SFB 1481
Sparsity and
Singular Structures

RWTH AACHEN UNIVERSITY

Workshop: Analysis and Simulation of Quantum and Molecular Systems

General Information

Time: 26th to 29th May 2026

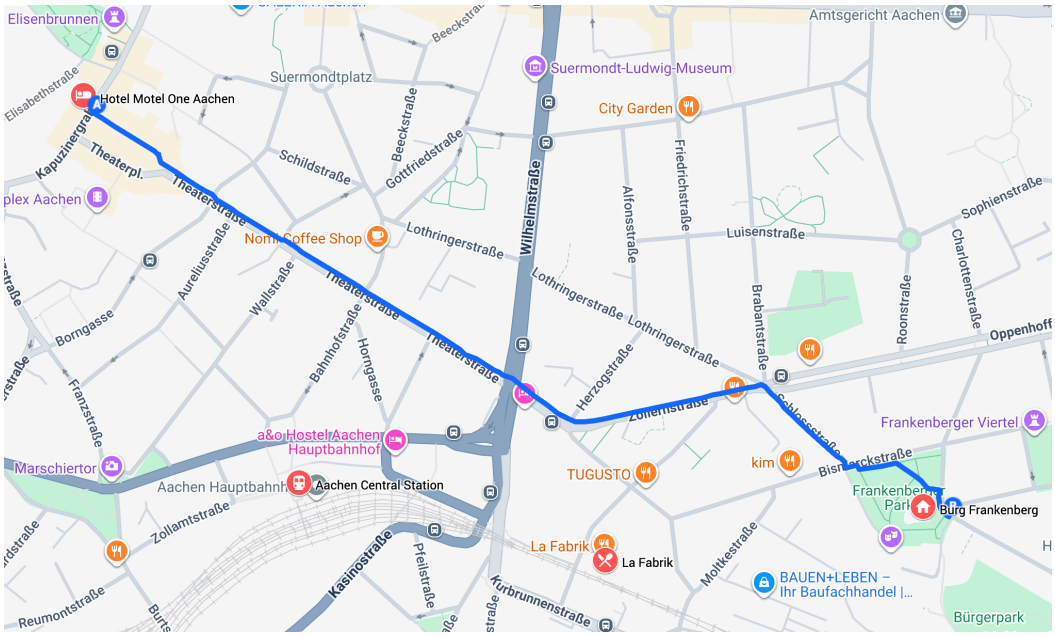
Venue: Burg Frankenberg, Goffartstraße 45, 52066 Aachen

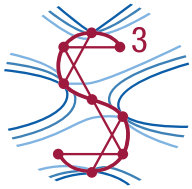
Workshop Hotel: Hotel Motel One, Kapuzinergraben 6-10, 52062 Aachen

Workshop Dinner: La Fabrik, Bachstraße 20, 52066 Aachen, Thursday (May 28th) at 19:00

Arriving at Aachen: We recommend arriving at Aachen Central Station by train. For international travelers, we recommend arriving at one of the nearby international airports (e.g. Frankfurt, Düsseldorf, Cologne or even Amsterdam) and then taking a train to Aachen.

Public Transport: Line 7/27/37 connect Hotel Motel One and Burg Frankenberg (Elisenbrunnen & Schlossstrasse); Line 11/21/51/SB63 connect Hotel Motel One and Aachen Central Station (Elisenbrunnen & Aachen Hbf).





