Koopman Methods in Classical and Classical-Quantum Mechanics

746. WE-Heraeus-Seminar

19 Apr - 23 Apr 2021
ONLINE

WILHELM UND ELSE
HERAEUS-STIFTUNG

Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see https://www.we-heraeus-stiftung.de

Aims and scope of the 746. WE-Heraeus-Seminar:

Following Koopman's Hilbert-space description of classical mechanics from the early thirties, Koopman operators are nowadays a crucial concept in ergodic theory. Within the areas of applied mathematics and quantum physics, Koopman operators are now being used successfully in fluid dynamics and Koopman-von Neumann wavefunctions have recently led to relevant developments, for example, in the studyof classical-quantum correspondence. Moreover, following an earlier proposal by George Sudarshan, Koopman wavefunctions have recently opened up promising avenues to model the interaction between classical and quantum systems beyond the use of standard semiclassical methods. However, despite these successes, Koopman methods are still little known outside the dynamical systems community and this seminar emerges as a unique opportunity for filling this gap between mathematical and physical sciences. Indeed, this meeting is meant to bring together communities from Mathematical Physics, Quantum Physics, and Chemical Physics working on different topics, including fluid dynamics, classical mechanics, and hybrid classical-quantum systems, with the intention of exploring the benefits of Koopman methods in different fields.

Introduction

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Program

Program

Monday, 19 April 2021		Time CET
08:55 – 09:00	Scientific organizers	**Welcome**
09:00 – 09:15	Stefan Jorda	**About the Wilhelm and Else Heraeus Foundation**
09:15 – 10:00	Wolfgang Schleich	**Schrödinger and Wigner wave functions revisited**
10:00 – 10:45	Lajos Diosi	**On Quantum-Classical Hybrid Canonical Dynamics**
10:45 – 11:15	*COFFEE BREAK*	
11:15 – 12:00	Aurelia Chenu	**On control of open quantum systems, with applications to thermalization**
12:00 – 12:30	Viktor Gerasimenko	**Evolution equations of quantum-classical systems**
12:30 – 14:00	*LUNCH BREAK*	
14:00 – 14:45	Raymond Kapral	**Quantum-classical wave functions and densities**
14:45 – 15:30	Stephen Fulling	**Quantum Field Theory in Curved Space-Time: Semiclassical in More Ways than One**
15:30 – 16:00	*COFFEE BREAK*	
16:00 – 16:30	Martin Bojowald	**Canonical description of quantum dynamics**
16:30 – 17:15	Igor Mezic	**A Transfer Operator Approach to Relativistic Quantum Wavefunction**
17:15 – 18:30	**Discussion session**	

Program

Tuesday, 20 April 2021		Time CET
15:15 – 16:00	Dorje Brody	**Phase-space approach to relativistic quantum theory**
16:00 – 16:45	Eberhard Gross	**Mixed-quantum-classical algorithms from the exact factorization**
16:45 – 17:15	*COFFEE BREAK*	
17:15 – 18:00	Cesare Tronci and Denys Bondar	**Koopman wavefunctions and hybrid quantum-classical models**
18:00 – 18:30	Hans-Thomas Elze	**Are they really 'out there'? On the ontology of quantum-classical hybrids**
18:30 – 20:00	*LUNCH BREAK*	
20:00 – 20:45	François Gay-Balmaz	**Symplectic geometry of hybrid quantum-classical dynamics**
20:45 – 21:15	Ilon Joseph	**Quantum Acceleration of the Koopman-von Neumann Approach to Nonlinear Classical Dynamics**
21:15 – 21:45	Ilya Dodin	**Operator methods for reduced modeling of waves in plasmas**
21:45 – 00:30	**Poster Session**	

Program

Wednesday, 21 April 2021		Time CET
09:15 – 10:00	Giovanni Manfredi	**Phase-space and hydrodynamic methods for polarized quantum plasmas**
10:00 – 10:45	Caroline Lasser	**Separation of scales and quantum-classical approximation**
10:45 – 11:15	*COFFEE BREAK*	
11:15 – 12:00	Irene Burghardt	**Towards a multi-configurational formulation of quantum-classical molecular dynamics**
12:00 – 12:30	Jean-Claude Zambrini	**Space-time stochastic control and Schrödinger's problem**
12:30 – 14:00	*LUNCH BREAK*	
14:00 – 14:45	Anthony Bloch	**Control and Geometry of Quantum Systems with Dissipation**
14:45 – 15:30	Paul Brumer	**A Koopman Type Approach in Quantum-Classical Correspondence: e.g., Chaotic Dynamics, The Born Rule and No-Cloning**
15:30 – 16:00	*COFFEE BREAK*	
16:00 – 16:30	Gerard McCaul	**Classical Influence Functionals**
16:30 – 17:00	Joanna Slawinska	**A Quantum Mechanical Approach for Data Assimilation of Dynamical Systems**
17:00 – 17:30	Andre Gontijo Campos	**The Dirac equation and its classical limit**
17:30 – 18:30	**Discussion session**	

Program

Thursday, 22 April 2021		Time CET
15:15 – 16:00	Maurice de Gosson	**On chalkboard motion**
16:00 – 16:45	Guiseppe Marmo	**Quantum Tomography and Schwinger's Approach to Quantum Mechanics**
16:45 – 17:15	*COFFEE BREAK*	
17:15 – 18:00	Ulf Klein	**Quantum theory as a randomized projection from phase space to configuration space**
18:00 – 18:30	Federica Agostini	**Simulating ultrafast non-radiative phenomena with the exact factorization**
18:30 – 20:00	*LUNCH BREAK*	
20:00 – 20:45	Nelida Črnjarić-Žic	**The Application of Koopman Operator-based Algorithms to Nonautonomous and Stochastic Systems**
20:45 – 21:30	Dimitris Giannakis	**Quantum Mechanical Embeddings of Classical Dynamical Systems**
21:30 – 22:00	*COFFEE BREAK*	
22:00 – 22:30	Francesco Di Maiolo	**Theoretical Approaches to Quantum Molecular Dynamics in Out of Equilibrium Environments**
22:30 – 23:15	Artur Izmaylov	**Quantum Nonadiabatic Dynamics in the Moving Crude Adiabatic Representation**
23:15 – 23:45	*BREAK*	
23:45 – 00:30	**Discussion session**	

Program

Friday, 23 April 2021		Time CET
09:15 – 10:00	Daniel Terno	**Quantum-classical hybrid dynamics**
10:00 – 10:45	Stefan Klus	**Kernel-based approximation of the Koopman generator and Schrödinger operator**
10:45 – 11:15	*COFFEE BREAK*	
11:15 – 11:45	Jonathan Oppenheim	**Classical-quantum General Relativity**
11:45 – 12:15	Benito A. Juárez-Aubry	**Semiclassical gravity in static spacetimes as a constrained initial value problem**
12:15 – 12:45	Dmitry Zhdanov	**Joint quantum-classical Hamilton variation principle in the phase space**
12:45 – 14:00	*LUNCH BREAK*	
14:00 – 14:45	Marcel Reginatto	**Classical-quantum interactions: observables, symmetries and uncertainties**
14:45 – 15:30	Ignacio Franco	**Quantum Coherence in Chemistry: Tackling the Decoherence Challenge**
15:30 – 16:00	Scientific organizers	**Closing remarks**

End of seminar

Posters

Posters

1	Bedros Afeyan	**Koopman Operators, Nonlinear Coherent Structures, Learning and Feedback Control in High Energy Density Plasmas**
2	Mustafa Amin	**Canonical Quantum-Classical Dynamics: Lessons from Phase Space**
3	Jacob Barandes	**The Koopman-von Neumann Formulation of Classical Physics and the Platonic Interpretation of Quantum Theory**
4	Basile Curchod	**Ab Initio Multiple Spawning with Informed Stochastic Selection**
5	David Freeman	**Quantum Mechanics for Stochastic Closures of Dynamical Systems**
6	Igor Gapyak	**Kinetic equations of the open quantum-classical systems**
7	Marek Gluza	**Recovering quantum correlations in optical lattices from interaction quenches**
8	Adrian Juan Delgado	**Quantum thermodynamics of an open quantum system periodically driven**
9	Shashaank Khanna	**Quantum Entanglement Percolation in a Monolayer Honeycomb Lattice**
10	Tonatiuh Miramontes	**Semiclassical theories as initial value problems**
11	Peter Morgan	**The collapse of a quantum state as a signal analytic sleight of hand**
12	Feliks Nüske + Boumediene Hamzi	**Generator EDMD: Data-Driven Approximation of the Koopman Generator**

