
Representing ensembles of quantum systems in phase space

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Abstract

Recently much progress has been made in the phase space representation of quantum systems. Specifically, we have shown how to construct Wigner and Weyl functions for any quantum system within a consistent framework [Phys. Rev. Lett. 117, 180401 (2016) and Phys. Rev. A 99, 012115 (2019)]. We will discuss how this new visualisations of systems such as atoms, molecules as well as atom-field interactions and the potential that such an approach offers. As an informationally complete description of quantum systems the Wigner and Weyl representations afford the capability of other representations but also make clear analogies to certain classical phenomena. We discuss the connection to classical statistical physics. Finally we speculate about potential applications to spin systems.

*Speaker

Correlated impurities, interfaces and photovoltaics out of equilibrium: Auxiliary Master Equation Approach

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I will present recent developments of a numerical scheme to address correlated quantum impurities out of equilibrium down to the Kondo scale. This Auxiliary Master Equation Approach [1,2,3] is also suited to address transport and photoexcitation effects in correlated interfaces within nonequilibrium Dynamical Mean Field Theory [4,5]. The method consists in an exponentially accurate mapping of the original impurity problem onto an auxiliary open quantum system including bath orbitals as well as a coupling to a Markovian environment. The intervening auxiliary orbitals allow for a treatment of non-Markovian dynamics at the impurity.

Green's functions are evaluated via (non-hermitian) Lanczos exact diagonalisation [2], by matrix-product states (MPS) [3], or by stochastic wave function approaches [6]. In particular, the Matrix-Product State implementation [5] of the resulting Lindblad equation produces highly accurate spectral functions for the Anderson impurity model in the Kondo regime. In equilibrium we obtain a remarkably close agreement to numerical renormalization group for intermediate values of the interaction.

I will show results for spectral and transport properties of selected quantum impurity systems out of equilibrium [3,6], and discuss photoexcitation induced transport across a Mott insulating gap in connection with the issue of impact ionization [5].

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* Speaker

Potential energy surfaces and Berry phases beyond the Born-Oppenheimer approximation

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Abstract

The starting point of essentially all modern electronic-structure techniques is the Born-Oppenheimer (BO) approximation. It not only makes calculations feasible, the motion of nuclear wave packets on the lowest BO potential energy surface often provides us with an intuitive and accurate picture of chemical reactions and, for small-amplitude motion, it yields an excellent way to determine vibrational spectra. To go beyond the adiabatic limit is notoriously difficult. Here we present a novel approach to non-adiabatic effects that is based on 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 for these wavefunctions lead to a unique definition of *exact* potential energy surfaces as well as *exact* geometric phases, both in the time-dependent and in the static case. We discuss a case where the exact Berry phase vanishes although there is a non-trivial Berry phase for the same system in Born-Oppenheimer approximation [2], implying that in this particular case the Born-Oppenheimer Berry phase is an artifact. In the time-domain, whenever there is a splitting of the nuclear wavepacket in the vicinity of an avoided crossing of BO surfaces, the exact time-dependent surface shows a nearly discontinuous step [3]. This makes the classical force on the nuclei jump from one to another adiabatic surface. Based on this observation, we deduce a novel mixed-quantum-classical algorithm whose unique feature is that the trajectories are coupled. Without recourse to Tully surface hopping and without any added decoherence correction, the new algorithm provides a rather accurate, (much improved over surface hopping) description of decoherence [4]. This is demonstrated for the photo-induced ring opening of oxirane [5]. We present a multi-component density functional theory [6,7] that provides an avenue to make the fully coupled electron-nuclear system tractable for very large systems. Finally, we explore the possibility of describing non-adiabatic effects in, e.g., proton transfer by R-dependent nuclear masses [8].

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Matrix-product-state methods for nonequilibrium dynamics, transport and dissipation in correlated electron-phonon wires

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Abstract

We present matrix-product-state methods for investigating the nonequilibrium dynamics, quantum transport and dissipation in one-dimensional correlated electron-phonon systems. The time-evolving block decimation method with local basis optimization (TEBD-LBO) [1] allows us to simulate the nonequilibrium dynamics of many-particle systems with strongly fluctuating bosonic degrees of freedom. Thus we can study nonlinear transport properties [2] including inelastic scattering and dissipation effects [1,3] as well as the relaxation of electronic excitations in the presence of a phonon bath [4].

We also show that the dynamical DMRG method combined with linear response theory [5] enables the calculation of the linear conductance in Luttinger liquids using a proper scaling of system length, zero-frequency current-current correlation functions, and broadening. This approach works for lattice models of Luttinger liquids including impurities, phonons or contacts to metallic leads.