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Workshop Schedule

Tuesday, May 26

Time	Event / Speaker & Title
9:00-9:30	Registration
9:30-9:40	Opening
9:40-10:30	Guido Falk von Rudorff: Perturbative Quantum Chemistry
10:30-11:10	Coffee Break
11:10-11:40	Alfred Kirsch: The thermodynamic limit of the one-body Green's function of quantum lattice systems.
11:40-12:10	Xiaoying Dai: Orthogonality Preserving Methods for Electronic Structure Calculations
12:10-14:00	Lunch Break
14:00-14:50	Mario Berta: Quantum Gibbs Samplers
14:50-15:20	Mi-Song Dupuy: Randomised sketching for tensor train rounding: application to quantum chemistry
15:20-16:00	Coffee Break
16:00-16:30	Julian Rincon: Operational characterization of entanglement–magic structure via magic-protected entanglement
16:30-17:00	Christian Schilling: Quantum Information Perspective on the Ground State Problem: What is Electron Correlation?
17:00	Reception

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Wednesday, May 27

Time	Event / Speaker & Title
9:00-9:50	Virginie Ehrlacher: Computing Dynamical Quantum Optimal Transport for Quantum Chemistry
9:50-10:20	Thiago Carvalho Corso: Density functional theory for one-dimensional systems: from Kohn-Sham to Kantorovich potentials
11:00-11:30	Noé Blassel: Shape-sensitive spectral asymptotics for overdamped Langevin dynamics
11:30-12:00	Harry Yserentant: The Laplace equation, measure concentration, and an application to quantum theory
14:00-14:50	Muhammed Hassan: The Numerical Analysis of the Finite Temperature Kohn-Sham LDA Pseudopotential Model for Perfect Crystals
14:50-15:20	Fabian Faulstich: A Robust and Efficient Gauge-Invariant Coupled-Cluster Solver
16:00-16:30	Jonas Beck: Interpolation Methods for Coupled Cluster
16:30-17:00	Shengyue Wang: A quasi-orthogonal iterative method in electronic structure calculations

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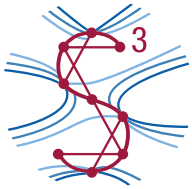
Thursday, May 28

Time	Event / Speaker & Title
9:00-9:50	Christoph Ortner: Inverse Problems Perspective on ML Surrogates for Particle Systems
9:50-10:20	Michael Herbst: Algorithmic differentiation (AD) in plane-wave DFT
11:00-11:30	Laura Grazioli: Differential geometry for excited states: a unified framework
11:30-12:00	Jonas Püschel: Energy-adaptive Riemannian optimization for Kohn-Sham type problems: an overview
14:00-14:50	Aihui Zhou: A Parallel Orbital-updating Approach for Electronic Structure Calculations
14:50-15:20	Antoine Levitt: Singular Brillouin zone integrals and spectral properties of periodic crystals
16:00-16:30	Camille Hernandez: Efficient construction and explicit dimensionality of Lie group-equivariant and permutation-invariant spaces
16:30-17:00	Gaspard Kemlin: Splitting methods for the Gross-Pitaevskii equation on the full space and vortex nucleation
19:00	Dinner



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Friday, May 29

Time	Event / Speaker & Title
9:00-9:50	Dante Kennes: Simulation of Light-Driven Quantum Matter
9:50-10:20	Andre Laestadius: A Non-Reflexive Moreau-Yosida Regularization for Density-Functional Theory
11:00-11:30	Yan Li: A Regularization Based Computational Method for the Quantum Incommensurate Problems
11:30-12:00	Clement Guillot: Low-complexity approximations with least-squares formulation of the time-dependent Schrödinger equation

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Titles and Abstracts

Perturbative Quantum Chemistry

Guido Falk von Rudorff

Understanding molecular properties across regions in chemical space requires methods that go beyond traditional one-by-one evaluations of individual systems. With "quantum alchemy", a perturbative approach, many diverse properties such as energies, orbital eigenvalues, electron densities, photoelectron circular dichroism parameters, protonation energies and more can be predicted for millions of related systems with a simple closed form expression. At heart, a Taylor or Padé approximant is built from the first low-order response functions of the property w.r.t. changes in the nuclear charges and geometry. End-to-end, this is typically five orders of magnitude cheaper than quantum chemistry methods of comparable accuracy.

