Posters

Time-dependent renormalized natural orbital theory for intense laser-atom interaction

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Natural orbital theory (NOT) is a computationally useful approach to the few and many-body quantum problem. While natural orbitals (NOs) are known and applied since many years in electronic structure applications [1], their potential for time-dependent problems is being investigated only since recently [2, 3, 4, 5, 6]. We give a short introduction to the time-dependent renormalized NOT (TDRNOT) and test it on cases where time-dependent density (TDDFT) functional theory fails (doubly excited states, Fano profiles in absorption spectra, and nonsequential double ionization). Exact numerical solutions of the time-dependent Schrdinger equation for a laser-driven one-dimensional He model atom serve as benchmarks and show that TDRNOT is a promising approach indeed.

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Dimensional reduction of Majorana modes at the boundary of a 3D topological superconductor

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We induce dimensional reduction of Majorana surface states in a 3D topological superconductor in the symmetry class DIII. To the boundary we introduce an effective Zeeman field with a pair of 1D domain walls. The 2D zero energy Majorana modes become localised at the 1D domain walls. Furthermore, we show that the boundary behaves as a pair of adjoined 2D topological superconductors in the symmetry class D that support Chern numbers of opposite sign. We also introduce a second 'checkerboard' configuration of the effective Zeeman field. This leads to a further reduction of the Majorana modes from 1D to 0D.

Propagating the two-particle reduced-density matrix of one- and two-dimensional Hubbard systems

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The Hubbard model is one of the simplest models for correlation in solid state physics but still beyond a full theoretical description. Ultra-cold Fermi gases in optical lattices allow to experimentally investigate the Hubbard model for large systems under well-controlled conditions [1]. Recently, experimental investigations have focused on the dynamics of these systems after quenches in two dimensions [2] and simultaneously in acquiring single-site resolution [3]. So far, an adequate theoretical description has been missing. We present a new theoretical approach to simulate the dynamics of Hubbard systems in the regime of weak inter-particle correlations which is applicable to higher-dimensional systems. We use the time dependent two-particle reduced-density matrix (TD-2RDM) method [4] to simulate the dynamics of finite Hubbard systems after potential quenches. One of the strengths of the TD-2RDM method is that it includes two particle correlations exactly. In the TD-2RDM method the timeevolution of the 2-RDM is coupled to two-particle and three-particle correlations via the interaction term of the underlying Hamiltonian. We manage to reconstruct three-particle correlations partially through a new ansatz [4] and using the Yasuda-Nakatusji approximation [5]. To benchmark our theory we investigate small systems that are still accessible to an exact numerical solution. We show results for one-dimensional Hubbard systems far from equilibrium where we overcome stability problems observed in [6] by employing purification [7] of the 2-RDM after each propagation step. We achieve better results than calculations with the non-equilibrium Greens function method [8]. Furthermore, we apply the TD-2RDM method for weak potential quenches and delimit its applicability. Finally, we show first results for density fluctuations caused by weak potential quenches for two-dimensional Hubbard nano-clusters. In future, we will study the two-dimensional Hubbard systems at sizes not treatable by exact methods and compare theoretical simulations to experimental results.

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Time-Dependent Two-Particle Reduced Density Matrix Theory for Atoms in Strong Laser Pulses

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Calculating the dynamics of correlated quantum many-body systems is one of the great challenges of modern theoretical physics. Essentially two competing approaches exist. On

one hand, the time-dependent density functional theory (TDDFT) allows for the treatment of hundreds of particles due to its favorable scaling with particle number. The drawback lies in the involved approximations for the correlation energy which have no universal quality and do not allow for systematic improvement. On the other hand, the multi-configurational time-dependent Hartree Fock (MCTDHF) ansatz (for a review see e.g. [1]) allows for an exact treatment but is limited to only small systems due to the factorial scaling with particle number. Motivated by recent progress in ground state calculations where the two-particle reduced density matrix (2RDM) has been used (see e.g.[2]), we bridge the gap between TDDFT and MCTDHF by developing a time-dependent quantum many-body theory which uses the 2RDM as the fundamental object. In doing so we fully incorporate two-particle correlations. The equations of motion for the 2RDM depend on the three-particle reduced density matrix which has to be approximated to obtain the equations of motion in closed form. This typically goes hand in hand with neglecting three-particle correlations completely [3]. Through a new ansatz [4] that ensures spin and energy conservation and by using approximations for the three-particle cumulant [5,6] we manage to reconstruct important parts of three-particle correlations. Additionally, we impose two necessary N-representability constraints during time evolution via a process called purification [7] thereby controlling dynamical instabilities previously observed [3]. To demonstrate the accuracy of the TD-2RDM method we calculate high-harmonic generation in atomic targets which sensitively probes correlated multi-electron dynamics. We find that the TD-2RDM method is in very good agreement with numerically exact solutions obtained from the MCTDHF method. Further, we find that the TD-2RDM method performs consistently better than TDHF and TDDFT within the adiabatic local-density approximation.