Posters

13	Martin Plávala	**Operational Theories in Phase Space: Toy Model for the Harmonic Oscillator**
~~**14**~~	*Cancelled at short notice*	~~**Koopman methods for reduced modeling of waves in plasmas**~~
15	Jonathan Rawlinson	**The bohmion method in nonadiabatic quantum hydrodynamics**
16	Adam Sawicki	**tba**
17	Abhijit Sen	**Free fall in KvN mechanics and Einstein's Equivalence principle**
18	Mauro Spera	**Geometric aspects of generalized Schroedinger equations**
19	Bartłomiej Spisak	**Parameterization of the Wigner distribution function and its consequences for the description of a quantum dynamical system in the phase space**

Abstracts of Lectures

(in alphabetical order)

Simulating ultrafast non-radiative phenomena with the exact factorization

F. Agostini[1]

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In this talk I will present various applications of the exact factorization [1] to describe ultrafast non-radiative phenomena, such as internal conversion [2, 3] and intersystem crossing [4]. A short introduction to the formalism will be given [5], that accounts for kinetic non-adiabatic coupling between electronic states of the same spin multiplicity and for spin-orbit coupling between states of different spin multiplicity. The generalized coupled-trajectory mixed quantum-classical (G-CT-MQC) algorithm [4] will be applied to the study of the photo-isomerization of a retinal chromophore [6] and to the simulation of singlet-to-triplet transitions [4]. Comparisons with vibronic-wavepacket dynamics and various trajectory-based schemes will be employed to evaluate the performance of G-CT-MQC. based on trajectories will be discussed as well.

References

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Control and Geometry of Quantum Systems with Dissipation

Anthony Michael Bloch, University of Michigan, abloch@umich.edu

In this talk we discuss aspects of the mathematics, control and geometry of quantum control systems interacting with their environment. In particular we discuss the control of a finite-dimensional dissipative Lindblad system by considering the geometry of its orbit and interorbit dynamics. This entails considering the geometry of the system, the structure of the Lindblad operator, and the convexity associated with the density equation. Applications are given to constructing pure states. We discuss controllability and also discuss optimality and optimal control in this setting. This talk includes work with Rooney, Rangan, Clark and Colombo.

Canonical description of quantum dynamics

M. Bojowald

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The relationship between classical and quantum physics can be analyzed by presenting the quantum state space as a phase space of classical type, with a Poisson bracket derived from the commutator. Recent progress in the derivation of canonical quantum degrees of freedom in a semiclassical setting offers a geometrical perspective on hybrid formulations of classical and quantum dynamics.

Koopman wavefunctions and hybrid quantum-classical models

Denys I. Bondar[1], Cesare Tronci[12]

[1]Tulane University, New Orleans, LA, USA
[2]University of Surrey, Guildford, UK

This talk aims at unfolding the role of Koopman wavefunctions in the formulation of quantum, classical, and quantum-classical models. First, we will introduce Operational Dynamical Modeling (ODM) [1], a methodology for deducing equations of motions from the dynamics of Ehrenfest expectation values. In this context, ODM can be used to derive evolution equations for both quantum and classical wavefunctions. We will uncover a family of phase space representations of quantum mechanics whose classical limit recovers different variants of the Koopman-von Neumann equation. Among these variants, the Koopman-van Hove equation allows to derive the quantum-classical hybrid model in [2] as a partial classical limit. Then, the talk proceeds by discussing quantum-classical hybrid dynamics in terms of the Dirac-Frenkel variational principle. This type of Hamiltonian hybrid dynamics is shown to overcome the issues previously emerging in Sudarshan's early work from '76. In particular, we will show how a new type of quantum-classical wave equation is capable of reproducing essential features, thereby leading to a new quantum-classical density operator and extending Bohmian trajectories to the hybrid setting [3]. Finally, we shall present exact solutions for the quantum-classical spin-boson model.

[1] Bondar DI, Cabrera R, Lompay RR, Ivanov MYu, Rabitz HA. 2012 Operational Dynamic Modeling Transcending Quantum and Classical Mechanics. Phys. Rev. Lett. 109: 190403.

[2] Bondar DI, Gay-Balmaz F, Tronci C. 2019 Koopman wavefunctions and classical–quantum correlation dynamics. Proc. R. Soc. A 475: 20180879.

[3] Gay-Balmaz F, Tronci C. 2019 Madelung transform and probability densities in hybrid quantum–classical dynamics. Nonlinearity 33: 5383–5424

Phase-space approach to relativistic quantum theory

Dorje Brody

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The phase space of a relativistic system can be identified with the future tube of complexified Minkowski space. As well as a complex structure and a symplectic structure, the future tube, seen as an eight-dimensional real manifold, is endowed with a natural positive-definite Riemannian metric that accommodates the underlying geometry of the indefinite Minkowski space metric, together with its symmetry group. A unitary representation of the 15-parameter group of conformal transformations can be constructed that acts upon the Hilbert space of square-integrable holomorphic functions on the future tube. These structures are rich enough to allow one to put forward a quantum theory of phase-space events. In particular, a theory of quantum measurement can be formulated in a relativistic setting, based on the use of positive operator valued measures, for the detection of phase-space events, hence allowing one to assign probabilities to the outcomes of joint space-time and four-momentum measurements in a manifestly covariant framework. This leads to a localisation theorem for phase-space events in relativistic quantum theory, determined by the associated Compton wavelength. (Based on joint work with L.P. Hughston.)

A Koopman Type Approach in Quantum-Classical Correspondence: e.g., Chaotic Dynamics, The Born Rule and No-Cloning

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The Hilbert Space structure of quantum and classical mechanics allows a framework In which the relationship between them is most evident. By defining eigenstates and eigenvalues of the Liouville Operator in both mechanics one gains a satisfying approach to quantum-classical correspondence and to quantum dynamics in the classical limit. This program, introduced decades ago [1,2], will be described, and the successful application to chaotic dynamics, to deriving the Born Rule[3], and to demonstrating classical no-cloning will be discussed.

[1] J. Wilkie and P. Brumer, Phys. Rev. A55, 27 (1997).
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Towards a multi-configurational formulation of quantum-classical molecular dynamics

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The time-dependent variational principle [1] provides a highly efficient approach for defining an optimal time evolution of approximate wavefunctions. For complex analytic parametrizations, the variational equations of motion exhibit a symplectic structure, corresponding to a generalized Hamiltonian flow. Here, we focus on multiconfigurational, correlated wavefunctions of hybrid type, which combine single-particle functions (SPFs) of the Multi-Configuration Time-Dependent Hartree (MCTDH) method [2] with Gaussian wavepackets (GWPs) in selected subspaces, yielding the so-called G-MCTDH approach [3]. Hierarchical tensorized wavefunctions of this type have recently been employed for quantum systems comprising hundreds of degrees of freedom [4,5]. Against this background, the present lecture focuses on an extension to a quantum-classical limit representation where hybrid configurations combine quantum SPFs with semiclassically scaled GWPs that are characterized by a classical parameter dynamics. As a result, a multiconfigurational Ehrenfest type dynamics is obtained that is able to capture quantum-classical correlations [6,7]. The mathematical underpinnings of this approach, based upon a dynamical separation of scales, are addressed in Ref. [8] (see the presentation by C. Lasser).

References

[1] C. Lubich, *From quantum to classical molecular dynamics: reduced models and numerical analysis*. Zurich Lectures in Advanced Mathematics, European Mathematical Society (EMS), Zurich (2008).

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On control of open quantum systems, with applications to thermalization

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Techniques known as shortcuts to adiabaticity (STA) tailor excitations in nonadiabatic processes to prepare a given state in a finite time, without the requirement of slow driving. Their developments in isolated quantum systems have found broad applications. I will first briefly present an experimental demonstration of STA in the control of compression and expansion of a Fermi gas, which results into friction-free strokes that can be implemented to increase the power output of a heat machine while maintaining a high efficiency [1].

STA are however severely limited to isolated systems. Extending such control techniques to open systems is highly desirable in view of applications to cooling, and more generally, in finite-time thermodynamics. I will present a universal scheme for the control of open systems, defining a trajectory-based equation of motion that allows for the control of any arbitrary dynamics [2]. Its application will be detailed for controlling the temperature and squeezing of a single-particle thermal state in a harmonic trap [3,4].