Moreover, the closed-form expression of quantum alchemy models can be analysed particularly well: it affords a way to make black-box predictors such as quantum chemistry calculations or machine learning models interpretable. This becomes possible through a unique decomposition of a global property into n-body k-order effects of individual atoms or functional groups. This is demonstrated through case studies on photoelectron circular dichroism (PECD) and NMR chemical shifts, where quantum alchemy improves understanding of the drivers of physical properties. For energies, this decomposition unravels approximate symmetries which must hold true for all conceivable systems of certain structural properties, which can help machine learning models by reducing the dimensionality of the search space. We show how contributions in this expansion can be used for estimating the intrinsic dimensionality of physical properties, thus allowing to explain different machine learning data efficiency.

The thermodynamic limit of the one-body Green's function of quantum lattice systems.

Alfred Kirsch

In modern strongly-correlated computational methods such as Dynamical Mean-Field Theory (DMFT) or GW, the one-body Green's function plays a crucial role. Indeed, this reduced one-body quantity enables to infer some important system properties, such as the

ground state energy, the one-body reduced density matrix or the conduction properties, all at a moderate computational cost. However, apart from the setting of dilute gases that has been studied by Ruelle in the 1970s, the very definition of this object in the thermodynamic limit is not fully understood mathematically. In this presentation, I will present our approach to defining this object with full mathematical rigor, for the special case of quantum lattice systems. The formalism associated with these systems, based on uniformly hyperfinite algebras, offers useful tools for proving the existence (and uniqueness at high temperature) of the one-body Green's function. If time permits, I will then focus on a class of Anderson Impurity Models, which is of paramount importance for DMFT computations.

Orthogonality Preserving Methods for Electronic Structure Calculations

Xiaoying Dai

To obtain convergent numerical approximations without orthogonalization operations is of great importance in electronic structure calculations. In this talk, we will introduce an extended gradient flow based Kohn-Sham DFT model, for which we prove that the flow is orthogonality preserving and that the solution evolves to the ground state. With the help of the extended gradient flow based Kohn-Sham DFT model, we propose some iteration schemes for the discretized Kohn-Sham model, which are proved to preserve the orthogonality of the Kohn-Sham orbitals automatically. With our schemes, the iterative approximations are guaranteed to converge to the Kohn-Sham orbitals without any orthogonalization operations when the initial orbitals are orthogonal.

Quantum Gibbs Samplers

Mario Berta

Randomised sketching for tensor train rounding: application to quantum chemistry

Mi-Song Dupuy

Randomisation has emerged as a powerful approach in numerical linear algebra, enabling the design of efficient and scalable algorithms for large-scale computations. In this talk, we explore the role of randomisation in the context of tensor trains, a powerful tensor decomposition technique widely used to compute low-lying states in solid-state physics and many-body quantum chemistry. We propose the TTStack sketch, interpolating between the Gaussian TT sketch and Kathri-Rao sketches. We are able to prove linear-scaling injection properties, improving the tensor-train rounding process, particularly for high-order tensors. The efficiency and accuracy of these randomised methods are illustrated through applications in quantum chemistry.

Operational characterization of entanglement–magic structure via magic-protected entanglement

Julian Rincon

Entanglement and nonstabilizerness ('magic') are widely regarded as key resources for quantum computation, yet their interplay in many-body states is not always captured by standard diagnostics. We introduce magic-protected entanglement as an operational characterization: it is the part of a state's entanglement that cannot be removed by any stabilizer (Clifford) processing. By construction, it quantifies the entanglement that survives optimal stabilizer preprocessing and thus serves as a diagnostic of nonlocal magic—highlighting correlations that remain even after stabilizer restructuring. This perspective motivates a resource-based separation between classes of states where magic is largely local and stabilizer processing can often simplify entanglement, and classes where entanglement is intrinsically stabilizer-resistant. We discuss implications for resource classification and for simulation of quantum many-body systems and quantum computing.

