QUANTUM TRANSPORT EQUATIONS AND APPLICATIONS

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1 Overview of the Field

Models for transport phenomena arise in several fields of pure and applied sciences. A lot of mathematical research, both theoretical and numerical approaches, has been done on these models in classical dynamical systems and, recently, also in quantum systems, especially in open quantum systems see References [10, 11, 7].

This workshop brought together people working in classical and quantum transport models and equations, open quantum systems, metrics on states of a C*-algebra, quantum stochastic calculus, models for heat conduction, quantum entropic methods, quantum phenomena as decoherence and dephasing, many particle systems and interacting Fock spaces and more generally evolution problems.

Contact points for future collaboration between researchers working on the above subjects have been identified, new methods and emerging ideas will be investigated.

The workshop exposed several young Mexican researchers to current ideas and technics in the field and allowed them to get in touch with internationally recognized experts for future collaboration and development of their scientific carriers.

2 Recent Developments and Open Problems

The main topics discussed in the workshop were:

1. Mathematical derivation through space-time scaling limits, of macroscopic conservation laws from the microscopic dynamics of molecules
2. Models for heat conduction and Fourier's law
3. Quantum Markov semigroups obtained from scaling limits of a system coupled to heat baths
4. Invariant states of quantum transport models
5. Structural properties of quantum Markov semigroups
6. Decoherence phenomena and the decoherence free sub algebra of a quantum Markov semigroup

7. Mean field limit for interacting quantum systems
8. Mean field transport equations
9. Entropy methods in quantum dynamics
10. Many particle systems and interacting Fock spaces
11. Metrics on states of a C*-algebra

The weak coupling and the low density limits are now established technics for the deduction of quantum Markovian master equations from physically meaning Hamiltonians of a system coupled with several reservoirs. Similar models have been studied for classical systems with Wiener noises playing the role of the heat baths. In this case the mechanism for heat conduction and transfer is understood. Classical models, as those presented by S. Olla, are often adapted to quantum systems by translating corresponding classical equation into some non-commutative versions. It would be desirable to have a fully quantum deduction treatment of these quantum master equations.

The analysis of the structure of weak coupling and low density limit Markov semigroups, in particular of those semigroups modeling quantum energy transport and photosynthesis, that have been deduced recently by means of the weak coupling limit, see references [1, 3], is a major challenge. The structure of its invariant states and other phenomena like the appearance of dark states should be well understood from the mathematical point of view. The relation of invariant states with the interaction (or decoherence) free subspaces is now clear and for that class of semigroups that do not allow explicit computations, the machinery of invariant subspaces and decoherence free subalgebra is available. The talks of L. Accardi, F. Guerrero, R. Quezada, J.C. García, F. Fagnola and E. Sasso are contributions in this direction.

A short list of open problems include:

- a complete description of the structure of QMSs,
- a characterization of the set invariant states of QMSs of weak-coupling and low-density limit type,
- characterize the set of invariant states and clarify the role of notions like energy flow (currents) and dark stationary states in models of quantum energy transport and photosynthesis

3 Presentation Highlights

The workshop included 19 talks given by the participants a well as three sessions of discussion on the main topics of the workshop by Stefano Olla, Luigi Accardi and Franco Fagnola.

In Stefano Olla's talk and discussion session on hydrodynamic limits from classical and quantum microscopic dynamics, one of the main problems in statistical mechanics was considered: the mathematical derivation, through space-time scaling limits, of macroscopic conservation laws, like compressible Euler equations or the heat equation, from the microscopic dynamics of molecules. Different space-time scalings, denoted as hydrodynamic limits, can lead to different macroscopic equations: the Euler system of equations governs the convergence to mechanical equilibrium (towards constant pressure) in a hyperbolic scaling, while at diffusive scaling (larger time) heat equation governs the convergence to thermal equilibrium (constant temperature), if thermal conductivity is finite. Deriving macroscopic limits from a deterministic (classical Hamiltonian or quantum) dynamics is a famous arduous problem. Some results can be obtained by adding to the dynamics some random terms such that momentum, energy and volume are still conserved but all other integrals of the motion are destroyed. The harmonic chain, despite the fact to be completely integrable, is an exception and, for the deterministic dynamics in thermal (global) equilibrium, the Euler equation are valid in the hyperbolic scaling. If the masses are random, thanks to Anderson localization, Euler equations are valid even out of thermal equilibrium. Furthermore, in the random mass case, the temperature profile remains constant in time at every later time scale, including the diffusive one, giving a further proof that thermal conductivity of this system is null. This results on the harmonic chain are extended to the corresponding quantum dynamics. Stefano Olla also presented a talk and discussion on energy transport in non-equilibrium stationary states.

