UNIVERSITY OF SASKATCHEWAN

Department of Mathematics& Statistics **Term 2, January 2010**

Mathematical modelling of nanosystems

MATH 498.3 (CRN 26936)/ MATH 818.3 (CRN 24505) Special Topics in Applied Mathematics-Nanosystem Modelling

Course Outline

Instructor: Artur Sowa, Department of Mathematics and Statistics, McLean Hall 225, 966-6114,

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Meeting hours: 3 times weekly, total of 39 lectures/-hours TBA

Prerequisites: Math 266.3: Linear Algebra II, and Math 338.6 Differential Equations II, or equivalent by permission of the instructor

Description: The course has been designed to bridge a gap between the traditional Applied Mathematics curriculum and the emerging trends in sciences and technology. It will be helpful to students specializing in either one of the following disciplines: Mathematics, Mathematical Physics, and Physics, various areas of Engineering, Statistics, Computer Science, Chemistry, or Biomolecular Structure Studies. The course will help students grasp the interconnectedness of sciences and mathematics. Students will be exposed to mathematical techniques and theoretical concepts necessary to make progress in the study of modern day quantum technologies. Students will build upon this foundation in their further studies and research in an interdisciplinary cutting edge science or applied mathematics.

The course consists of two modules:

- **Quantum information:** As technology progresses toward higher scales of integration, and engineers engage in manipulation of matter at the nanoscale, there emerges a need to develop methods for the analysis of signals that have been forged in strongly quantum environments. Therefore, it is becoming necessary to include the notion of quantum information alongside that of the classical information in the foundational framework of signal processing. This module will be devoted to the discussion of the rudiments of the quantum information theory.
- **Nanosystem modelling:** Partial differential equations (PDE) are indispensable in the modeling of various physical systems. We often wish to use PDE models in order to simulate a given physical system on a computer, e.g. as an efficient alternative to an experiment. While PDE models are relevant to both the classical and the quantum realm, we often encounter a complexity barrier when it comes to simulating relatively large quantum systems. In many cases this barrier can be circumvented by substituting a somewhat simplified model with manageable complexity, which nevertheless captures the essential characteristic of the system. In this module we will discuss the nature of the complexity barrier and some examples of reduced-complexity models in the context of nanosystem modeling

List of topics by week:

Week 1: The rudiments of Hilbert space theory and the principles of Quantum Mechanics

Week 2: Nonlocality and quantum information

Week 3: Evolution of a quantum state

Week 4: The fundamentals of Hamiltonian systems

Week 5: Open quantum systems and the Markovian master equation in Lindblad form

Week 6: Review of the Schrödinger-equation based model of the hydrogen atom

Week 7: The formalism of the many-body quantum mechanics

Week 8: Introduction to the Hartree-Fock theory

Week 9: A model for the conduction of a molecule between two metal contacts

Week 10: Another look at the conduction of a molecule, the Nonequilibrium Green's Function Formalism

Week 11: A crash-course in functional analysis for quantum-mechanical calculations

Weeks 12 and 13: An outline of nonlocal dynamics and its applications

Texts and other sources: S. Stenholm, K.-A. Suominen, Quantum approach to informatics, (Wiley 2005), M. Paulsson, F. Zahid, S. Datta, Resistance of a molecule, in: W.A. Goddart III et al. (editors), Handbook of Nanoscience, Engineering, and Technology, (CRC Press 2003), R. Alicki and M. Fannes, Quantum Dynamical Systems, (Oxford University Press 2001), and many selections from scientific literature

Grading: Your grade will be computed as follows:

<u>20% Assignments</u> - A set of mathematical problems will be proposed weekly, or as appropriate. Each student will work on the problems independently.

<u>30% Projects and Presentations</u> - There will be a longer term assignment focused about computer system modelling. Students will work in groups, performing a study of suggested literature, and computer experimentation, including Matlab programming. Groups will make presentations on their assigned subjects.

<u>50% Final exam</u> -The final exam will consist of a set of problems, and responses to more open-ended questions focused about the applicability of mathematics to quantum technologies.

Anyone interested: Please contact Prof. Artur Sowa, 966-6114, sowa@math.usask.ca