Quantum Information Perspective on the Ground State Problem: What is Electron Correlation?

Christian Schilling

Describing strongly interacting electrons is one of the crucial challenges in the modern quantum sciences. A comprehensive solution to this electron correlation problem would simultaneously exploit both the pairwise interaction and its spatial decay. By taking a quantum information perspective, we explain how this structure of realistic Hamiltonians

gives rise to two conceptually different notions of correlation and entanglement [1]. The first one describes correlations between orbitals [2] while the second one refers more to the particle picture [3]. We illustrate those two concepts of orbital and particle correlation and present measures thereof. In particular, we show how they provide a deeper understanding of chemical bonding [4]. Furthermore, we propose a systematic approach to enhancing wave function methods for strongly correlated electron systems [5,6], relevant to both classical and quantum computing. Altogether, these insights highlight the deep connection between quantum information and quantum chemistry, demonstrating fruitful synergies that can foster the second quantum revolution.

[1] D.Aliverti-Piuri, K.Chatterjee, L.Ding, K.Liao, J.Liebert, C.Schilling, Faraday Discuss. 254, 76 (2024)

[2] L.Ding, S.Mardazad, S.Das, S.Szalay, U.Schollwöck, Z.Zimborás, C.Schilling, J. Chem. Theory Comput. 17, 79 (2021)

[3] D. Aliverti-Piuri, J. Liebert, C. Schilling, forthcoming

[4] L.Ding, E.Matito, C.Schilling, arXiv:2501.15699, to appear in Nature Commun.

[5] L.Ding, S.Knecht, C.Schilling, J. Phys. Chem. Lett. 14, 11022 (2023)

[6] K.Liao, L.Ding, C.Schilling, J. Phys. Chem. Lett. 15, 6782 (2024)

Computing Dynamical Quantum Optimal Transport for Quantum Chemistry

Virginie Ehrlacher

(joint work with Geneviève Dusson and Etienne Obermeyer) Quantum optimal transport provides a geometric framework for comparing and interpolating density matrices, which play the role of non-commutative probability measures in quantum mechanics and quantum chemistry. In this talk, I will focus on a dynamical formulation of quantum optimal transport inspired by the Benamou–Brenier formulation of classical optimal transport and by the Carlen–Maas construction of transport metrics on density matrices.

I will present a numerical method for computing quantum optimal transport geodesics between finite-dimensional density matrices. The method combines a time-discretized continuity equation with a sequential quadratic programming strategy, an interior-point

logarithmic barrier, and a regularization procedure designed to handle positive semidefinite and low-rank matrices. This is particularly relevant in quantum-chemistry settings, where one-particle density matrices arise naturally and are often low-rank. The computed geodesics are visualized through their integral kernels and diagonal densities, allowing a qualitative comparison with classical optimal transport and with reference curves obtained from electronic-structure computations.

Density functional theory for one-dimensional systems: from Kohn-Sham to Kantorovich potentials

Thiago Carvalho Corso

In this talk we present some recent developments on the mathematical foundations of density functional theory for one-dimensional systems. We start by presenting a complete solution of the v-representability question for arbitrary interaction potentials. We then discuss the regularity of the Levy-Lieb constrained search functional and the adiabatic density-to-potential map. Finally, we present some results on the asymptotics of the adiabatic potential in both the weakly interacting limit, where we recover the Görling-Levy perturbation formula, and in the strongly interacting limit, where we recover the Kantorovich potential.