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^{*}Speaker

Quantum Spin Liquids: Signatures of Fractionalization

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Abstract

I will discuss emergent gapped and gapless quantum spin liquid (QSL) phases in the phase diagram of the Kitaev model on a honeycomb lattice with bond-dependent spin exchange interactions as a function of an externally applied magnetic field. In a QSL magnetic long-range order is destroyed due to quantum fluctuations so it cannot be characterized by a local order parameter. Instead we use the topological entanglement entropy to characterize the gapped QSL. For the gapless QSL we determine the Fermi surface of the neutral $S=1/2$ spinons. I will discuss material platforms that realize the Kitaev model and signatures of fractionalization in thermal transport and inelastic neutron scattering.

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*Speaker

Cluster formation in nuclear systems

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Abstract

Light clusters (mass number $A \leq 4$) in nuclear matter at subsaturation densities are described using a quantum statistical approach to calculate the quasiparticle properties and abundances of light elements. Virial coefficients are derived from continuum contributions to the partial densities which depend on temperature, densities, and total momentum. The Pauli blocking is modified taking correlations in the medium into account. Both effects of continuum correlations lead to an enhancement of cluster abundances in nuclear matter at higher densities. The properties of light clusters and continuum correlations in dense matter are of interest for nuclear structure calculations, heavy ion collisions, and for astrophysical applications such as the formation of neutron stars in core-collapse supernovae.

*Speaker

Basic microscopic plasma physics from N-body mechanics

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Abstract

Computing is not understanding. This is exemplified by the multiple and discordant interpretations of Landau damping still present after 70 years. For long deemed impossible, the mechanical N-body description of this damping, not only enables its rigorous and simple calculation, but makes unequivocal and intuitive its interpretation as the synchronization of almost resonant passing particles. This synchronization justifies mechanically why a single formula applies to both Landau growth and damping. As to the electrostatic potential, the phase mixing of many beam modes produces Landau damping, but it is unexpectedly essential for Landau growth too. Moreover, collisions play an essential role in collisionless plasmas. In particular, Debye shielding results from a cooperative dynamical self-organization process, where "collisional" deflections due to a given electron diminish the apparent number of charges about it. The finite value of exponentiation rates due to collisions is crucial for the equivalent of the van Kampen phase mixing to occur in the N-body system. As to Coulomb scattering, there is a smooth connection between impact parameters where the two-body Rutherford picture is correct, and those where a collective description is mandatory. The N-body approach reveals two important features of the Vlasovian limit: it is singular and it corresponds to a renormalized description of the actual N-body dynamics.

*Speaker

Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations

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Abstract

One of the main goals of electronic structure theory is to precisely describe increasingly complex polyatomic systems. It is widely accepted that size extensive methods based on the coupled-cluster (CC) theory and their extensions to excited states via the equation-of-motion (EOM) formalism are excellent candidates for addressing this goal. Indeed, when applied to molecular properties and chemical reaction pathways, the CC hierarchy, including CCSD, CCSDT, CCSDTQ, etc., rapidly converges to the limit of the exact, full configuration interaction (FCI), diagonalization of the Hamiltonian, allowing one to capture the relevant many-electron correlation effects in a conceptually straightforward manner through particle-hole excitations from a single Slater determinant. One of the key challenges has been how to incorporate higher-than-two-body components of the cluster operator, needed to achieve a quantitative description, without running into prohibitive computational costs of CCSDT, CCSDTQ, and similar schemes, while eliminating failures of the more practical perturbative approximations of the CCSD(T) type in multi-reference situations, such as chemical bond breaking. In this talk, we examine a radically new way of obtaining accurate energetics equivalent to high-level CC calculations, even when electronic quasi-degeneracies become significant, at the small fraction of the computational cost, while preserving the black-box character of single-reference computations. The key idea is a merger of the deterministic formalism, abbreviated as $CC(P;Q)$ [1,2], with the stochastic CI [3,4] and CC [5] Quantum Monte Carlo (QMC) approaches [6]. We also demonstrate that one can take the merger of the stochastic and deterministic ideas to the ultimate level and use it to enable precise extrapolations of the exact, FCI, energetics based on the early stages of FCIQMC propagations [7]. The advantages of the new methodologies will be illustrated by molecular examples, where the goal is to recover the nearly exact, CCSDT and CCSDTQ, and exact, FCI, energetics in multi-reference situations involving chemical bond dissociations and reaction pathways. Extensions of this work to excited electronic states by a combination of stochastic CIQMC and deterministic EOMCC computations [8] and converging FCI energetics in strongly correlated systems, such as those involved in modeling metal-insulator transitions [9], will be discussed as well.

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^{*}Speaker

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Exotic features of superfluidity far from equilibrium

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Abstract

Superfluidity and superconductivity are remarkable manifestations of quantum coherence at a macroscopic scale. The existence of superfluidity has been experimentally confirmed in many condensed matter systems, in ^3He and ^4He liquids, in nuclear systems including nuclei and neutron stars, in both fermionic and bosonic cold atoms in traps, and it is also predicted to show up in dense quark matter. The interplay between spin-polarization and superfluidity gives rise to fascinating phenomena manifested in Josephson- π junction or in exotic phases like FFLO or Sarma (interior gap) phase, which involve nontrivial behavior of the order parameter.