References

[1] F. S. Deng, A. Chenu, P. Diao, F. Lu, S. Yu, I. Coulamy, A. del Campo, H. Wu. Superadiabatic quantum friction suppression in finite-time thermodynamics, Sci. Adv. 4:5909 (2018).

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The Application of Koopman Operator-based Algorithms to Nonautonomous and Stochastic Systems

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In practice, a complex dynamical system often include some time-dependent or random forcing so that it can not be modeled as autonomous system. Therefore, the extension of the Koopman operator theory to nonautonomous and stochastic systems is of great importance. It brings a new viewpoint to the existing theory of nonautonomous and random dynamical systems, particularly, with application of Koopman operator-based data-driven algorithms.

We consider the nonautonomous Koopman operator family based on the skew-product definition of the nonautonomous dynamical system. Similarly, we introduce the stochastic Koopman operator family associated with the given random dynamical system. In both cases, we state basic properties of the operator and discuss the application of Koopman-operator based algorithms on the considered systems. The performance of the algorithms is illustrated in the context of discovering the spectral objects of the system, as well as, on the reconstruction and prediction of the system behaviour.

On chalkboard motion

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In the usual approaches to mechanics (classical or quantum) the primary object of interest is the Hamiltonian, from which one tries to deduce the solutions of the equations of motion (Hamilton or Schrödinger). In the present work we reverse this paradigm and view the motions themselves as being the primary objects. This is made possible by studying arbitrary phase space motions, not of points, but of (small) ellipsoids with the requirement that the symplectic capacity of these ellipsoids is preserved. This allows us to guide and control these motions as we like, and the project them on subpaces corresponding to subsstems.

Theoretical Approaches to Quantum Molecular Dynamics in Out of Equilibrium Environments

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The description of quantum molecular dynamics as influenced by a polarizable and dynamically evolving environment is critical to understand the nature of various physical processes, from solvation phenomena to photobiological processes in protein environments, and transport of charge carriers and excitons in nanostructures. Indeed, experimental molecular systems, S, are not closed systems due to the interaction with the surrounding environment, generically denoted the bath, B. Large effects on S dynamics can be expected depending on the nature of the environment as well as on the SB interaction strength. The typically used dielectric continuum picture for B is likely to fail when dealing with nonequilibrium solvation effects. On the other hand, fully atomistic first principles quantum calculations are hardly feasible due to the large number of environmental degrees of freedom.

Against this background, we present the effect of a dynamic environment on a time-evolving molecular system, using the Quantum-Classical Reduced Hydrodynamic (QCRH) approach [1]. In particular, the hydrodynamic formalism naturally describes density, current and heat transport phenomena. Accordingly, the QCRH theory can describe molecular relaxation in condensed dynamic phases, complementing typically used dielectric continuum models for the environment. At present, we have extended the QCRH approach in order to deal with orientational solvation processes in charge-transfer phenomena, using a Maxwellian closure for the hydrodynamic hierarchy.

References

[1] I. Burghardt, B. Bagchi, Chem. Phys. **329**, 343-356 (2006)

On Quantum-Classical Hybrid Canonical Dynamics

Lajos Diósi

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Over the decades, desire of a hybrid of quantum and classical dynamics came from many fields spanning from quantum chemistry to cosmology, from foundations to open system theories, also from such special fields like quantum control. Koopman's quantum formalism of classical dynamics or Wigner's classical phase-space formalism of quantum dynamics are two opposite options to create the hybrid formalism. My topics is about a third option, kind of "in the middle". To construct natural coupling between a classical system's canonical formalism and a quantum system's operator formalism, Aleksandrov constructed a hybrid of the Poisson and Dirac brackets, Gerasimenko proposed an equivalent structure. This is remarkable and useful phenomenology but incorrect mathematically. Additional terms to the hybrid bracket can cure the defect, while the reversibility of the resulting hybrid dynamics becomes lost.

Operator methods for reduced modeling of waves in plasmas

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Simulations of linear and weakly nonlinear radiofrequency (RF) waves in plasmas, particularly those used in fusion applications, typically rely on analytic models of the plasma linear conductivity. The conductivity operator is readily calculated for homogeneous media, but full-wave modeling of waves in realistic inhomogeneous plasmas (i.e., direct solution of Maxwell's equations with a prescribed conductivity) is more challenging. The corresponding operator is usually extrapolated from homogeneous-plasma models *ad hoc*. This makes full-wave modeling imprecise and often brings in significant spurious effects, because singling out weak dissipation from strong dispersive effects in inhomogeneous plasma is typically a subtle matter.

The difficulty is due to the fact that the plasma response is usually calculated along characteristics of the linearized kinetic (Vlasov) equation [1], which are nonlinear and thus intractable without significant simplifications unless the underlying medium is homogeneous. However, the solution can also be expressed through the Perron-Frobenius operator, which is linear. Then, the conductivity becomes a superposition of linear operators and can be approximated using methods of operator analysis and the Weyl calculus. This approach also yields a more explicit and rigorous formulation of the classic oscillation-center quasilinear theory [2-4] (of plasma interaction with wave turbulence) as a manifestly local conservative theory. Resonant and nonresonant particles are described on the same footing, and both quasilinear diffusion and ponderomotive effects (time-averaged effects caused by rapidly oscillating fields) are captured.

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Are they really ‘out there’?
On the ontology of quantum-classical hybrids

Hans-Thomas Elze

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The *Cellular Automaton Interpretation* of Quantum Mechanics will be briefly recalled, which has been proposed by Gerard ‘t Hooft recently, see, e.g., ref. [1]. An example of a “classical” Ising spin chain will be shown that follows deterministic dynamical rules, yet is ‘arbitrarily close’ to a genuine quantum many-body system, namely a relativistic field theory [2]. Considering interaction of two such systems, we discuss the possibility of a “quantum-classical hybrid” [3,4,5,6], a classical object interacting with a quantum mechanical one, and argue that this is fundamentally not tenable.

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Quantum Coherence in Chemistry: Tackling the Decoherence Challenge

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A subject of considerable current interest in Chemistry is the possibility of using non-trivial quantum mechanical effects, such as coherence and interference, to enhance molecular function. This possibility is hindered by decoherence processes that prevent matter from fully exhibiting its quantum features. In this talk, I will summarize our progress [1-7] understanding decoherence in molecular processes, and in particular electronic decoherence. I will focus the discussion on topics at the boundary of quantum and classical mechanics, including a theory of dissipation pathways in open quantum systems [1], a discussion of the utility of classical noise models in capturing the decoherence [2], and a theory of decoherence timescales that offer light into the utility of mixed quantum classical approaches to capture the decoherence [3, 6].

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Quantum Field Theory in Curved Space-Time: Semiclassical in More Ways than One

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The term "semiclassical" has two completely different meanings. Both are vitally important in the quantum theory of fields in curved space-times. The first refers to a dynamical theory in which a quantum system is coupled to a classical system, as when one tries to calculate the effect of a quantized field on the background gravitational field. The second refers to approximations of the WKB type to solutions of differential equations, where each derivative in the equation is formally associated with a small parameter, often identified with Planck's constant. The basic idea is that the scale of variation of the gravitational background is much larger than the wavelength of the solution, so that, locally, the background can be treated to lowest order as flat. The first meaning fits well with the Koopman formalism, which disguises a classical dynamical system as quantum theory. The second one is associated with the Madelung formalism, which disguises a quantum-mechanical system as classical hydrodynamics.

Symplectic geometry of hybrid quantum-classical Dynamics

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We present the geometric properties underlying a Hamiltonian model recently proposed by the authors for hybrid quantum-classical systems. This model is based on the Koopman-van Hove (KvH) formulation of classical mechanics. It is obtained by writing the KvH wave equation for two classical particles and applying canonical quantization to one of them. In particular, we elucidate several concepts from symplectic geometry underlying the quantum-classical Madelung transform and show that the joint quantum-classical distribution arises as a momentum map for a unitary action naturally induced from the van Hove representation on the classical-quantum Hilbert space. By developing a Lie group equivariant setting and using the tools of geometric quantization, we extend this Hamiltonian classical-quantum model to systems governed by Lie-Poisson brackets, with a focus on the interaction of classical and quantum spins.

