Mathematical Horizons for Quantum Physics

A workshop held at the

Institute for Mathematical Sciences
National University of Singapore

Session 3: Non-Equilibrium Statistical Mechanics

August 25 – September 14, 2008

Final Report

1 Aim and Organization

This 4 sessions workshop was organized in a somewhat unconventional way. Rather than giving to participants the opportunity to report on the recent progresses in their respective fields of interest, the well named MHQP-program was designed with the idea of looking forwards into the future of these fields.

The aim of the organizers was to bring together small teams of scientists sharing common interests in mathematical problems related to quantum physics and offer them the opportunity to think about *open problems*. In each session a limited number of discussion themes were identified and discussion leaders were responsible to launch the work of the team through a Review presentation of these themes. Then followed a period of intense and close collaboration between the session participants, possibly in smaller groups, under the guidance of the discussion leaders. Overlapping sessions also offered nice opportunities for more informal but nevertheless very fruitful cross-session discussions. The outcome of the session's team work was presented in a final round-table discussion.

In parallel to these research activities, each session has also provided one or several more pedagogical Tutorial presentation, aimed at graduate students and non-experts.

2 Participants

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3 Themes and Reviews

Session 3 – non-equilibrium statistical mechanics – was organized around two central themes:

- *Non-Equilibrium steady states (NESS).*

  Discussion leader C.-A. Pillet.

- *Quantum fluctuations out of equilibrium.*

  Discussion leader J. Dereziński.

For each theme, several important open problems were addressed during the session (see Section 5).

Despite recent progresses, non-equilibrium statistical mechanics, as a physical theory, as well as its mathematical foundations are still in an early stage of development. To the mathematical physicists, they offer many challenging problems related to a large spectrum of mathematical knowledge: operator algebras, spectral analysis, scattering theory, non-commutative probability theory and stochastic calculus, completely positive semigroups, ...

To setup some of these problems and expose their mathematical framework, three Review presentations were proposed:

- *Non-equilibrium steady states of open quantum systems,*

  by C.-A. Pillet.
- *The extended weak coupling limit,*

  by J. Dereziński.
- *Fluctuations in open quantum systems,*

  by W. De Roeck.

4 Tutorial

Scattering theory plays a fundamental role in the theory of quantized fields. It turned out to be also an important tool in recent developments of non-equilibrium quantum statistical mechanics. It was therefore natural to schedule a pedagogical Tutorial presentation on this subject during session 3:

- *Scattering in quantum field theory I, II and III,*

  by J. Dereziński.

Despite the apparent and somewhat surprising lack of interest in this subject from graduate students, these 3 two-hours lectures were a success among the participants to sessions 3 and 4. They also turned out to be quite useful for some of the research worked out during the session.

5 Results

1. Thermal relaxation. The first problem addressed during the session was to extend the Liouvillean approach to thermal relaxation (return to equilibrium and more generally construction of NESS) to open systems with many degrees of freedom (i.e. where the “small” system is spatially confined but has an infinite dimensional Hilbert space. In mathematical terms its Hamiltonian is unbounded above but has compact resolvent). Since the Liouvillean approach is based on the study of dynamical resonances, the mathematical problem faced here is perturbation theory of infinitely degenerate embedded point spectrum. Solving this problem requires understanding the spectrum of a so-called level-shift operator. For finite small system, this operator has a spectral gap which controls the relaxation processes. For infinite systems, it was not clear, prior to discussions, whether such a gap was to be expected. Even though we did not expect to solve this hard problem during the session, some progresses in understanding its physical origin have been made through discussions between M. Merkli, C.-A. Pillet, W. De Roeck and V. Bach (session 4). High energy fluctuations are rare events because the ultra-violet cutoff on the interaction prevents direct “jumps” over large energy scales. For the very same reason such events are long-lived: it takes a long time for the system to recover from such a rare event. It is therefore natural to expect the relaxation process to be slow, non-exponential. This directly leads to the conjecture that the level-shift operator has no spectral gap in this situation. Of course, this implies that spectral analysis of the level-shift operator will be much more delicate.