I will present certain aspects of superfluidity in nonequilibrium conditions, which originate from dynamics of the order parameter both in unpolarized and spin-imbalanced systems. In particular, I will discuss properties of quantum vortices in the context of quantum turbulence. I will also explore the role of pairing dynamics, leading to the appearance of solitonic excitations, in nuclear collisions. Finally, I will describe quasiparticle scattering on the pairing nodal surfaces leading to the creation of stable, spin-polarized droplets (*ferrons*) in superfluid ultracold atomic gases. Properties of these hypothetical objects will be discussed.

*Speaker

Symmetry-broken and -restored many-body perturbation theory in ab initio nuclear structure

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Abstract

The *ab initio* description of medium-mass open-shell nuclei using accurate nuclear Hamiltonians poses a formal and computational challenge in state-of-the-art nuclear structure calculations. The presence of strong correlations and the breakdown of conventional approaches due to the onset of (quasi-)degeneracies require extensions of already existing formalisms. In particular, exploiting symmetry breaking in a many-body expansion enables to lift such degeneracies and obtain a well-behaved, i.e., non-singular correlation expansion. Recently, the use of particle-number broken reference states, conveniently obtained from a Hartree-Fock-Bogoliubov (HFB) mean-field calculation, has shown great promise to account for the nuclear superfluidity in singly open-shell nuclei.

In this talk I will introduce the so-called *Bogoliubov many-body perturbation theory* (BMBPT), i.e., a perturbative expansion based on a particle-number broken HFB vacuum. Ground-state energies along medium-mass isotopic chains are compared to large-scale calculations performed with state-of-the-art non-perturbative many-body schemes using realistic nuclear Hamiltonians.

Additionally, the restoration of the broken symmetry is discussed accounting for the conservation of particle number in a finite quantum system. The resulting *particle-number projected BMBPT* (PBMBPT) constitutes the first framework in which a continuous symmetry is consistently broken and restored beyond the mean-field level in a realistic nuclear structure application.

*Speaker

Neural-Network Quantum States

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Abstract

Machine-learning-based approaches, routinely adopted in cutting-edge industrial applications, are being increasingly adopted to study fundamental problems in science. Recently, their effectiveness has been demonstrated also for many-body physics. In this seminar I will present applications to the quantum realm. First, I will discuss how a systematic machine learning of the many-body wave-function can be realized. This goal has been achieved in [1], introducing a variational representation of quantum states based on artificial neural networks. This representation can be used to study both ground-state and unitary dynamics, with controlled accuracy. I will discuss several applications in diverse domains, including Quantum State Tomography of highly-entangled states [2], frustrated spin systems [3], and as an alternative to the standard path integral [4].

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*Speaker

Thermodynamic properties of the Shastry-Sutherland model and SrCu₂(BO₃)₂

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Abstract

Modern numerical methods for simulating quantum many-body systems allow for determining finite-temperature properties of two-dimensional frustrated lattice systems. We apply the thermal pure quantum state (TPQ) technique and infinite projected entangled pair states (iPEPS) to study the thermodynamics of the Shastry-Sutherland spin model. The former employs the concept of quantum typicality to extend the system sizes accessible to perform exact diagonalizations, while the latter is a tensor network based approach. We demonstrate convergence as a function of system size in TPQ calculations and complete agreement with iPEPS results. Our methods reveal a remarkably sharp and low-lying feature in the magnetic specific heat around the quantum phase transition from the dimer to the intermediate phase, whose origin appears to lie in multi-triplon bound states. We also find close agreement of experimental thermodynamical quantities measured for the compound SrCu₂(BO₃)₂. We thereby assess up to which precision the material SrCu₂(BO₃)₂ is described by the Shastry-Sutherland model.

^{*}Speaker

Spin-polarized fermions at unitarity: a complex Langevin study

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Abstract

The unitary Fermi gas, situated "right in the middle" of the crossover between Bardeen-Cooper-Schrieffer superfluidity and Bose-Einstein condensation, is one of the most intensely studied many-body system in recent years. However, its strongly-correlated nature renders a theoretical treatment challenging. While the spin-balanced scenario is accessible with Quantum Monte Carlo methods, its spin-imbalanced counterpart suffers from a sign problem and is thus out of reach for such approaches.

Through recent advances with the complex Langevin (CL) method, we are now able to treat spin-polarized fermions at unitarity in an ab initio fashion and extract thermodynamic properties such as the particle density and magnetization. From these equations of state we obtain response functions such as the compressibility and magnetic susceptibility. In the spin-balanced case we observe excellent agreement of our non-perturbative results with existing state-of-the-art results from other methods as well as with experimental data. At low fugacity, we find excellent agreement with the virial expansion for spin-polarized systems. Away from the limit where the virial expansion is valid, we provide predictions for the equations of state for a wide range of spin asymmetries. In addition to thermodynamic quantities we investigate the pairing behavior and we show first results for two-body correlation functions.

*Speaker