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Evolution equations of quantum-classical systems

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The talk will deal with a review of some approaches to the description of the evolution of many-particle quantum-classical systems [1]-[3]. In particular, it will be considered the links between fundamental and approximate evolutionary equations of interacting particle systems composing of two subsystems, one of which behaves classically while the other requires a quantum description.

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Quantum Mechanical Embeddings of Classical Dynamical Systems

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We present a framework for simulating a measure-preserving, ergodic dynamical system by a finite-dimensional quantum system amenable to implementation on a quantum computer. The framework is based on a quantum feature map for representing classical states by density operators (quantum states) on a reproducing kernel Hilbert space, *H*, of functions on classical state space. Simultaneously, a mapping is employed from classical observables into self-adjoint operators on *H* such that quantum mechanical expectation values are consistent with pointwise function evaluation. Meanwhile, quantum states and observables on *H* evolve under the action of a unitary group of Koopman operators in a consistent manner with classical dynamical evolution. To achieve quantum parallelism, the state of the quantum system is projected onto a finite-rank density operator on a 2^N-dimensional tensor product Hilbert space associated with *N* qubits. In this talk, we describe this "quantum compiler" framework, and illustrate it with applications to low-dimensional dynamical systems. In addition, we discuss a related quantum mechanical approach for data assimilation of partially observed systems, with applications to climate dynamics.

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The Dirac equation and its classical limit

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The formalism of Operational Dynamical Modeling [Bondar et al., Phys. Rev. Lett. 109, 190403 (2012)] is employed to analyze dynamics of spin half relativistic particles. We arrive at the Dirac equation from specially constructed relativistic Ehrenfest theorems by assuming that the coordinates and momenta do not commute. Forbid- ding creation of antiparticles and requiring the commutativity of the coordinates and momenta lead to classical Spohn's equation [Spohn, Ann. Phys. 282, 420 (2000)]. Moreover, Spohn's equation turns out to be the classical Koopman-von Neumann theory underlying the Dirac equation.

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Mixed-quantum-classical algorithms from the exact factorization

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Most of modern simulation techniques are based on the assumption that the motion of nuclei is well described by classical trajectories while the electrons are treated quantum mechanically. The forces on the nuclei usually come from a mean-field-like approximation or from a single Born-Oppenheimer surface. However, some of the most fascinating phenomena in physics and chemistry, such as the process of vision, the dynamics of excitons in photovoltaic systems or the Nobel-prize-winning femto-chemistry experiments of Ahmed Zewail, occur in the so-called non-adiabatic regime where the coupled motion of electrons and nuclei beyond the dynamics on a single Born-Oppenheimer surface is essentional. To tackle this problem, we start from the exact factorization [1] of the full electron-nuclear wave function into a purely nuclear part and a many-electron wave function which parametrically depends on the nuclear configuration and which has the meaning of a conditional probability amplitude. The equations of motion of these two wave functions provide an ideal starting point to develop efficient algorithms for the study non-adiabatic phenomena. The successful prediction of ultrafast laser-induced isomerization processes [2], the description of decoherence within mixed quantum-classical algorithms [3], calculations of the molecular Berry phase without invoking the Born-Oppenheimer approximation [4], evaluation of electronic currents [5] associated with nuclear motion and accurate predictions of vibrational spectroscopies [6], especially dichroism, will demonstrate the power of this novel approach.

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Quantum Nonadiabatic Dynamics in the Moving Crude Adiabatic Representation

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On-the-fly quantum nonadiabatic dynamics for large systems greatly benefits from the adiabatic representation readily available from electronic structure programs. However, conical intersections frequently occurring in this representation introduce nontrivial geometric or Berry phases, which require a special treatment for adequate modeling of the nuclear dynamics. I analyze two approaches for nonadiabatic dynamics using the time-dependent variational principle and the adiabatic representation. The first approach, the global adiabatic representation, employs adiabatic electronic functions with global parametric dependence on the nuclear coordinates. The second approach, the moving crude adiabatic representation, uses adiabatic electronic functions obtained only at the centers of moving localized nuclear basis functions (e.g., frozen-width Gaussians). Unless a gauge transformation is used to enforce single-valued boundary conditions, the global adiabatic representation fails to capture the geometric phase. In contrast, the moving crude adiabatic representation accounts for the geometric phase naturally because of the absence of the global nuclear coordinate dependence in the electronic functions. In addition, the moving crude adiabatic representation does not suffer from appearance of the second order nonadiabatic couplings and allows us to avoid approximate Taylor series expansions of potential energy surfaces for wave-packet dynamics.

Quantum Acceleration of the Koopman-von Neumann Approach to Nonlinear Classical Dynamics

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In principle, quantum algorithms can accelerate the solution of a number of important numerical algorithms. However, quantum computation is limited to the application of linear unitary transformations, and, hence, it is not immediately clear how to accelerate the solution of nonlinear non-Hamiltonian dynamical systems. The Koopman-von Neumann (KvN) formulation of classical mechanics recasts the conservation of the probability distribution function on phase space, expressed by the Liouville equation, as an equivalent Schrodinger equation on Hilbert space with a Hermitian Hamiltonian operator and a unitary propagator for the KvN wavefunction. Thus, a quantum computer with finite resources can be used to simulate a finite-dimensional approximation of the unitary KvN evolution operator. Using this approach to quantum simulation is exponentially more efficient than a deterministic Eulerian discretization of the Liouville equation if the KvN Hamiltonian is sparse [1]. Using amplitude estimation for the calculation of observables and quantum walk techniques for state preparation can lead to up to a quadratic improvement over probabilistic Monte Carlo algorithms [1].

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Semiclassical gravity in static spacetimes as a constrained initial value problem

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Semiclassical gravity is the theory in which gravity is treated as a classical field -- the spacetime metric -- and matter is treated in the framework of quantum field theory. The gravitational field and matter interact through the semiclassical Einstein equations: matter sources the dynamics of the spacetime metric via the expectation value of the stress-energy tensor of the quantum fields, while the quantum fields propagate in curved spacetime. It is currently unknown whether semiclassical gravity has a well-posed initial value formulation even for free fields. In this contribution, I will discuss the situation in static spacetimes, which greatly reduce the difficulty of the problem, and where one can show well-posedness. I will also discuss how to generalise these results to non-static spacetimes under some special circumstances. Based on arXiv:2011.05947 and some unpublished work in progress.

Quantum-classical wave functions and densities.

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When constructing models for physical systems, it is often useful consider quantum systems comprising a subsystem coupled to a bath. It may be computationally convenient or physically reasonable to construct quantum-classical theories where the bath is treated classically. It is well known that such theoretical descriptions suffer from difficulties due to a lack of a Lie algebraic structure. Nevertheless, necessity has prompted many attempts to construct such theories.

One way to construct a quantum-classical dynamical description is to start with a full quantum description and take a suitable classical limit on the bath.[1-3] The starting point is the quantum Liouville equation for its evolution. Following a partial classical limit on the quantum Liouville operator one obtains the quantum-classical Liouville equation. The resulting quantum-classical density matrix, or the average values of observables derived from it, can no longer be written in terms of wave functions.

Another route to quantum-classical dynamics instead starts from the classical equations of motion for the density function, constructs a classical Koopman wave function [4], and then carries out a partial quantization procedure to obtain a quantum-classical Schroedinger equation [5-6]. In this case the density operator and the average values of observables are expressed in terms of the quantum-classical wave function and are not closed in the density.

These two approaches, quantum dynamics to quantum-classical dynamics or classical mechanics to quantum-classical dynamics, do not coincide. I will discuss wave functions and densities for quantum-classical systems, and describe differences that arise when the quantum-classical dynamics is constructed from these different perspectives, along with comparisons will full quantum dynamics.