Shape-sensitive spectral asymptotics for overdamped Langevin dynamics

Noé Blassel

So-called accelerated dynamics methods (Hyperdynamics, TAD, Parallel Replica) rely on local metastability to accelerate the sampling of long, asymptotically unbiased trajectories of molecular systems. These techniques rely on a separation of timescales assumption within well-chosen subsets of the configurational space called metastable states. Given a configurational domain Ω, this assumption states that the system started in Ω will quickly reach a local equilibrium inside Ω, much faster than the expected exit time from this local equilibrium. The validity of this assumption strongly relies on appropriate definitions of the state Ω. In the dynamical setting of reversible elliptic diffusions, one can interpret this separation of timescales quantitatively, as a ratio of eigenvalues $\frac{\lambda_2(\Omega)

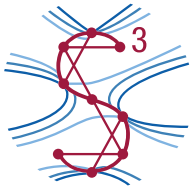
\lambda_1(\Omega)}{\lambda_1(\Omega)}$, where the eigenvalues are those of the infinitesimal generator of the evolution semigroup, endowed with Dirichlet boundary conditions on $\partial\Omega$. Motivated by the question of how to maximize the separation of timescales with respect to Ω, we study low-temperature asymptotics of these eigenvalues for families of domains $(\Omega_{\alpha,\beta})_{\beta>0}$, jointly parametrized by the inverse temperature parameter β, and a shape-design parameter α. This study is equivalent to that of semiclassical asymptotics of the Witten Laplacian in presence of a h-dependent Dirichlet boundary. Under suitable geometric conditions, we compute previously unknown spectral asymptotics, which are only sensitive at first-order to β and the design parameter α, resolving the shape of sharp transitions in the spectrum of the Witten Laplacian, when the boundary of the domain crosses critical points of the potential. As a byproduct, these results allow to define asymptotically optimal metastable states with respect to the efficiency of the Parallel Replica algorithm, within the class of domains satisfying our geometric assumptions.

The Laplace equation, measure concentration, and an application to quantum theory

Harry Yserentant

The potential in the electronic Schrödinger equation depends on the distances between the electrons. The electronic wave functions therefore possess singularities at the points in R3N where two of the considered N electrons meet. Orbital-based approaches are not well suited to resolve these singularities. It is therefore an attractive idea to use ansatz functions that explicitly depend on the differences of the particle positions. The talk will present an approach that allows to treat such ansatz functions in a tensor framework. The idea is to represent the wave functions as traces of even higher-dimensional separable functions. The main tool is a fast iterative method for solving Laplace-like equations with right-hand sides that themselves are traces of such functions. The amazing properties of this iterative method are based on a measure concentration effect.

H. Yserentant, An iterative method for the solution of Laplace-like equations in high and very high space dimensions; Numerische Mathematik (2024) 156:777–811 expanded and extensively revised version: arXiv:2403.00682 [math.NA]



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The Numerical Analysis of the Finite Temperature Kohn-Sham LDA Pseudopotential Model for Perfect Crystals

Muhammed Hassan

A Robust and Efficient Gauge-Invariant Coupled-Cluster Solver

Fabian Faulstich

The coupled-cluster (CC) equations are most frequently solved by a fixed-point (FP) iteration. When CC equations are formulated in a different gauge such as in atomic orbital CC theory, a simple FP iteration can be slow to converge or diverge completely. A remedy is an energy level shift and a direct inversion of iterative subspace (DIIS), which motivate quantum chemistry packages to include their own equation solvers. However, developing and maintaining dedicated solvers to perform consistently across variants of CC theories costs significantly more effort than using an off-the-shelf solver, and there is little theoretical reason to expect an advantage. On the contrary, Chao et al. [Frontiers in chemistry 8 (2020): 590184.] showed an opposite wall-time advantage in canonical CC using a standard preconditioned Newton Krylov (PNK) method. In this study, we generalize the preconditioner to arbitrary gauges by replacing the energy denominator with GMRES, which removes the need for an energy level shift and makes the iteration count of PNK gauge-invariant. We therefore argue that PNK consistently outperforms fine-tuned FP iteration across different gauges.

