRIAS 09**  
**ICARAI NITEROI, , RJ 24220**  
**BR**

---

**10/31/2023**  
**Final Technical Report**

**Controlled By:** USAF AFOSR  
**CUI Category:**  
**Distribution Statement:**  
**POC:** JAMES LYKE/IOSB

Air Force Research Laboratory  
Air Force Office of Scientific Research  
Arlington, Virginia 22203  
Air Force Materiel Command

## REPORT DOCUMENTATION PAGE

PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ORGANIZATION.

<b>1. REPORT DATE</b> 20231031		<b>2. REPORT TYPE</b> Final		<b>3. DATES COVERED</b>	
				<b>START DATE</b> 20190801	<b>END DATE</b> 20230430
<b>4. TITLE AND SUBTITLE</b> Foundations of Statistical Mechanics and Quantum Correlations					
<b>5a. CONTRACT NUMBER</b>		<b>5b. GRANT NUMBER</b> FA9550-19-1-0361		<b>5c. PROGRAM ELEMENT NUMBER</b>	
<b>5d. PROJECT NUMBER</b>		<b>5e. TASK NUMBER</b>		<b>5f. WORK UNIT NUMBER</b>	
<b>6. AUTHOR(S)</b> thiago de oliveira					
<b>7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)</b> UNIVERSITY FEDERAL FLUMINENSE RUA MIGUEL DE FRIAS 09 ICARAI NITEROI RJ 24220 BR				<b>8. PERFORMING ORGANIZATION REPORT NUMBER</b>	
<b>9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)</b> Air Force Office of Scientific Research 875 N. Randolph St. Room 3112 Arlington, VA 22203			<b>10. SPONSOR/MONITOR'S ACRONYM(S)</b> AFRL/AFOSR IOS		<b>11. SPONSOR/MONITOR'S REPORT NUMBER(S)</b> AFRL-AFOSR-VA-TR-2024-0022
<b>12. DISTRIBUTION/AVAILABILITY STATEMENT</b>					
<b>13. SUPPLEMENTARY NOTES</b>					
<b>14. ABSTRACT</b> In this project, we studied the equilibration of isolated quantum systems and the effects of quantum correlations in quantum engines using two baths or quantum measurements. In particular, we obtained bounds for the equilibration time of isolated quantum systems and related this to well know speed limit bounds. We then studied how to emulate the dynamics of isolated quantum systems using the propagation of a laser after passing through aperiodic diffracting structures. We also studied how equilibration changes when we prepare initial states whose initial magnetization has low resolution. Concerning quantum engines, we studied magnetic quantum engines and how the coupling between the spins may change the behavior and efficiency of the engine and the role of non-adiabatic driving of the engine. Thus we analyzed the possibility to implement it using dinuclear metal complexes. Finally, we studied the effects of coupling in quantum measurement engines. In total, the results were published in 6 articles in International Journals [10, 13, 16, 11, 12, 15] and one manuscript that is under review [17]. Four post-docs, one Ph.D. student, one master's student, and one undergrad student participated and were financed by the project.					
<b>15. SUBJECT TERMS</b>					
<b>16. SECURITY CLASSIFICATION OF:</b>			<b>17. LIMITATION OF ABSTRACT</b>		<b>18. NUMBER OF PAGES</b>
<b>a. REPORT</b> U	<b>b. ABSTRACT</b> U	<b>c. THIS PAGE</b> U	SAR		7
<b>19a. NAME OF RESPONSIBLE PERSON</b> JAMES LYKE				<b>19b. PHONE NUMBER (Include area code)</b> 000-0000	

Department of Defense  
Air Force Office of Scientific Research  
Research Interests of the Air Force Office of Scientific Research

Final Performance Report on grant number FA9550-19-1-0361  
Ago 19 - Apr 23

Foundations of Statistical Mechanics and Quantum Correlations

Thiago R de Oliveira

Instituto de Física, Universidade Federal Fluminense, Av. Gal. Milton Tavares de Souza  
s/n, Gragoatá 24210-346, Niterói, RJ, Brazil

August 1, 2023

# 1 Abstract

In this project, we studied the equilibration of isolated quantum systems and the effects of quantum correlations in quantum engines using two baths or quantum measurements. In particular, we obtained bounds for the equilibration time of isolated quantum systems and related this to well know speed limit bounds. We then studied how to emulate the dynamics of isolated quantum systems using the propagation of a laser after passing through aperiodic diffracting structures. We also studied how equilibration changes when we prepare initial states whose initial magnetization has low resolution. Concerning quantum engines, we studied magnetic quantum engines and how the coupling between the spins may change the behavior and efficiency of the engine and the role of non-adiabatic driving of the engine. Thus we analyzed the possibility to implement it using dinuclear metal complexes. Finally, we studied the effects of coupling in quantum measurement engines. In total, the results were published in 6 articles in International Journals [10, 13, 16, 11, 12, 15] and one manuscript that is under review [17]. Four post-docs, one Ph.D. student, one master's student, and one undergrad student participated and were financed by the project.