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Quantum theory as a randomized projection from phase space to configuration space

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We show that quantum theory (QT) can be derived from the probabilistic description of classical particles with the help of a few reasonable assumptions. Our starting point is an ensemble of particle trajectories that is defined by a Hamiltonian H(q,p). We introduce two associated fields in phase space, the probability density $\rho_H(q,p,t)$, and the classical action $S_H(q,p,t)$. Our first fundamental assumption is that the independent variables of all physical fields must be the space-time variables q,t. This implies a projection onto configuration space: the independent variables p have to be replaced by fields $M_H(q, t)$. It turns out that the fields M_H are unsuitable as dynamical variables and must be replaced by potentials. The result is a nonlinear theory of quasi-classical type. Although it still describes the movement of particles, it is unstable due to the nonlinearity. This almost inevitably leads to our second fundamental assumption, which says that the emerging theory in configuration space must be linear. The linearization can also be viewed as a randomization; as an implementation of a kind of local statistics, using the concept of Fisher information. Performing this second step, the possibility of describing trajectories is lost and QT for the observable H is obtained. The order of these two steps does not matter, in principle, but allows different insights in each case. In a similar way, QT may be derived for any other observable A. The QT's of two observables A and B are compatible if the Poisson brackets of A and B vanish. In this way one can derive the occurrence of operators as observables, their non / commutativity, the form of the evolution equations, the existence of eigenvalue equations, and Born's rule. If one carries out the projection onto the configuration space as first step, this has the advantage that one has precise control over the structure of $M_H(q,t)$. If one assumes an irrotational momentum field (with a single potential), one obtains Schrödinger's equation. However, for the important case of a single free particle there must be three functionally independent potentials, corresponding to the three-dimensionality of space. This leads to the conclusion, which is in agreement with empirical evidence, that all structureless massive particles in nature must have spin 1/2.

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Kernel-based approximation of the Koopman generator and Schrödinger operator

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Many dimensionality and model reduction techniques rely on estimating dominant eigenfunctions of associated dynamical operators from data. Important examples include the Koopman operator and its generator, but also the Schrödinger operator. We will present a kernel-based method for the approximation of transfer operators and differential operators in reproducing kernel Hilbert spaces and show how eigenfunctions can be estimated by solving auxiliary matrix eigenvalue problems. We will illustrate the results with the aid of guiding examples and highlight potential applications in molecular dynamics, fluid dynamics, and quantum mechanics.

Separation of scales and quantum-classical approximation

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We consider complex quantum-dynamical systems that can be partitioned into weakly interacting subsystems, similar to system-bath type situations. Using a factorised wave function ansatz, we mathematically characterise dynamical scale separation. In particular, we consider the situation where one of the sets of variables is semiclassically scaled and derive a quantum-classical formulation. We analyse the error for the wave function and for the action of observables. This is recent joint work with I. Burghardt, R. Carles, C. Fermanian Kammerer, and B. Lasorne (*Separation of scales: a quantum-classical approach for complex systems and a system-bath ansatz*, arXiv:2012.08373).

Phase-space and hydrodynamic methods for polarized quantum plasmas

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Dense quantum plasmas ($n > 10^{28}$ m^{-3}) are routinely encountered in metallic nanostructures, compact astrophysical objects, and high-intensity laser-plasma experiments. To investigate the quantum plasma dynamics, recent works [1] made use of Wigner's phase-space representation of quantum mechanics. These works disregarded the effects due to the electron spin (Zeeman effect and spin-orbit coupling), which play an important role in experiments on magnetic nano-objects.
Simulations of spin plasmas in the phase space are computationally challenging, as the corresponding Wigner distribution is not a scalar quantity, but rather a 2X2 matrix [2-4]. It is also possible to define an equivalent scalar probability distribution that evolves in an extended 8D phase space [5], where the spin is treated as a classical two-component vector on the unit sphere.
In our research group, we have derived a semiclassical Vlasov equation with spin effects by expanding the full quantum model to first order in the Planck constant. This "spin-Vlasov" equation may be coupled to the Maxwell equations to form a self-consistent mean-field model. By taking velocity moment of the spin-Vlasov equation, one can also further a set of quantum hydrodynamic equations with spin effects [3].
We have used the extended-phase-space formalism to construct a particle-in-cell (PIC) code that solves the coupled nonlinear spin-Vlasov-Maxwell equations [6].
As an example of application, we studied the impact of spin effects on the interaction of an intense laser source with a dense plasma, focusing in particular on stimulated Raman scattering (SRS). SRS is a parametric instability where the incident electromagnetic wave drives two waves inside the plasma: a scattered electromagnetic wave and a longitudinal electron plasma wave. We used the spin-Vlasov-Maxwell PIC code to study SRS for spin-polarized electrons, investigating how the SRS instability progressively destroys the spin coherence of the electron gas.

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Quantum Tomography and Schwinger's Approach to Quantum Mechanics

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The description of any physical system, be it classic or quantum, requires the identification of i) States; ii)Observables ; iii) Probability map, a pairing between states and observables with values in the space of probability measures on the real line ; iv) Evolution ; v) Composition rule ,to construct systems out of elementary ones.

Heisenberg , Born ,and Jordan started from observables as primary objects .They constructed Matrix Mechanics (later developed into the C*-algebraic approach).
Schrödinger ,Dirac ,and von Neumann started from vector states (the Hilbert-space approach) as primary objects.
Quantum Tomography deals with statistical-probabilistic aspects as primary objects.It may be considered as "Quantum Mechanics on Phase Space" ,and may be ascribed ,mainly ,to Wigner and Weyl. Tomography describes quantum states by means of fair probability distributions (marginal distributions) associated with quasi-distributions on phase-space introduced by Wigner .In this respect it allows to deal with "quantum" and "classical" systems by means of the same ingredients.
On the other hand ,Schwinger's approach (The Algebra of Atomic Measurements) has been formalized recently [1,...] by means of groupoids. This approach ,stemming from Stern-Gerlach experiment, was presented as "purely quantum".But as Einstein used to say : " I do not believe in micro and macro laws, but only in (structural) laws of general validity",we will argue that the groupoid approach allows to deal with quantum and classical systems in the same structural setting.

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Classical Influence Functionals

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The longstanding question of how stochastic behaviour arises from deterministic Hamiltonian dynamics is of great importance, and any truly holistic theory must be capable of describing this transition. For quantum mechanical systems, this process can be described by the *influence functional*. Using this tool, it is possible to derive exact stochastic evolution equations from a Hamiltonian system. Here we show that an equivalent classical influence functional exists for systems described by Koopman-von Neumann dynamics. Using the classical influence functional, we are able to show that the proper classical limit of stochastic quantum dynamics corresponds non-trivially to a generalised Langevin equation. This provides a further unifying link between open quantum systems and their classical equivalent, highlighting the utility of influence functionals and their potential as a tool in both fundamental and applied research.

A Transfer Operator Approach to Relativistic Quantum Wavefunction

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We introduce a transfer-operator based wavefunction formalism and obtain an evolution equation for the wavefunction of 0-spin and spin 1/2 particles. The equation features a non-hermitian term associated with the local divergence of trajectories that can be generated e.g. by gravitational effects. In the special relativity limit the scalar wavefunction of Dirac spinors satisfies the new equation. In the non-relativistic case we obtain the Schrodinger equation in the limit when trajectories have small deviations from inertial motions. However, when changes in trajectory curvature are not small, classical effects arise, and when divergence of trajectories is present, non-hermitian effects arise.

Classical-quantum General Relativity

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I will give an overview of a theory of classical general relativity coupled to quantum field theory. The dynamics is linear, completely positive and trace preserving and doesn't suffer from the pathologies of semi-classical gravity. It reduces to Einstein's equations in the appropriate limit. The theory can be regarded as an effective theory describing the backreaction of quantum fields on space-time, or as fundamental. There is a discrete and continuous version, each with a modified constraint algebra. We introduce general theorems which severely constrain any hybrid classical-quantum coupling, and which allow the quantum nature of gravity to be tested experimentally.

https://arXiv:1811.03116v1 [hep-th] 7 Nov 2018

https://arxiv.org/abs/2011.15112

https://arxiv.org/abs/2011.06009

Classical-quantum interactions: observables, symmetries and uncertainties

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Finding a physically consistent approach to modelling interactions between classical and quantum systems is a highly nontrivial task. While many proposals based on various mathematical formalisms have been made, most of these efforts run into difficulties of one sort or another. One of the first detailed descriptions was given by Sudarshan and his collaborators who, motivated by the measurement problem in quantum mechanics, proposed a Hilbert space formulation of classical-quantum interactions which made use of the Koopman-von Neumann description of classical systems. Other descriptions of classical-quantum interactions include the mean field approach, in which classical observables appear as parameters in a quantum Hamiltonian operator, the trajectory approach, which relies on modifying the de Broglie–Bohm formulation of quantum mechanics, and the configuration ensemble approach, which is based on a general formalism for describing physical systems in terms of ensembles evolving on a configuration space, with dynamics specified by an action principle. While each of these approaches have proven useful for given applications (e.g., to provide an approximate description of a system where it is desirable to model some components classically while the rest of the system is modelled quantum mechanically), the question of their validity in a more general sense still needs to be evaluated. I address this issue by considering and contrasting two particular hybrid theories, the Hilbert space formulation which goes back to Sudarshan and collaborators [1-4] and the configuration ensemble approach [5-6], and focus on their respective definitions of classical and quantum observables, how the representation of fundamental symmetries can be carried out for certain simple examples, and the question of the uncertainties associated with the combined classical-quantum interacting system. The aim is to clarify certain issues about the application of these hybrid models to problems in foundations of physics.