Interpolation Methods for Coupled Cluster

Jonas Beck

The coupled cluster method is widely regarded as one of the most accurate approaches for calculating ground-state energies. It provides a systematically improvable and size-consistent framework, although this accuracy comes at a high computational cost. This limitation becomes particularly significant when many coupled cluster calculations must be performed across different nuclear geometries, such as during geometry optimization. Unfortunately, straightforward interpolation across geometries cannot reliably reduce the number of calculations, as orbital energy crossings at the Hartree–Fock level make such interpolation problematic.

In this talk, a framework to circumvent these challenges is presented, along with an introduction to a polynomial-like interpolation method. Furthermore, error estimates of the interpolation, the associated computational difficulties, and possible solutions are discussed.

A quasi-orthogonal iterative method in electronic structure calculations

Shengyue Wang

Computing many mutually orthogonal eigenvectors is a core requirement in electronic structure simulations. Traditional numerical methods rely on explicit orthogonalization, creating computational bottlenecks and limiting scalability for large-scale systems. Recent orthogonality-preserving approaches avoid this step but require orthogonal initial data and lack robustness against numerical perturbations. To address these limitations, we propose a quasi-orthogonal iterative method. This scheme eliminates explicit orthogonalization and orthogonal initial conditions. Iterates inherently maintain quasi-orthogonality and asymptotically converge to the Stiefel manifold. Numerical experiments demonstrate robustness against perturbations and high-precision numerical orthogonality.

Inverse Problems Perspective on ML Surrogates for Particle Systems

Christoph Ortner

Machine learning surrogates for many-body particle interactions have become a mainstream modelling tool for materials and molecular modelling over the past few years. Two paradigm examples are ML interatomic potentials (MLIPs) and ML tight binding (MLTB) models. I will briefly review a unifying many-body expansion framework for efficient and physics-informed parameterization in those contexts. The natural question arises "what object is being learned", or conversely, "what data is required to learn the object of interest" (e.g., energy, hamiltonian operator)? For MLTB, i.e. learning a hamiltonian, this is related to the classical ill-posed spectral inverse problem: it is impossible to identify a Hamiltonian operator from its spectrum. I will show how to construct additional quantum mechanical observables to augment the spectrum from which

the Hamiltonian can be uniquely recovered (up to a gauge). The result suggests a new approach to learning MLTB models. (joint work with Dexuan Zhou, Huajie Chen and Bernie Hsu).

Algorithmic differentiation (AD) in plane-wave DFT

Michael Herbst

Reliable algorithmic differentiation techniques offer great promise for the inverse design of materials, improved density-functional theory (DFT) models or the propagation of uncertainties in first-principle modelling: three topics of current interest with direct consequences to improve accuracy and reliability of materials simulations. In recent work [1] we equipped the density-functional toolkit (DFTK, https://dftk.org) --- our in-house Julia-based DFT code --- with algorithmic differentiation capabilities. I will present some of the required algorithmic developments to robustly solve the arising linear response equations and discuss the perspectives of this framework following examples such as the inverse design of a semiconductor band gap, the learning of exchange-correlation functional parameters, or the propagation of DFT parameter uncertainties to relaxed structures.

[1] N.F. Schmitz, B. Ploumhans, M. F. Herbst. npj Computational Materials 12, 6 (2025). DOI https://doi.org/10.1038/s41524-025-01880-3

Differential geometry for excited states: a unified framework

Laura Grazioli

In exact theory, excited states correspond to higher-energy solutions of the Schrödinger equation. For an exact wave function, these states appear as saddle points of the electronic energy functional, and for a Morse function they can be classified by the number of negative eigenvalues of the Hessian matrix—the nth excited state having Morse index n. When the linear Schrödinger equation is solved within a nonlinear wave-function parameterization, however, spurious critical points may emerge.