Markov generators of stochastic limit type where presented by Luigi Accardi who introduced some general properties of that generators, explored the notion dark stationary states in chlorophyll systems and gave an introduction to quantum Markov chains.

The general properties of low density limit type generators where illustrated in the talk by Fernando Guerrero-Poblete who discussed on the structure of quantum Markov generators describing the reduced dynamics of a test particle interacting with a diluted Bose gas in the low density limit. He also presented some results concerning the structure of invariant states in the generic case.

The mechanisms of quantum transport have attracted the attention of researchers from different areas (biology, physics, chemistry, mathematics), who have produced an important amount of scientific, experimental or theoretical work focused on describing and modeling these complex mechanisms. Due to their characteristics as complex systems, semigroups of weak coupling limit type, with degenerate Hamiltonian, are suitable for modeling these phenomena.

The general structure of the stationary states of excitation energy transport models and weak coupling limit type generators was discussed by Roberto Quezada, he started with the case of a non-degenerate reference Hamiltonian and presented the structure of stationary states belonging to the annihilator of all Krauss operators, including detailed balance and local detailed balance states. He also presented a talk on the dark stationary states in a model of photosythesis [3].

In his talk, Julio C. García discussed the mathematical structure of the infinitesimal generator of some semigroups modeling quantum energy transport and the set of their stationary states. He also discussed on the decoherence free subalgebra of a quantum transport model of [1].

Franco Fagnola described the structure of generators of norm-continuous quantum Markov semigroups with atomic decoherence-free subalgebra providing a natural decomposition of a Markovian quantum open system into its irreducible components and noiseless components. As an application, he discussed the structure of invariant states of certain quantum Markov semigroups of weak coupling limit type.

In her talk, Emanuela Sasso explained the relationships between the atomicity of the decoherence-free subalgebra, environmental decoherence, ergodic decomposition of the trace class operators, and the structure of fixed points. In particular, she showed that, for a Quantum Markov Semigroup (QMS) with a faithful normal invariant state, the atomicity of the decoherence-free subalgebra and environmental decoherence are equivalent. Moreover, she characterized the set of reversible states and explicitly described the relationship between the decoherence-free subalgebra and the fixed point subalgebra for QMSs with the above equivalent properties. Loosely speaking one can say that, for QMSs with a faithful invariant state, the same conclusions can be drawn replacing finite dimensionality of the system Hilbert space by atomicity of the decoherence-free subalgebra.

George Androulakis explored the notion of quantum Kac's chaos which was implicitly introduced by Spohn and explicitly formulated by Gottlieb. He proved the analogue of a result of Sznitman which gives the equivalence of Kac's chaos to 2-chaoticity and to convergence of empirical measures. He gave a simple, different proof of a result of Spohn which states that chaos propagates with respect to certain Hamiltonians that define the evolution of the mean field limit for interacting quantum systems.

Hölder-type inequalities for norms of Wick products generated by a subclass of Meixner random variables was discussed by Aurel Stan. The class of Meixner random variables can be described in terms of a Lie Algebra structure generated by their quantum operators. This Lie Algebra structure is useful in computing first the kernels that give the second quantization operators, and then the Wick products generated by these random variables. Special attention was given to three of the most important types of Meixner random variables: Gaussian, Poisson, and Gamma, and presented some Hölder inequalities for the norms of the Wick products generated by them. He showed that these inequalities are related to sharp inequalities from classic Harmonic Analysis concerning the norms of some convolution-type products.

Jorge Bolaos explored the spectrum of completely positive Toeplitz Operators and Weak Coupling Limit type generators. The notion of circulant completely positive map was extended to the Toeplitz case together with the usual technique of invariant subspaces in order to study the operator itself and its spectrum. Some results and simple cases were reviewed. The relation between Toeplitz maps and a family of (non degenerate) WCLT generators was described together with some simple results regarding the spectrum.