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Schrödinger and Wigner wave functions revisited

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When Erwin Schrödinger was challenged by Peter Debye in a colloquium in Zürich in 1925 to propose a wave equation for matter he understandably faced a tremendous challenge. Therefore, it is not surprising that he first proposed several equations before he settled for the one that we call today the time-dependent Schrödinger equation. Unfortunately, he did not provide much motivation for his choice.

In the present talk we provide a brief history of the birth of the Schrödinger equation and review our work [1] on this topic which centers around three characteristic features of quantum mechanics: (i) it displays a symmetric coupling between the amplitude and the phase of the quantum wave, (ii) it allows for more freedom in phase than the one given by the classical action, and (iii) it incorporates gauge invariance.

We also build the bridge to the Wigner formulation [2] of quantum mechanics and present vivid examples of the power of this approach. In this way we connect these topics to the theme of this Heraeus seminar.

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A Quantum Mechanical Approach for Data Assimilation on Dynamical Systems

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We present a framework for data assimilation (filtering) combining aspects of operator-theoretic ergodic theory and quantum mechanics. This framework adapts the Dirac-von Neumann formalism of quantum dynamics and measurement to perform data assimilation (filtering) of a partially observed, measure-preserving dynamical system, using the Koopman operator on the $L2$ space associated with the invariant measure as an analog of the Heisenberg evolution operator in quantum mechanics. In addition, the statistical state of the data assimilation system is represented by a trace-class operator analogous to the density operator in quantum mechanics, and the assimilated observables by self-adjoint multiplication operators. We present a data-driven formulation of the quantum mechanical data assimilation approach, utilizing kernel methods from machine learning and delay-coordinate maps of dynamical systems to represent the evolution and measurement operators via matrices in a data-driven basis. Applications to data assimilation of two-layer Lorenz and El Nino Southern Oscillation are discussed.

Quantum-classical hybrid dynamics

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We discuss consistency of quantum-classical hybrid dynamics using both the Hilbert space (Koopman) and the phase-space (Moyal) formalisms. Variously coupled harmonic oscillators provide a sufficiently rich structure to describe uses and limitations of these scheme. One of the arguments a theory of gravity should be quantal is based on the failure to describe the interaction of classical gravity and quantum matter. We use the linearized gravity coupled to scalar field to make this argument more precise.

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Space-time stochastic control and Schrödinger's problem

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Schrödinger's problem can be regarded as a probabilistic counterpart of the classical Least Action principle whose solution is a stochastic boundary value problem. Formulated in 1931 as an analogy with Quantum Mechanics, it has been elaborated in the mid-eighties and re-discovered recently in Mass Transportation Theory. It was defined originally on a fixed time interval.
We shall describe a space-time generalization of this variational problem and explain why it should be of interest far beyond its initial motivations.

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Joint quantum-classical Hamilton variation principle in the phase space

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At first glance, the Hamilton variation principle cannot be formulated for quantum particles since they lack well-defined trajectories. I will show how to overcome this seemingly formidable obstacle using Husimi representation of quantum mechanics based on our recent result [1].

The dynamics of a closed quantum system in Husimi representation can be treated as a flow of multidimensional probability fluid in the phase space [2]. By introducing the classical counterpart of Husimi representation in close analogy to Koopman-von Neumann theory, one can largely unify the formulations of classical and quantum dynamics. I will prove that the motions of elementary parcels of both classical and quantum Husimi fluid obey Hamilton variation principle, and the differences between associated action functionals stem from the differences between classical and quantum pure states.

Husimi action functionals are not unique and defined up to the Skodje flux gauge fixing [2]. The gauge choice can dramatically alter flux trajectories. For instance, I will show that the Bohmian mechanics is nothing but the Husimi representation in a different gauge. I will also briefly outline an application of the presented formalism for improving semiclassical initial value representations employed in quantum many-body simulations [3].

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Abstracts of Posters

(in alphabetical order)

Koopman Operators, Nonlinear Coherent Structures, Learning, and Feedback Control in High Energy Density Plasmas

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We will examine methods of controlling laser-plasma instabilities in high energy density plasmas. The use of Spike Trains of Uneven Duration and Delay (STUD pulses) will be Highlighted. For nonlinear optical processes such as Resonance Absorption or Stimulated Raman Scattering, taming of instabilities will be demonstrated by learned pulse sequence designs. Vlasov (Kinetic) simulation models as well as fluid coupled-mode equation models will be considered. We plan to find neural net surrogates, train them and deploy them in more complex configurations as our longer-term goals. Highlights of these learning challenges will be introduced. Experiments to test these results are scheduled on the ALEPH laser at Colorado State University as part of the LASERNET US program.

Work supported by the DOE FES-NNSA Joint Program in HEDLP

Canonical Quantum-Classical Dynamics: Lessons from Phase Space

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Studying the interaction between classical and quantum systems is useful for practical applications where it is computationally simpler to treat some degrees of freedom as classical. It may also shed light on foundational questions like the possibility of treating gravity as fundamentally classical or analyzing the process of quantum measurement. However, no-go theorems in the literature found that quantum-classical dynamics is inconsistent because, unlike the quantum commutator or the classical Poisson bracket, the hybrid dynamical bracket does not obey the Jacobi identity or the Leibniz rule.

Analyzing the problem from the phase-space approach to quantum mechanics, we found a single consistency condition that, if satisfied, guarantees the Jacobi and Leibniz properties for the hybrid dynamical bracket [2]. This conditions suggests the possiblility of circumventing the no-go theorems. It leads us to recognize the importance of ``composition products'' for dynamical variables. We show that to satisfy the consistency condition, we can either construct a non-trivial composition product for hybrid variables, or allow only a restricted set of hybrid variables into the dynamical framework. The latter of these possibilities lead to the restriction of allowed quantum-classical interactions.

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The Koopman-von Neumann Formulation of Classical Physics and the Platonic Interpretation of Quantum Theory

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Given a collection of random variables representing the quantifiable properties of a physical system, the Gelfand-Naimark-Segal (GNS) construction produces a corresponding Hilbert-space picture. For a classical system, the random variables naturally make up a commutative C*-algebra, and the GNS construction yields the Koopman-von Neumann (KvN) formulation of the system. For the quantum case, the random variables form a noncommutative C*-algebra, and the GNS construction yields the usual Hilbert-space picture formulation found in standard textbooks. This parallel between the classical and quantum cases suggests that Hilbert spaces are not fundamental ingredients of quantum theory, but are merely convenient mathematical tools. This parallel also motivates a new interpretation of quantum theory that sheds new light on the measurement problem, entanglement, and other mysterious features of the theory.

Ab Initio Multiple Spawning with Informed Stochastic Selection

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What happens to a molecule once it has absorbed UV or visible light? How does the molecule release or convert the extra-energy it just received? Answering these questions clearly goes beyond a pure theoretical curiosity, as photochemical and photophysical processes are central to numerous domains like energy conversion and storage, radiation damages in DNA, or atmospheric chemistry, to name a few. Different theoretical tools have been developed to simulate the excited-state dynamics of molecules [1]. Ab initio multiple spawning (AIMS) describes the dynamics of nuclear wavepackets using adaptive linear combinations of traveling frozen Gaussians [2]. Trajectory surface hopping portrays the nuclear dynamics with a swarm of independent classical trajectories that can hop between potential energy surfaces for this task [3].

With this poster, I intend to present some of our recent work aiming at developing new approximate techniques based on the multiple spawning framework. In particular, I will introduce the stochastic selection AIMS approach [4] and compare it to trajectory surface hopping [5].