# 2 Introduction

Statistical Mechanics and Thermodynamics are very successful theories that describe the behavior of macroscopic objects. On the other hand, Quantum Mechanics is very successful to describe the physics of microscopic objects. However, there is still debate on how to connect the microscopic description of Quantum Mechanics with the macroscopic description of Thermodynamics and Statistical Physics: how the macroscopic behavior emerges from the microscopic. Many fundamental questions appear, for example, the justification of the second law of thermodynamics and the possibility of macroscopic superpositions (Schrodinger Cats). These questions, while debated since the origins of the theories, have regained new attention in part due to the experimental possibility to isolate larger systems and observe their quantum behavior: with cold atoms, for example, it is now to isolate up to 50 atoms [1]. These questions are also relevant to the advances of new technologies using quantum effects, as quantum computation.

One approach to obtain the macroscopic behavior from a microscopic, quantum, or classical, description is to introduce probabilities distribution to describe the microscopic behavior. While this approach works, one has to justify the introduction of the probabilities. Another possibility, that has regained interest, is to use a full microscopic quantum description of an isolated system [2]. In this case, the system would never stop evolving and its entropy would be constant; we would never obtain the usual thermalization of macroscopic systems, or the second law. However many new results have shown that for large systems, when one has access to only a few degrees of freedom, the system behavior looks like the usual macroscopic one [2].

Another interesting problem is to use the techniques, formalism, and concepts from thermodynamics to describe small quantum systems. There is also a renewed interest in this problem in a new area that has been named quantum thermodynamics [3]. It has important fundamental and practical questions, such as the definition of work and heat for microscopic quantum systems and the possibility to build small quantum thermal engines with better performance than the classical ones. In quantum thermodynamics, there is an expectation that, as in quantum computing, quantum correlation may allow for enhanced performance over the classical scenario.

# 3 Accomplishments

## 3.1 Research Objectives

One of the objectives of the present project is to study the mechanism of equilibration of isolated quantum systems, in particular the times scales involved, the relevant physical properties, and the roles of quantum correlations. Related to this we also want to study the role of quantum correlations in quantum thermal

engines and possible enhancement in its performance. The technical approach used are analytical calculations and numerical simulations of spin chains.

### 3.2 Details of the accomplishments

In the first year of the project, we studied measured base engines using the Otto cycle. This is a new type of engine where instead of exchanging energy in the form of heat with thermal baths, a quantum measurement is made on the system. This measurement disturbs the system and transfers energy to it in a random and irreversible way [5]. A thermal engine where the hot bath is replaced by a quantum measurement was studied for the Otto cycle in [6]. In particular, they showed that minimally disturbing measures always increase the system energy and that for a single spin-1/2 particle the efficiency is the same as the classical engine. Thus no quantum advantage was obtained for this simple system. In order to study more complex systems and the role of quantum correlations the same engine with two spin-1/2 coupled with the Heisenberg interaction was analyzed in [7]. An increase in the efficiency with the coupling was obtained and it was suggested it may be due to the quantum correlations between the two particles.

We studied a measurement base Otto cycle with more general coupling between the spins; allowing for anisotropies for example. We showed that the increase in the efficiency is not due to the quantum correlations between the spins, but to the structure of the energy levels: the fact that some of the levels do not change during the adiabatic process and therefore do not contribute to the work. We also characterized the measurements that increase the efficiency. These results were obtained by a master's student and published in [11].

We also showed that energy level structure is responsible for the increase in the efficiency of the same system operating with two thermal baths, and not the quantum correlation as was suggested [4]. Moreover, in this case, we found a new counter-intuitive phenomenon: it can cease to operate as an engine if the hot bath becomes too hot, or if the cold bath becomes too cold; even in the limit of absolute zero. This work was done by me (PI) and a collaborator [10].

In the second year of the project, we extended the analyses considering the effects of an adiabatic process at a finite time for the two bath engines. As expected there is a decrease in the efficiency and we studied how this decrease change in the coupling and the adiabatic time. Interestingly we found that the non-intuitive phenomenology may be preserved if the adiabatic time is not too short. This work has been conducted by a post-doc hired in the second year of the project [13].

We also studied the interplay between quantum speed limits and the equilibration time of isolated quantum systems. We obtained several upper bounds on the equilibration time, based on the quantum speed limit, and analyzed them for spin chains. This work was conducted by a second post-doc [12].

In the third year of the project, we studied the effects of a lack of resolution in the preparation of magnetized initial states in its equilibration. We showed that this lack of resolution, or coarse-graining, in the magnetization may induce the equilibration of the state for non-integrable Hamiltonians. This work was done by two post-docs and a master's student and is already under review [17].