To address this, we develop manifold-constrained saddle-point search algorithms defined on the manifold of admissible electronic states. These methods target saddle points of fixed index k. A global exploration of the energy landscape is first performed using stochastic algorithms adapted to Riemannian manifolds, to identify regions likely to contain saddle

points. Within these regions, local critical-point algorithms are then employed, relying on the Riemannian gradient and selected information from the Riemannian Hessian. A careful treatment of the underlying manifold geometry is essential in both stages, enabling the construction of stable algorithms for locating saddle points, which are naturally unstable.

In quantum chemistry, excited states are also commonly computed through linear response theory, which analyses the linearized dynamics around a stable ground state. Although linear response formulations exist for many variational theories, their derivations are often technically involved and rely on ad-hoc constructions. We provide a unified derivation for variational theories by exploiting the geometric structure of Kähler manifolds.

Both excited-state characterisations—saddle-point theory and linear response theory—are developed and applied first within Hartree–Fock theory, represented by a Grassmann manifold, and subsequently within Complete Active Space Self-Consistent Field (CASSCF) theory, represented by a flag manifold. A comparison of the results obtained by using manifold-constrained saddle-point search algorithm with those given by already established quantum chemical methods is also shown for test systems.

Energy-adaptive Riemannian optimization for Kohn-Sham type problems: an overview

Jonas Püschel

Kohn–Sham type problems form the computational core of density functional theory and give rise to large-scale, nonlinear eigenvalue problems whose accurate and efficient solution remains a central challenge in electronic structure calculations. In this talk, we provide an overview of energy-adaptive Riemannian optimization strategies for the numerical solution of Kohn–Sham type equations. This includes theoretical foundations like construction of the energy-adaptive metric for the different Riemannian manifolds, practical aspects like the gradient calculation and general choice of parameters, and challenges and limitation of energy-adaptive approaches. The talk concludes with an illustration of practical performance in numerical experiments.

A Parallel Orbital-updating Approach for Electronic Structure Calculations

Aihui Zhou

In this presentation, we will introduce a parallel orbital-updating approach for electronic structure calculations. This approach is based on our understanding for the single-particle equations of independent particles that move in an effective potential. With this approach, the solution of the single-particle equation is reduced to some solutions of independent linear algebraic systems and a small scale algebraic problem, for instance. This approach can be applied to not only Galerkin discretizations but also Ritz discretizations. It is demonstrated by theory and numerical experiments that this approach is supercomputer-firendly and efficient for electronic structure calculations for a class of molecular systems. This presentation is based on joint works with Xiaoying Dai, Xingao Gong, Yan Li, Zhuang Liu, Yan Pan, Bin Yang, Xin Zhang, and Jinwei Zhu

Singular Brillouin zone integrals and spectral properties of periodic crystals

Antoine Levitt

The computation of spectral properties (Green functions, densities of states...) of periodic crystals relies on singular integrals in momentum space. I will describe algorithms to compute these integrals, with applications to solid state physics.

Efficient construction and explicit dimensionality of Lie group-equivariant and permutation-invariant spaces

Camille Hernandez

Most of the physical properties of interest arising in molecular simulations exhibited certain symmetries, including Lie Group Equivariance and Permutation Invariance. In this presentation, we propose a practical construction of group-equivariant and group-equivariant and permutation-invariant multi-variable functions from the knowledge of a one-variable basis stable with respect to the group action. In particular, this construction avoids explicitly symmetrizing over permutations which significantly reduces the computational cost. In the special case of the groups SO(3) and SU(2), it allows us to compute the exact dimensionalities of the group-equivariant and group-equivariant and permutation-invariant spaces. We also present numerical simulations to show that the cost

of the proposed method scales linearly, which is way faster than other methods from the literature and can thus deal with a larger number of variables.