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Quantum Mechanics for Stochastic Closures of Dynamical Systems

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When modelling chaotic dynamical systems, notably in climate prediction models, the use of deterministic local parametrization can cause a loss in the model's ability to capture important dynamics of the original system. To circumvent this issue, stochastic non-local parametrization schemes can be implemented. We propose such a parametrization scheme incorporating a data assimilation method based on quantum mechanics and employing use of the Koopman operator. We also outline a basic general iterative formula for the implementation of this method. Given a system in which some component of the state is unknown, this method involves defining the system as being in a time-dependent "quantum-state" which influences the tendency of a random draw of the unknown component of the classical state. The quantum state is an operator on the RKHS of classical observables and evolves over time under an action by the Koopman operator. The quantum state also updates with new data-points according to a quantum Bayes' law. The RKHS property is used to generate kernel functions which allow the quantum Bayes' law to be approximated numerically. We analyze the results of this methodology applied to the Lorenz 63' system and show that this method can preserve large-scale chaotic dynamics.

Kinetic equations of the open quantum-classical systems

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In the talk, we consider the rigorous approach to the description of the kinetic evolution of a many-particle system composed of a trace quantum particle and an environment of finitely many hard spheres [1]. Using the method of kinetic cluster expansions developed in [2], we prove that the evolution of the state of a trace quantum particle in an environment of hard spheres can be described within the framework of the marginal density operator governed by the generalized kinetic equation and by an infinite sequence of the explicitly defined functionals of a solution of this kinetic equation.

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Recovering quantum correlations in optical lattices from interaction quenches

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Quantum simulation experiments with ultra-cold atoms have lead to numerous insights into the physics of strongly correlated quantum systems, e.g., realizing and observing anti-ferromagnets with substantial evidence of string patterns. It is fair to say that there has been steady progress towards realizing the ambitious long-term goals set for quantum simulators. In the future developing diagnostic tools regarding genuine quantum correlations in such systems will become key. The atom gas microscope is the state-of-the-art diagnostic tool and enables a level of inquiry into ultra-cold atoms in optical lattices unparalleled in any other quantum many-body system opening an exciting pathway towards understanding strongly interacting quantum systems. However, currently a direct measurement of a coherent current is out of reach. In this work, we show how to unify the two principal read-out techniques in optical lattice quantum simulators by using atom microscope measurements together with time-of-flight expansion into an optical superlattice. For this, we establish a data analysis method not resorting to the far-field approximation which reliably recovers the full covariance matrix, including off-diagonal correlations representing coherent currents. The signal processing builds upon semi-definite optimization, providing bona fide covariance matrices optimally matching the observed data. We demonstrate how the obtained information about non-commuting observables allows to lower bound entanglement at finite temperature which opens up the possibility to study quantum correlations in quantum simulations going beyond the capabilities of classical computers.

We consider fermionic atoms in optical lattices and show how to use readily available quench protocols to perform tomographic reconstructions based on atom microscope measurements. Our protocol consists of four steps: (a) Prepare a fermionic state, (b) Double-up the lattice locally, (c) Quench to the nearest-neighbour hopping Hamiltonian in the new lattice, (d) Measure on-site particle numbers using the atom microscope. The results of the numerical reconstruction, involving semi-definite positivity constraints, of correlations in a thermal state are presented in Fig. 1. It is crucial that *i)* there is no need of new experimental developments, our novel reconstruction method is the innovation, *ii)* the measurements need not be perfect and Fig. 1 includes statistical noise, *iii)* in the submitted paper we show that the reconstruction allows to quantify entanglement present in the system using a novel entropic witness. These three points are fully in line with very encouraging feedback from experimentalists who have shown much interest in our new tomographic reconstruction method and applying it experimentally is now our main focus.

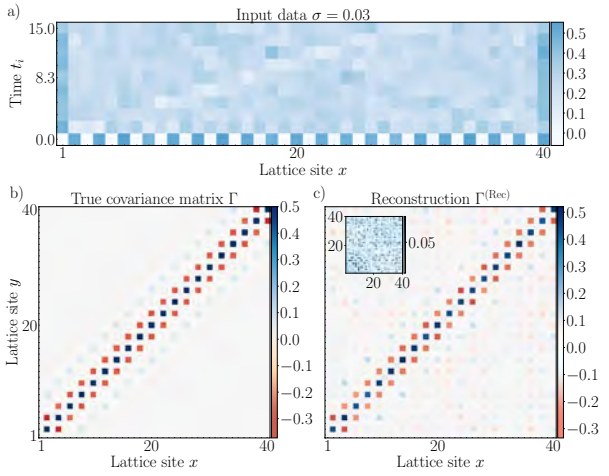

FIG. 1. **Tomographic reconstruction.** *a)* Input data for the reconstruction based on out-of-equilibrium data of local particle numbers $N_x(t_i)$ as would be measured by the atom microscope. *b)* The true input covariance matrix representing a thermal state. We have chosen a temperature so that there are relatively large currents to be recovered. The covariance matrix Γ is shown after step (b) after the sub-lattice has been created. Note that besides the new checker-board pattern, the correlations between sites are assumed to be exactly preserved. *c)* Results of the reconstruction $\Gamma^{(\mathrm{Rec})}$ which works even in presence of statistical noise.

Quantum thermodynamics of an open quantum system periodically driven

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We study the thermodynamics of an open system that is periodically driven and offer a comparison of different formal definition of heat and work. We consider a two-level atom interacting with a dephasing and electromagnetic bath. The master equation is rigorously obtained thanks to the Floquet theorem, that allows splitting the evolution operator. We solve the dynamical evolution to compute the thermodynamics properties using two different approaches. Thus, we compare results from the standard approach, in which the Hamiltonian basis is preferred and the heat variation is related to the density matrix evolution, and from a recently proposed entropy-based approach, in which the density matrix basis is preferred and the heat variation is considered as that part of the energy exchanged related to the entropy variation of the system. We find that the atom returns to the equilibrium regardless of the approach used, hence, the dynamics of the model is consistent with the thermodynamics laws. In doing so, we highlight the limitation of the adiabatic approach that lead to thermodynamics inconsistencies in systems with time-dependent Hamiltonian.

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Quantum Entanglement Percolation in a Monolayer Honeycomb Lattice

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The problem of establishing Bell and Greenberger-Horne-Zeilinger states between faraway places or distant nodes of a circuit is a difficult and an extremely important one, and a strategy which addresses it is entanglement percolation. We provide a method for attaining the end through a quantum measurement strategy involving three-, two-, and single-qubit measurements on a single-layer honeycomb lattice of partially entangled bipartite entangled states which would call for less noise effects in an actual experimental realisation.

We explicitly compare our result of using QEP on the monolayer honeycomb lattice with that of using CEP on the same lattice in Ref. [2]. The table below makes evident that the number of measurements we require for the final result is lesser than CEP in Ref.[2] and thus it is plausible that noise effects on a realisation of our strategy will be lower than the same on the one in Ref. [2].

Comparison of the Number of Measurements in the 2 strategies

Type of Measurement	QEP	CEP in Ref. [2]
Single Qubit Measurements	$2l^2 + O(l)$	$6l^2 + O(l)$
Two Qubit Measurements	$O(l)$	$O(l)$
Three Qubit Measurements	$2l^2 + O(l)$	
Total Number of Measurements	$4l^2 + O(l)$	$6l^2 + O(l)$

The number of measurements shown here are for an **$l \times l$** square box encompassing a part of a hexagonal lattice. We have also compared our measurement strategy with the one used in Ref.[3] where the authors had to carry out **4-5 measurements per unit cell** of their lattice for the success of their strategy. But our strategy does the job in **3 measurements per unit cell,** thus calling for less noise effects.

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Semiclassical Theories as Initial Value Problems

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Motivated by the initial value problem in semiclassical gravity, we study the initial value problem of a system consisting of a quantum scalar field weakly interacting with a classical one. The quantum field obeys a Klein-Gordon equation with a potential proportional to the classical field. The classical field obeys an inhomogeneous Klein-Gordon equation sourced by the renormalised expectation value of the squared quantum field in a Hadamard state, $\langle\Psi|\Phi^2\,\Psi\rangle$. We show that a unique asymptotic solution for the system can be obtained perturbatively at any fixed finite order in the weak coupling from initial data provided that the interaction is switched on and off smoothly in a spacetime region to the future of the initial data surface. This allows one to provide “free” initial data for the decoupled system that guarantees that the Wightman function of the quantum field be of Hadamard form, and hence that the renormalised $\langle\Psi|\Phi^2\,\Psi\rangle$ exist (in a perturbative sense) and be smooth.

