MHQP Final Report: Session I

MHQP Session I: Quantum Control and Dynamics

Organizer:

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Discussion Leaders: (parentheses indicate the period of stay)

Goong Chen (July 28-August 15, 2008)
Stephan DeBievre (July 28-August 6, 2008)
Arne Keller (July 28-August 6, 2008)
Hans-Rudolf Jauslin (August 3-August 15, 2008)

Core Participants:

Andre Bandrauk (August 10-August 15, 2008)
Zhonghai Ding (July 28-August 15, 2008)
Raymond Ooi (August 5-August 15, 2008)
Viswanath Ramakrishna (July 28-August 15, 2008)

Objectives:

There are three main objectives of study in this MHQP Session I Program:

(1) Molecular quantum control;
(2) Laser driven quantum computing devices;
(3) Quantum chaos.

Tutorials and survey talks on these topics were given on July 28, July 29 and August 4, plus many small group discussions and presentations, as well as interactions with the NUS local groups and researchers. See the list of talks in

`http://www.ims.nus.edu.sg/Programs/mhqp08/activities1.htm`

(There are many other small group tutorials and discussions not included in the above.) Overall, the schedules of the program were quite tight and intense, and the benefits to the participants were numerous and profound.

Round Table Discussions (August 15, 2008, 2-3:30pm)

It took place in the Meeting Room of IMS and there were about 30–40 participants. Prof. Berge Englert first briefed the participants about the organization process of and financial support for MHQP, which took nearly two years of planning and reviewing to receive the final approval.

Prof. Goong Chen then gave a summary of the program topics, activities and progress:

Main topics:

(1) Molecule alignment and orientation problem: Discussion leader: Arne Keller, who gave tutorials on the state-of-the-art mathematical techniques and models, and guided problem discussions.

(2) Quantum chaos: Discussion leader: Stephan de Bievre, who gave a nice survey of quantum chaos and recent progress on the sensitivity and topological transitivity issues. We were hoping to connect quantum chaos with the limitations of quantum computing.

(3) Applications of the Floquet theory to laser driven quantum systems:

> Discussion leader: Hans-Rudolf Jauslin, who really showed his finesse on this subject, tutored the group about major techniques of the Floquet theory, plus many examples of applications.

(4) Quantum computing devices:

> Discussion leader: Goong Chen, discussed the problem of isomorphism between different quantum computing gates with Ramakrishna. Hopefully a paper can be written on this topic in the forthcoming months.

(5) Computational chemistry and physics of dynamic phenomena involving atoms and molecules in intense laser fields: Andre Bandrauk gave a fascinating talk; he will be organizing a conference at the Centre de Mathematiques in the Universite de Montreal in 2009.

(6) Other general problems in atomic and molecular quantum mechanics; e.g. Maxwells demon, entropy change in quantum control, etc.

Unfortunately, the topics of fractional quantum Hall effects and topological quantum computer design could not be covered.

Prof. Wayne Lawton and Dr. Anders Mouritzen have given talks and participated particularly actively throughout the entire Session I. Prof. Baowen Li and his group have also contributed a full day program of nice talks on quantum chaos, BEC, quantum rotors and other quantum physical processes. Their contributions and participation are gratefully acknowledged.

More discussions ensued. Andre Bandrauk has raised a question whether there are attempts to design quantum algorithms for solving difficult partial differential equations. Reinhardt Werner commented that solving of ground states involves complicated many body problem. Mary Beth Ruskai mentioned adiabatic quantum computing and lattice gas dynamics and Type II Quantum Computers. Etc.

Hans Jauslin then presented a more detailed technical discussion of the many problems of interest to Session I, including optimal control in an infinite dimensional Hilbert spaces, genetic algorithms, etc. See more details in the next section.

Specific Research Topics Discussed and Open Problems Introduced in MHQP Session I

(1) Entanglement witness for two coupled Quantum Arnold maps (S. de Bièvre, A. Keller, H.R. Jauslin) The goal is to analyse the incidence on entanglement of two quantum systems that can be precisely characterized with respect to their quantum chaos properties. The analysis can be permormed in terms of some of the recently proposed tools of entanglement witnesses. An intersting aspect will be the behavior of the entanglement witness with respect to the semi-classical limit.

(2) Floquet model for Raman spectroscopy in strong field plasmons on nano-structured surfaces (A. Keller, H. R. Jauslin)

(3) Extension of adiabatic Floquet theory to the control of the nonlinear dynamics of Bose-Einstein condensates (H.R. Jauslin and L. Morales-Molina (Dept. Physics, NUS)). This involves several open subproblems:

   (a) Extension of resonant averaging techniques to nonlinear systems to models for the control by electromagnetic fields of Bose–Einstein condensates.

   (b) Analysis of adiabatic processes in non-integrable Hamiltonian systems involving chaotic regions of phase space.

(4) Factorization of an arbitrary matrix in U(N) as the product of exponential of diagonal and tri-diagonal anti-hermitian matrices. Applications to impulse control processes (V. Ramakrishna, A. Keller).

(5) Control theory for quantum systems in infinite-dimensional Hilbert spaces (V. Ramakrishna, Z. Ding, S. de Bièvre, A. Keller, G. Chen, H.R. Jauslin)

   (a) For quadratic Hamiltonians; control problem for the symplectic group

   (b) For models of alignment and orientation of molecules by strong laser pulses. Analysis of the Galerkin approximations.

(6) Numerical techniques for determining the energy and eigenfunction of H^- (Z. Ding, G. Chen, M.B. Ruskai).

(7) Control of molecular processes by atto-second laser pulses (A. Bandrauk)
Open problems:

   (a) control of continuum states

   (b) decoherence of time dependent states

   (c) Control of Maxwell–Schrödinger equations (solitons, etc.)

   (d) Time series for multiscales (electron an nuclear motion)

   (e) Treatment of boundary conditions in parallel computing of quantum dynamics

(8) Conditions of applicability of adiabatic approximations in quantum dynamics (L.C. Kwek and D.M. Tong (Dept. Physics, NTU), H.R. Jauslin)

Summary

Laser driven dynamic quantum mechanical and molecular systems governed by the Schrödinger equation are very timely topics in chemical physics, quantum computation and information, and general quantum technology. There are many newly emerged problems of great interdisciplinary interest to the physics, chemistry and applied mathematics communities, and with immense application potential. On the other hand, quantum chaos is a more established subject, continuing to attract the attention of many mathematical physicists.

Overall, we are delighted to report that the responses from participants have been totally positive and favorable. Within the next few months, research papers should begin to be written and published which are either direct consequences of the many discussions made at MHQP, or outcomes indirectly impacted by MHQP Session I. Acknowledgements to MHQP, IMS and NUS will be cordially registered. We wish to express our sincerest thanks to NUS local participants (Prof. Lawton, Dr. Mouritzen, Prof. Baowen Li and his group, Mr. L. Morales-Molina) for their active participation and contributions, to IMS staff (Ms. Claire Fong and Agnes Wu) for their help and service, and to the Organizing Committee (Profs. Araki, Englert, Kwek, and Dr. Suzuki), IMS Director Prof. Louis Chen, Centre for Quantum Technologies of NUS, the Lee Foundation and Faculty of Science of NUS for the financial support and hospitality for the MHQP Session I Program.