2. Leaky QED cavity. The Liouvillean approach to thermal relaxation has also been successfully applied to Repeated Interaction Quantum Systems. In such systems, the environment consists in a chain of independent, identical subsystems (e.g. 2-level atoms) which successively interact with the “small” system. This class of model is widely used in physics to describe the dynamics of a QED cavity interacting with a beam of atoms (one-atom masers). The problem raised during the session was to incorporate the effect of an imperfect (leaky) cavity into this description. This can be done by coupling the cavity to a heat bath. The question is to study the competition between this reservoir which wants to bring the system in thermal equilibrium and the repeated interactions with the chain which drives it to a non-equilibrium stationary state. A. Joye and M. Merkli, who had already worked together (with L. Bruneau, Cergy University) on the perfect cavity models, have made substantial progress on this problem during the session.

3. The Rotating Wave Approximation. As already mentioned, scattering theory plays a important role in non-equilibrium statistical mechanics. To develop scattering theory beyond the perturbative regime (Schwinger-Dyson) is a major challenge which could allow us to extend the domain of application of these techniques. On the other hand, stationary formulas for scattering operators are essential ingredients in the description of stationary currents in quasi-free fermionic open systems (Büttiker-Landauer formalism, shot noise statistics). It is an open problem to extend such formulas to locally interacting fermions. With these two motivations in mind, discussions took place to setup a tractable mathematical problem and start working on it. At the outcome of the first stage of the discussion, the spin-boson model in the rotating wave approximation was elected as the simplest non-trivial model. This model was then further investigated by J. Dereziński, A. Joye and C.-A. Pillet. The existence of asymptotic creation/annihilation operators turned out to be an easy problem for this model. Further investiations are needed, however, to proceed towards some form of asymptotic completeness and to derive stationary formulas for the scattering operators. In the first non-trivial (1 boson) sector, the Friedrichs Hamiltonian emerges. The spectral and scattering theory of this operator is well known and was part of J. Dereziński's Tutorial lecture. We then succeeded in the analysis of the 2 boson sector, getting a complete picture of the analytic structure of the resolvent on the second sheet. The general structure of the Hamiltonians in higher (n bosons) sectors is well understood. A collaboration has been setup in order to continue this work towards a precise spectral and resonance analysis of these operators.

4. Quantum generating functionology. Generating functions for fluctuations of entropy production and currents are at the center of new results in classical non-equilibrium statistical mechanics. Their Legendre transform are rate functions of large deviation principles for these fluctuation. As a result of Evans-Searles and Gallavotti-Cohen fluctuation theorems these generating functions display a symmetry (colloquially coined the GC-symmetry). Several quantum generating functions for the statistics of fluctuations of the entropy production and currents which display the GC-symmetry have been recently proposed, either on the basis of ideal physical measurement processes or on a mathematical analysis of the modular structure of the underlying von Neumann algebras. One of them relates to what physicists call full counting statistics, but the others are still lacking a physical interpretation. A discussion has been launched on the possible physical meaning of these new generating functions. Y. Ogata proposed an interesting relation with quantum hypothesis testing for discriminating the state of the system at time t

and its time reversed. Such a relation leads to a clear physical interpretation of the new generating functions. She has been working in this direction and has obtained some encouraging results. Efforts in this direction will be continued. Another aspect of quantum generating functionology is the actual calculation of these generating functions for concrete models. In particular, this seems to be the only currently available route to check the validity of GC-symmetry for generating functions computed on NESS. Some progresses have been achieved in this direction by Y. Ogata and C.-A. Pillet who succeeded in developing a general scheme for computing various generating functions for quasi-free fermionic open systems. In these systems, the generating functions can be expressed in terms of energy integrals of determinants involving the on-shell scattering matrix of the system.

6 Acknowledgements

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