FRI 2: Many-Body Quantum Dynamics III

Time: Friday 10:45–12:15 Location: ZHG002

FRI 2.1 Fri 10:45 ZHG002

Geometric speed limit of state preparation and curved control spaces — Maximilian Goll[1,2] and •Robert H. Jonsson[2] — [1]Freie Universität Berlin, Germany — [2]Nordic Institute for Theoretical Physics, Stockholm University, Sweden

The preparation of quantum many-body systems faces the difficulty that in a realistic scenario only few control parameters of the system may be accessible. In this context, an interesting conjecture was put forward by Bukov et al. in 2019, that the minimal length of any accessible state preparation protocol, as measured by the Fubini-Study metric, may lower bound the integrated energy fluctuation during any state preparation protocol.

We show that the conjecture holds if the accessible parameter space has no extrinsic curvature, when embedded into the space of all dynamically accessible states. However, we construct counter examples to the general form of the conjecture for qubits and harmonic oscillators.

[1] arXiv:2504.15175

FRI 2.2 Fri 11:00 ZHG002

Quantum phase transitions and collective excitations in long-range interacting spin XX models with superconducting qubits — •Benedikt J.P. Pernack, Mikhail V. Fistul, and Ilya M. Eremin — Theoretische Physik III, Ruhr-Universität Bochum, Bochum 44801, Germany

We investigate the emergence of collective quantum phases in coherent networks of superconducting qubits described effectively by interacting spin XX models with both short- and long-range couplings, subject to tunable local longitudinal and transverse magnetic fields. The spin interactions are engineered via the direct embedding of π-Josephson junctions in dissipationless transmission lines, enabling precise control over the interaction range and local field strengths [1]. Using advanced numerical techniques, including density matrix renormalization group (DMRG) analysis, we map out the phase diagram and identify quantum phase transitions between distinct ground states. Analytically, we employ a hard-core boson approach to characterize the ground state properties, order parameters, and the spectrum of Bogoliubov collective modes. Our results reveal a rich landscape of quantum phases, including paramagnetic, compressible superfluid, and weakly compressible superfluid states, and provide insight into the interplay between interaction range, local fields, and collective excitations in engineered quantum systems.

[1] B.J.P. Pernack, M.V. Fistul, I.M.Eremin, Phys. Rev. B 110, 184502 (2024)

FRI 2.3 Fri 11:15 ZHG002

Computational fluid dynamics simulation of dipolar gases in the hydrodynamic regime — •Michael Mayle[1], Reuben R. W. Wang[2,3], and John L. Bohn[4] — [1]Fakultät Angewandte Mathematik, Physik und Allgemeinwissenschaften, Technische Hochschule Nürnberg Georg Simon Ohm, Nürnberg, Germany — [2]ITAMP, Center for Astrophysics | Harvard & Smithsonian, Cambridge, Massachusetts 02138, USA — [3]Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA — [4]JILA, NIST, and Department of Physics, University of Colorado, Boulder, Colorado 80309, USA

In a recent theoretical effort, a hydrodynamic model of ultracold, but not yet quantum condensed, dipolar gases has been derived. Within this model, the dipolar scattering results in an anisotropic viscosity tensor. Effects of the anisotropy have been predicted to be observable in the weltering motion, i.e., the collective oscillations of a dipolar Fermi gas, as well as in its acoustic behavior.

In this contribution, we approach dipolar fluids from a computational fluid dynamics (CFD) perspective. To this end, previously derived analytic expressions of the anisotropic viscosity tensor are implemented in the finite-element software COMSOL Multiphysics. This allows us to investigate a whole spectrum of fluid flow situations but now including the inherent anisotropy of dipolar scattering. We present first results of such CFD simulations with an emphasis on effects attributable to the special characteristics of the anisotropic viscosity tensor.

FRI 2.4 Fri 11:30 ZHG002

Fully numerical Hartree-Fock calculations for atoms and small molecules with quantics tensor trains — •Paul Haubenwallner and Matthias Heller — Fraunhofer Institut für Graphische Datenverarbeitung IGD, Darmstadt, Deutschland

We present a fully numerical framework for the optimization of molecule-specific quantum chemical basis functions within the quantics tensor train format using a finite-difference scheme. The optimization is driven by solving the Hartree*Fock equations (HF) with the density-matrix renormalization group algorithm on Cartesian grids that are iteratively refined. In contrast to the standard way of tackling the mean-field problem by expressing the molecular orbitals as linear combinations of atomic orbitals (LCAO) our method only requires as much basis functions as there are electrons within the system. Benchmark calculations for atoms and molecules with up to ten electrons show excellent agreement with LCAO calculations with large basis sets supporting the validity of the tensor network approach. Our work therefore offers a promising alternative to well-established HF-solvers and could pave the way to define highly accurate, fully numerical, molecule-adaptive basis sets, which, in the future, could lead to benefits for post-HF calculations.

FRI 2.5 Fri 11:45 ZHG002

Long-range polarization models for reactive molecular systems. — •Shuran Xu and Stefan Ringe — Department of chemistry, Korea University, Seoul, Republic of Korea.

The combination of the molecule-based many-body expansion (MBE) with machine learning interatomic potentials (MLIP) has proven highly potent in generating surrogate potential energy surfaces for fast computational sampling of condensed phases. Key to accurate MBE-MLIP potentials is an accurate description of long-range electrostatics which requires the definition of element-specific fixed atomic parameters such as atomic charges and polarizabilities. In the case of reactive systems, such a treatment falls short due to significant charge transfer generating atomic environment-dependent atomic charges and polarizabilities. In this work, we systematically investigate this problem at the example of protonated water clusters and discuss possible solution strategies from Thole-type polarization models up to MBE-corrected models.

FRI 2.6 Fri 12:00 ZHG002

Role of many-body electronic structure effects on carbon monoxide surface distribution and dynamics on copper — •Seungchang Han and Stefan Ringe — Korea University, Seoul, Republic of Korea

Electrochemical CO2 reduction offers a promising and sustainable approach to producing valuable chemicals and fuels. Copper (Cu) stands out as the sole catalyst capable of yielding substantial quantities of higher reduced products such as ethylene, ethanol, and methane. The complex nature of the active site environment, including facet, site, and coverage dependencies of the central carbon monoxide (CO) intermediate, is known to influence product selectivity significantly. To investigate these adsorption phenomena and their energetic profiles, studies often use the Perdew-Burke-Ernzerhof (PBE) functional based on the generalized gradient approximation (GGA). Although widely used, this approach relies on error compensation, which can limit its applicability to systems for which the error is unknown. It also leads to an inconsistent prediction of adsorption trends across different surface facets and adsorption sites. Applying many-body corrections based on the random phase approximation (RPA) has been shown to improve the prediction of facet- and site-dependent stability significantly. In this study, we investigate the initial relationships between facet and site dependencies that affect adsorption energies, incorporating results derived from the RPA. Additionally, we elucidate coverage-dependent adsorption energy trends to deepen understanding of surface interactions.