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Spectral properties of reduced fermionic density operators and parity superselection rule

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We consider pure fermionic states with varying number of quasiparticles and demonstrate that spectra of partial states (reduced with respect to some bipartition) are not identical as it takes place for bosons and conventional states in spaces with tensor product structure. We fully characterize pure states with equispectral partial states and show that they are related via local unitary operations with states satisfying the parity superselection rule. Thus, valid purifications for fermionic density operators are found. As a byproduct, the positive semidefinite density matrix for fermions is constructed without implying the state gaussianity. The developed formalism clearly indicates that the conventional partial trace methods are not applicable to fermionic systems.

The semiclassical propagator of two anyons

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I present a systematic derivation of the semiclassical limit of the propagator of two free anyons. Thereby, a sum over the discrete eigenvalues of the canonical angular momentum of the relative motion of the particles turns into an integral over a continuous variable, and the stationary points of this integral coincide with the classical value of the relative momentum. The treatment reveals the origin of a discontinuity of the semiclassical propagator and relates the validity of the semiclassical approximation to the angular part of the classical action.

SDPs for solving the quantum ground state problem

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The Institute of Photonic Sciences

We report on methods to solve the quantum ground state problem with semi-definite programming techniques based on the NPA-hierarchy in spin and fermionic systems.

The Symmetric Extendability Problem

Joel Klassen
The Institute for Quantum Computing Waterloo

The symmetric extendability problem is an instance of a quantum marginal problem. It asks: Given a set of identical reduced density matrices living in overlapping Hilbert spaces, does there exist a global symmetric state compatible with these reduced density matrices. This problem is an adaption of an old problem in quantum chemistry called the N-representability problem. It has broad applicability in quantum information theory.

Reduced Density Matrices in Quantum Chemistry

Arseny Kovyrshin
ETH Zürich

The role of the 1- and 2-order RDM's in Quantum Chemistry will be discussed.

Current Correlations from a Mesoscopic Anyon Collider

Ivan Levkivskyi
ETH Zürich

Fermions and bosons are fundamental realizations of exchange statistics, which governs the probability for two particles being close to each other spatially. Anyons in the fractional quantum Hall effect are an example for exchange statistics intermediate between bosons and fermions. We analyze a mesoscopic setup in which two dilute beams of anyons collide with each other, and relate the correlations of current fluctuations to the probability of particles excluding each other spatially. While current correlations for fermions vanish, negative correlations for anyons are a clear signature of a reduced spatial exclusion as compared to fermions.

Density functionals with the help of matrix product states

Michael Lubasch
University of Oxford

In the context of strongly correlated fermions on a one-dimensional lattice, we propose to use matrix product states for the construction of density functionals. Focussing on the exchange-correlation energy, we construct a functional that includes the local density approximation and improves systematically upon it.

Topology of configuration space for indistinguishable particles on tree graphs

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We outline a procedure of computing homology groups over integers for configuration spaces of particles on tree graphs. This work is inspired by a paper of J. M. Harrison, J. P. Keating, J. M. Robbins and A. Sawicki (Commun. Math. Phys, 33(3), 1293-1326), where the first homology group for particles on a simple graph has been calculated. This in turn allowed to prove the existence of anyon statistics for particles on simple graphs. Firstly, we describe a construction of the configuration space and show that it is a cubic complex. Regarding a tree graph as a set of star graphs, wel show how to construct a basis of homology group of any order using only a basis of the first homology group of a star graph. Such an approach proves to be more effective than the sole use of the discrete Morse theory, which has been applied in this context. This is a preliminary result of a joint project with Adam Sawicki, which aims to compute homology groups of the configuration space for any simple graph.