The collapse of a quantum state as a signal analytic sleight of hand[1]

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The collapse of a quantum state is a mathematical sleight of hand that allows the construction of a joint probability density even for operators that are noncommutative. We can formalize that construction as a non-commutative, non-associative collapse product that is nonlinear in its left operand as a model for joint measurements at time-like separation, in part inspired by the sequential product for positive semi-definite operators. A collapse picture, in which a quantum state collapses after each measurement, can therefore be equivalent to a no-collapse picture that uses a different state and Quantum Non-Demolition (QND) measurement operators to model the same joint probability density for consecutive measurements. The collapse of a state is a mathematical construction that can also be a useful tool when noncommutative operators are used in classical mechanics and signal analysis. This construction helps us understand the connection between Koopman's Hilbert space formalism for classical mechanics[2] and quantum mechanics by normalizing the mathematics of "The Collapse of the Wave Function", allowing us to equate the resulting joint probability densities with what we would obtain from a commutative algebra of operators.

The material presented in this poster was presented as the central part of a talk given at IQOQI, Vienna (by Zoom), on March 17th, 2021, which is available as a YouTube video[3].

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Generator EDMD: Data-Driven Approximation of the Koopman Generator

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[2] University of Surrey, Surrey, U.K.

I will present a powerful framework to compute a Galerkin approximation of the Koopman generator of a (stochastic) dynamical system based on simulation data. I will explain how such an approximation can be used to analyze the system, determine reduced models, and solve associated control problems. The framework can also be used if the Galerkin subspace is a reproducing kernel Hilbert space, enabling the use of powerful approximation spaces. Lastly, I will point out how the same strategy can be employed to the approximation of more general linear differential operators, as long as a suitable dynamical system can be associated to the weak formulation of that differential operator. An application to model systems from quantum physics will serve as illustration.

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Operational Theories in Phase Space: Toy Model for the Harmonic Oscillator

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We construct a toy model for the harmonic oscillator that is neither classical nor quantum. The model features a discrete energy spectrum, a ground state with sharp position and momentum, an eigenstate with non-positive Wigner function as well as a state that has tunneling properties. The underlying formalism exploits that the Wigner–Weyl approach to quantum theory and the Hamilton formalism in classical theory can be formulated in the same operational language, which we then use to construct toy model with well-defined phase space. The toy model demonstrates that operational theories are a viable alternative to operator-based approaches for building physical theories.

Various ideas have been proposed to generalize quantum theory, among others also operational approaches to physical theories, which are built on the assumption that convexity represents mixtures of states and are collected under the term general probabilistic theories [1]. Within this framework, for example, thermodynamics [2], dynamics [3], and recently even the operational consequences of gravitational effects [4] were investigated. But the aforementioned research within the framework is bound to black-box-like and finite-dimensional prototheories, which do not describe actual physical systems, but rather information-theoretic effects, like, for example, bounds on violations of Bell inequalities. Our goal is to construct a bridge between operational theories in the above sense and quantum theory. We accomplish this by incorporating continuous position and momentum into an operational theory, thus we are able to formulate a toy model for the harmonic oscillator. Our construction demonstrates that there are alternatives to quantization for building physical theories and that one can use the operational approach for such a construction. In order to construct a toy theory of harmonic oscillator, we reformulate both quantum and classical theory in a way that allows us to express observables in terms of spectral measures on phase space. The key idea behind the reformulation and introduction of those phase space spectral measures is the Wigner function formalism of quantum theory.

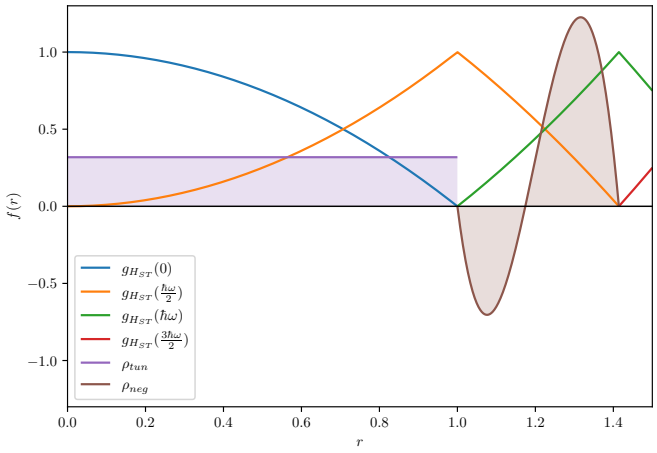

FIG. 1. Phase space spectral measure and phase space states for the sawtooth oscillator. The functions of the phase space spectral measure for the energies $E_0 = 0$, $E_1 = \frac{\hbar\omega}{2}$, $E_2 = \hbar\omega$, and $E_3 = \frac{3\hbar\omega}{2}$ are shown in blue, orange, green, and red, respectively. The "tunneling" state ρ_{tun} and the eigenstate ρ_{neg} for the energy E_2 are shown in purple and brown, respectively, with the area under the functions filled. The energy observable is $H_{\mathrm{ST}} = \hbar\omega r^2/2 = (p^2/2m) + (m\omega^2 q^2)/2$ (not shown).

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The bohmion method in nonadiabatic quantum hydrodynamics

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Starting with the exact factorization of the molecular wavefunction, we presents the results from the numerical implementation in nonadiabatic dynamics of the recently proposed bohmion method. Within the context of quantum hydrodynamics, we introduce a regularized nuclear Bohm potential admitting solutions comprising a train of δ−functions which provide a finite-dimensional sampling of the hydrodynamic flow paths. The bohmion method inherits all the basic conservation laws from its underlying varia-tional structure and captures electronic decoherence. The method is applied to the well-known Tully models, which are used here as benchmark problems. In the present case of study, we show that the new method accurately reproduces both electronic decoherence and nuclear population dynamics.

Free fall in KvN mechanics and Einstein's Equivalence principle

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The implementation of Einstein's principle of equivalence in the framework of Koopman-von Newmann (KvN) mechanics is discussed. Both in KvN mechanics and in quantum mechanics, a propagator in a homogeneous gravitational field is simply related with a free propagator. As a result, the wave function in a homogeneous gravitational field in a free falling reference frame differs from the free wave function only in phase. Also the fisher information does not depend on the magnitude of the homogeneous gravitational field and hence this is formulation of Einstein's principle of equivalence that is valid both in quantum mechanics and KvN mechanics.

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Geometric aspects of generalized Schroedinger equations

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In this contribution we review several geometric aspects concerning Schroedinger's and Pauli's equations, mostly based on [3,4]. First, we resume the Madelung–Bohm hydrodynamical approach to quantum mechanics and recall the Hamiltonian structure of the Schroedinger equation. The probability current provides an equivariant moment map for the group G = sDiff(R^3) of volume-preserving diffeomorphisms of R^3 (rapidly approaching the identity at infinity) and leads to a current algebra of Rasetti–Regge type. The moment map picture extends, mutatis mutandis, to the Pauli equation and to generalized Schroedinger equations of the Pauli–Thomas type. A gauge theoretical reinterpretation of all equations is outlined via consideration of suitable Maurer–Cartan gauge fields and it is then related to Weyl geometric and pilot wave ideas. A general framework accommodating Aharonov–Bohm and Aharonov–Casher effects is presented within the gauge approach. Connections with geometric quantum mechanics, coherent state and Fisher information theoretic aspects are highlighted throughout.

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Parameterization of the Wigner distribution function and its consequences for the description of a quantum dynamical system in the phase space.

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The Wigner distribution function belongs to the class of the non-classical distribution functions that are used for studying quantum dynamical systems in phase space [1]. Some of these functions can be unified owing to certain parameterization as it was discussed in [2]. This observation allowed one to think about the general form of the equation of motion for such parameterized distribution functions and consequences concerning dynamical aspects of the quantum systems in the classical limit.

This report aims to derive and analyze the equation of motion for the parameterized Wigner distribution function [3]. This parameterization directly results from some modification of the linear transformation of the spatial variables which is used to derive the original Wigner distribution function and its equation of motion. Depending on the value of this real parameter the corresponding Wigner distribution function can be a real or complex one. Additionally, one of the unexpected consequences of this parametrization is appertaining an additional term in the equation for this function. Presented analysis is focused on the influence of the parameter on individual terms in this equation and the gradient approximation for the non-local potential. Apart from that is discussed the relationship between the introduced Wigner function and its interpretation as a probability amplitude of finding a particle at a certain point in the classical phase space [4].

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