In his talk, Alex Wiedemann discussed quantum dynamical semigroup generator induced digraphs. Digraph induced generators of quantum dynamical semigroups have been introduced and studied, particularly in the context of unique relaxation. In his talk he aconsidered the converse construction to show every generator

$\mathcal{L}$ naturally gives rise to a digraph $G_{\mathcal{L}}$. In specialized cases he used properties of $G_{\mathcal{L}}$ to explicitly compute all invariant states of the semigroup. In the general case he discussed relaxation and the number of invariant states of the semigroup in terms of several other generator induced graphs

In his talk " From quantum random walks to quasifree stochastic cocycles", Alexander Belton explained that Attal and Joye (J. Funct. Anal. 247, 2007) studied a repeated-interactions model driven by particles in a faithful normal state. As they observed, the limit dynamics obey a Langevin equation driven by quantum noises which satisfy the commutation relations for a quasifree state. Inspired by this example, he describe a general framework to handle such quasifree random walks. The theory of quasifree quantum stochastic integration required to describe the limit cocycles builds on early work of Hudson and Lindsay, together with more recent work of Lindsay, Margetts and Weatherall.

Duncan Wright discussed on the nonlinearity of quantum dynamical entropy. He showed that the quantum dynamical entropy introduced by Slomczynski and Zyczkowski is nonlinear in the time interval between successive measurements of a quantum dynamical system. This is in contrast to Kolmogorov-Sinai dynamical entropy for classical dynamical systems, which is linear in time. He also computed the exact values of quantum dynamical entropy for the Hadamard walk with varying Lüders-von Neumann instruments and partitions.

D. Bures defined a metric on states of a C*-algebra as the infimum of the distance between associated vectors in common GNS representations. Now there are modifications and extensions of this notion to completely positive maps. Rajarama Bhat presented some recent results in the area.

4 Scientific Progress Made

We think that this workshop provided an invaluable outline on the main lines of research and contact points between researchers working on open quantum systems, quantum probability, partial differential equations and its applications to classical and quantum transport problems, creating a fertile ground for the emergence of new methods and ideas.

The workshop also helped at exposing several young Mexican researchers to current ideas and methods in the field in order to establish a broad and continuous cooperation with internationally recognized experts.

Several problems in QMSs and, more generally, in Quantum Probability, were born from concrete problems in Quantum Physics or Quantum Information. To study nontrivial and meaningful classes of models as a paradigm for quantum transport phenomena in equilibrium and local equilibrium conditions the machinery of QMSs is now available. The class of weak coupling limit type generators with a degenerate reference Hamiltonian, exhibit a complex behavior that seems to be appropriate for modeling excitation energy transfer. The analysis of models of quantum transport and photosynthesis deduced through the stochastic limit method gave important insight and has stimulated further research in this direction in the forthcoming years.

We know from e-mail contacts we had after the meeting that, in particular:

- Franco Fagnola and Roberto Quezada, discussed with Alvaro Hernández-Cervantes on recent progress in his PhD project concerning the structure of the set of invariant states of weak coupling limit type semigroups.
- Marco A. Cruz de la Rosa counted with L. Accardi's advice on his research on non-equilibrium stationary states of multi-photon absorption and emission semigroups and a possible postdoctoral stage in Roma.
- Julian Agredo discussed with Julio C. García and Roberto Quezada on their work on the decoherence free sub algebra of weak coupling limit type generators.
- José Manuel Valdovinos had the opportunity to discuss with Aurel Stan on his work initiated in Ohio State University.
- Luigi Accardi, Roberto Quezada and Fernando Guerrero discussed on the class of low density limit semigroups and started collaboration on this topic.

5 Outcome of the Meeting

This workshop has been a dynamic arena for discussion on classical and quantum transport equations and models. In particular, the quantum transport models discussed in the workshop strongly suggest that degenerate (with degenerate reference Hamiltonian) open systems interacting with several reservoirs are appropriate to model quantum transport phenomena. It is clear now that the role of notions like energy flow (currents) and dark state may be of fundamental importance and deserve further investigation.

Important progress on some joint works has been made during the workshop.

The workshop served for a number of young PhD's and post-docs from Mexico and United States (at least eleven) to stablished contact with experienced researchers in the field.

Finally let us quote the testimonials of two participants.

Rajarama Bhat: " ... I came to know of several recent developments in my field and also some of them have given me some new ideas to work on. I also met some younger mathematicians whom I had not met before..."

Marco A. Cruz de la Rosa: "The workshop helped me a lot; for the topics of interest addressed, for the contacts I could make that I would not have had otherwise, for reinforcing the ones I already had, and above all for the chance of a postdoctoral stay abroad"

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