We also studied the effects of coarse-graining in Typicality results that are relevant to understand the thermalization of macroscopic systems. It has been shown that if one picks a pure state at random in the Hilbert space, it may seem like a thermal state when looking at small regions [8]. To obtain these results one has to sample the Hilbert space using the uniform Haar measure. However, most of the states of the Hilbert space are nonphysical; they have a lot of entanglement and would not be generated by local Hamiltonian in a polynomial time. Thus there is an effort to consider how the typicality results would change when considering more physical sets of states (see [9], for example). One possibility is to sample the Hilbert space with the Haar measure but to apply a coarse-graining in the states that would generate a more physical set of states. We showed that the typicality of the set of random states can increase after coarse-graining by a degree that depends on the entropy of the quantum map that characterizes the coarse-graining. These results seem very interesting and may be useful tools for studies of thermalization and equilibration. We are finishing writing a draft with the results that will be sent for publication.

We also participate in a study of the regimes of operation of quantum engines with coupled spins, but

using the Stirling cycle. In this work, we also showed that it may be possible to use a dinuclear metal complex to build such a quantum engine [16].

Finally, we finished a collaboration with the experimental group to simulate the revival dynamics of isolated quantum systems by light [15].

Unfortunately, we were not able to study the quantum fluctuations involved in the operation of the magnetic quantum engine. We are starting to analyze this problem and hope to have results in the next six months;

### 3.3 Dissemination

The work was disseminated to the physics community through participation in several conferences where the works were presented. In particular in international conferences such as "Quantum Thermodynamics Conference" of 2020-2023 and "Frontiers of Quantum and Mesoscopic Thermodynamics" of 2022. We also presented the works at the annual fall conference of the Brazilian Physical Society from 2020 to 2022. Besides, we also gave seminars to other research groups in Brazil about the results.

With respect to outreach activities, we presented the results for undergrad students in seminars at the Physics Institute of Federal Fluminense University and participated in "Pint of Science"; an event to present research for the general public.

## 4 Impacts

The results of the project help to advance the understanding of the equilibration of isolated quantum systems and quantum thermodynamics. The results in [12] is one of the first attempts to connect results from quantum speed limit to equilibration of isolated quantum systems. The results in [17] helped to better understand the physical properties of initial states that are relevant for equilibration besides energy resolution.

We also made a collaboration with experimentalists to emulate the evolution of isolated quantum systems using light propagation [15].

The study of typicality under coarse-graining can help to study typicality for classes of random states with more physical motivation and improve our understanding of the role of typicality on the foundations of statistical mechanics. It may also allow the study scenarios beyond the usual subsystem and canonical ensembles.

For thermal engines, our studies showed a new mechanism for the efficiency increase of quantum engines that does not involve quantum coherence or correlation, as used expected from the quantum information community [10, 13].

In relation to human resources, four post-doc participated in the project, one Ph.D., one master's student, and one undergrad. While the post-docs were fully financed by the project the other students had an complement to their university fellowship.

## References

- [1] I. Bloch, J. Dalibard, and S. Nascimbene, *Nature Phys.* 8, 267 (2012).
- [2] Equilibration, thermalization, and the emergence of statistical mechanics in closed quantum systems C. Gogolin, J. Eisert, *Rep. Prog. Phys.* 79, 056001 (2016).
- [3] S. Deffner and S. Campbell, *Quantum Thermodynamics: An introduction to the thermodynamics of quantum information* (Morgan and Claypool Publishers, 2019). arXiv:1907.01596 [quant-ph]
- [4] G. Thomas and R. S. Johal, *Physical Review E* 83, 031135 (2011).
- [5] C. Elouard, D. Herrera-Martí, B. Huard, and A. Auffèves, *Phys. Rev. Lett.* 118, 260603 (2017).

- [6] J. Yi, P. Talkner, and Y. W. Kim, *Physical Review E* 96, 022108 (2017).
- [7] A. Das and S. Ghosh, *Entropy* 21, 1131 (2019).
- [8] Sandu Popescu, Anthony J. Short and Andreas Winter, *Nature Physics* 2, 754 (2006).
- [9] Silvano Garnerone, Thiago R de Oliveira, Stephan Haas, Paolo Zanardi, *Physical Review A* 82, 052312 (2010).
- [10] Thiago R. de Oliveira, D Jonathan *Physical Review E* 104, 044133 (2021).
- [11] Maron F. Anka, Thiago R. de Oliveira, D Jonathan, *Physical Review E* 104, 054128 (2021).
- [12] Diego P Pires, Thiago R de Oliveira *Physical Review A* 104, 052223 (2021).
- [13] Cleverson Cherubim, Thiago R. de Oliveira, D Jonathan, *Physical Review E* 105, 044120 (2022).
- [14] Maximilian Schlosshauer, *Phys. Rev. A* 72, 012109 (2005).
- [15] M. R. Maia, D. Jonathan, Thiago R. de Oliveira, A. Z. Khoury, and D. S. Tasca, *Opt. Express* 30, 27180-27195 (2022).
- [16] Clebson Cruz, Hamid Reza Rastegar Sedehi, Maron Freitas Anka, Thiago R. de Oliveira, Mario S Reis, *Quantum Sci. Technol.* 8, 035010 (2022)
- [17] Gabriel Dias Carvalho, Luis Fernando dos Prazeres, Pedro Silva Correia, Thiago R de Oliveira, arXiv:2305.11985 [quant-ph]