UNIVERSITY OF KWAZULU-NATAL
INYUVESI YAKWAZULU-NATALI
School of Chemistry and Physics

MINI WORKSHOP ON QUANTUM DYNAMICS and NON-HERMITIAN HAMILTONIANS

University of KwaZulu-Natal, Pietermaritzburg Campus
Science Building, Physics Students' LAN

- December 3, 2014 - 11:00 a. m. (45 mins + questions)
  Dr Eva-Maria Graefe
  Quantum and classical dynamics generated by non-Hermitian Hamiltonians I

- December 4, 2014 - 11:00 a. m. (45 mins + questions)
  Dr Daniel A. Uken
  Simulating quantum dynamics in the partial Wigner representation

- December 5, 2014 - 11:00 a. m. (45 mins + questions)
  Dr Eva-Maria Graefe
  Quantum and classical dynamics generated by non-Hermitian Hamiltonians II

- December 8, 2014 - 11:00 a. m. (45 mins + questions)
  Prof Dorje Broody
  Quantum heat bath

INFORMATION

Dr Eva-Maria Graefe is a Junior Research Fellow in Mathematics at the Imperial College of London http://www.imperial.ac.uk/people/e.graefe

Prof Dorje Broody is Chair in Mathematics in the Department of Mathematical Sciences at Brunel University West London and visiting Professor at the Imperial College of London http://www.brunel.ac.uk/cedps/mathematics/people/professor-dorje-brody
http://www.imperial.ac.uk/people/d.brody

Dr Daniel A. Uken is a postdoctoral NRF researcher in the group of Dr A. Sergi
http://physicspmb.ukzn.ac.za/index.php/Dr_Alessandro_Sergi

COFFEE, SWEETS AND COOKIES WILL BE SERVED BEFORE EACH SEMINAR AT 10:30 A. M.

For additional information contact: Dr Alessandro Sergi (sergi@ukzn.ac.za)

Quantum and classical dynamics generated by non-Hermitian Hamiltonians I and II

Dr Eva-Maria Graefe
Department of Mathematics
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Quantum mechanics traditionally focuses on Hermitian operators for the description of closed systems. However, there is a rapidly growing interest arising from different areas in the use of non-Hermitian operators. The first is the field of open quantum systems where the overall probability decrease in time, which can be described via complex energies. Applications include, for example, decay, transport, and scattering phenomena. The second motivation arises from the observation that there is a class of non-Hermitian operators (often called PT-symmetric) yielding purely real eigenvalues that have been proposed as candidates for generalised quantum theories for closed systems. The main focus in the field lies on spectral properties of these systems and only recently there is considerable interest in their dynamical properties as well. Interestingly, the classical analogues of non-Hermitian quantum theories have hitherto remained almost unexplored.
In these talks I will give a brief overview of non-Hermitian quantum theories, and present some results on quantum evolution of Gaussian wave packets generated by a non-Hermitian Hamiltonian in the semiclassical limit of small h-bar. This yields the non-Hermitian analog of the Ehrenfest theorem for the dynamics of observable expectation values. An illustrative example of a non-Hermitian harmonic oscillator will be discussed in detail.

Simulating Quantum Dynamics in the partial Wigner Representation

Dr Daniel A. Uken
School of Chemistry and Physics
University of KwaZulu-Natal

Due to the enormous computational resource requirements for simulating interacting many-body quantum systems accurately, it is often impossible to perform numerical calculations on anything but systems with a small number of degrees of freedom. However, there are many instances when one is led to consider a system comprising a few quantum degrees of freedom, with a discrete representation, coupled to an environment of harmonics modes, eventually perturbed by a finite number of higher order anharmonic terms. In such cases, it is highly convenient to adopt a partial Wigner representation of the problem. According to this, the discrete quantum degrees of freedom retain their standard operatorial representation while the environment is represented in a classical-like phase space. Such a representation greatly reduces the computational complexity of the problem. Moreover, when certain approximations can be taken, the von Neumann equation, obeyed by the density matrix, becomes the quantum-classical Liouville equation (QCLE), describing a hybrid quantum-classical dynamics where nonadiabatic effects can be rigorously addressed.
In this talk, trajectory-based techniques will be discussed in order to simulate both quantum-classical nonadiabatic dynamics in arbitrary environments and fully quantum adiabatic dynamics in harmonics baths. It will also be discussed how numerical grids can be used to simulate the coherent quantum dynamics of discrete degrees of freedom coupled to continuous variables under the action of a polynomial potential.

Quantum heat bath

Prof Dorje Brody
Dept. of Mathematics
College of Engineering, Design and Physical Science
Brunel University West London

A model for a quantum heat bath is introduced. When the bath molecules have finitely many degrees of freedom, it is shown that the assumption that the molecules are weakly interacting is sufficient to enable one to derive the canonical distribution for the energy of a small system immersed in the bath. While the specific form of the bath temperature, for which we provide an explicit formula, depends on (i) spectral properties of the bath molecules, and (ii) the choice of probability measure on the state space of the bath, we are in all cases able to establish the existence of a strictly positive lower bound on the temperature of the bath. The results can be used to test the merits of different hypotheses for the equilibrium states of quantum systems. Two examples of physically plausible choices for the probability measure on the state space of a quantum heat bath are considered in detail, and the associated lower bounds on the temperature of the bath are worked out.