Mapping the electronic changes in MgO-nanoclusters using quantum mechanics: Effects on HOMO-LUMO gaps and Coulomb properties by symmetry and surface alterations

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Advanced materials and surfaces are key components in nanotechnology and are applied given their magnetizable and spintronic properties, high-frequency scattering, and other features attributed to nanoelectronics and nanomagnetic functionalities. Earth oxides are a group of materials with catalytic effects in nanocrystalline formats, and electronic field effects with promising applications in nanomagnetics and in memory processing units. However the electronic properties og MgO clusters, when subjected to small changes in the surface are not fully mapped in detail, and as nanoclusters have different properties from bulk material, the electronic character of MgO clusters in large, small and irregular forms are hereby studied using density functional theory. Initial results show that the Coulomb energy is positive and close to zero for small MgO clusters and vanishes the larger the MgO grow. However, this pattern is changed when MgO assumes the exact cubic Td geometry composed of 32 MgO units, which gains a significant positive Coulomb energy at the expense of the kinetic energy and experiences a reduction in HOMO-LUMO gap. The removal of single MgO units from the cluster surface affects the particles in an interesting fashion, leading to expansions of the lattice and also a reduced H-L gap. The charge landscape of the clusters and the magnetization properties are furthermore affected, delineating that potential pathways of erosion of MgO materials affect not only structural formation, but also increase reactivity and alter magnetizability.

Topological Edge States are Monogamous

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We propose an alternative approach to assessing topologically induced edge states in free and interacting fermionic systems. We do so by focussing on the fermionic covariance matrix of the ground state. This matrix is often tractable either analytically or numerically and it captures the relevant correlations. By invoking the concept of monogamy of entanglement we show that highly entangled states supported across a system bi-partition are largely disentangled from the rest of the system. We then define an entanglement qualifier that identifies the presence of topological edge states in terms of singular values of the covariance matrix. We demonstrate the versatility of this qualifier by applying it to free and interacting fermionic topological systems.

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On the computational limits of a full quantum mechanical treatment for few-body systems

Andrea Muolo
ETH Zürich

The difficult aspects of our pre-Born-Oppenheimer theory with respect to computational efficiency are discussed.

Exchange statistics on graphs

Adam Sawicki
University of Bristol

We develop a full characterization of abelian quantum statistics on graphs. We explain how the number of anyon phases is related to connectivity. For 2-connected graphs the independence of quantum statistics with respect to the number of particles is proven. For non-planar 3-connected graphs we identify bosons and fermions as the only possible statistics, whereas for planar 3-connected graphs we show that one anyon phase exists. Our approach also yields an alternative proof of the structure theorem for the first homology group of n-particle graph configuration spaces.

Active Orbital Space Selection Based on Density Matrices

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Quantum-chemical multi-configurational methods allow for a calculation of qualitatively correct wave functions for molecules with close-lying frontier orbitals. This class of methods, however, requires the manual selection of a subset of so-called active orbitals within which all possible configurations are considered. A poor choice of this subset leads to the exclusion of important configurations and therefore even qualitatively wrong results. Currently, these active orbitals are selected based on empirical rules[1] or natural orbital occupation numbers obtained from the one-particle density matrix of a precedent calculation.[2] We propose selection criteria that additionally take entropy based orbital entanglement measures into account.[3] These entanglement measures are calculated from the one- and two-orbital reduced density matrices (1-, 2-oRDMs).[4] The density matrix renormalization group algorithm (DMRG) allows for an efficient approximation of the 1- and 2-oRDM from partially converged calculations. This and the ability of DMRG to handle active orbital spaces of up to one-hundred orbitals around the Fermi level enable the automated identification of a set of active orbitals for a converged calculation. Here, we present results obtained with this approach for challenging molecules such as oxo-Mn(salen) and Cu2O22+. With the protocol presented here we overcome the tedious and error prone active orbital selection step in multi-configurational calculations.

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Lagrange method based on natural orbitals

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A Lagrange function is proposed to optimise the energy directly in the basis of natural orbitals.