Splitting methods for the Gross-Pitaevskii equation on the full space and vortex nucleation

Gaspard Kemlin

In this talk, we prove the convergence in Zhidkov spaces of the first-order Lie-Trotter and the second-order Strang splitting schemes for the time integration of the Gross-Pitaesvkii equation with a time-dependent potential and non-zero boundary conditions at infinity. We also show the conservation of the generalized mass and the near-preservation of the Ginzburg-Landau energy balance law. Numerical accuracy tests performed on a one dimensional dark soliton corroborate our theoretical findings. We finally investigate the nucleation of quantum vortices in two experimentally relevant settings. This is joint work with Quentin Chauleur (Inria Lille).

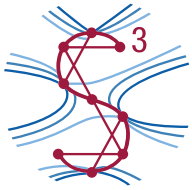
Simulation of Light-Driven Quantum Matter

Dante Kennes

Periodic electromagnetic fields provide a way to modify the effective behavior of quantum systems, opening the possibility of creating or controlling phases of matter away from equilibrium. A key question is how far this idea can be pushed before the drive simply heats the system and destroys the desired quantum correlations.

I will discuss this problem in a one-dimensional interacting quantum chain, studied using time-dependent density matrix renormalization group simulations directly in the infinite-size limit. The model has two familiar regimes: a gapless Luttinger liquid and an ordered charge-density-wave phase. By analyzing the real-time response to a periodic drive, the work shows how the ramp protocol, drive frequency, and initial phase of the system determine whether the driven state retains coherent quantum correlations or evolves toward an effectively thermal state.

The results illustrate both the analytical structure and numerical simulation challenges of driven quantum many-body systems, and connect naturally to broader questions in the control, stability, and simulation of quantum and molecular systems far from equilibrium.



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A Non-Reflexive Moreau-Yosida Regularization for Density-Functional Theory

Andre Laestadius

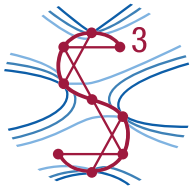
Standard density-functional theory faces a fundamental mathematical challenge: the universal functional is discontinuous on the natural non-reflexive Banach space $L^1 \cap L^3$. In this talk, I will elaborate on a non-reflexive formulation of Moreau-Yosida regularization that resolves this issue. This problem is interesting in its own right but is also motivated by approximation schemes that require a continuous density functional, such as neural network approximations.

A Regularization Based Computational Method for the Quantum Incommensurate Problems

Yan Li

Quantum incommensurate systems have attracted considerable interest from mathematicians and physicists because of their distinctive electronic, optical, and transport properties. However, due to the incommensurate nature, a rigorous mathematical understanding of the spectral properties and wavefunction behavior of the associated Schrödinger operators is still lacking, posing significant challenges to numerical computation and further understanding of the underlying physics for such systems. Based on a spectral analysis of the associated Schrödinger operators, we propose a regularization based computational method for incommensurate systems. Using our method, physical observables in incommensurate systems become well-defined and can be further computed efficiently. This method provides a novel and practical framework for analyzing and computing such systems.

Low-complexity approximations with least-squares formulation of the time-dependent Schrödinger equation



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Clement Guillot

We introduce a novel variational formulation for the time-dependent Schrödinger equation, showing that its solution can be uniquely characterized as the minimizer of a global space–time quadratic functional arising from a least-squares principle. The least-squares functional is constructed by reformulating the evolution problem using free dynamics—similarly to scattering theory—and is defined within a space with well-established regularity properties in both space and time. The functional comprises two terms: the first measures the L^2 norm of the residual for the twisted evolution equation, while the second enforces the initial condition similarly to a penalty term. We prove that this framework is applicable to the many-body Schrödinger equation with Coulomb singularities by using results from Kato's smoothing theory. Beyond providing a foundation for numerical schemes, this formulation enables the construction of dynamical low-rank approximations based on a variational principle distinct from the classical Dirac–Frenkel approach, and for which global-in-time existence of solutions can be established. In particular, combining the approach with a greedy algorithm, we derive a numerically stable procedure to compute an approximation of the solution as a sum of complex Gaussian wave packets. Since Gaussian wave packets efficiently represent high-dimensional functions with relatively few parameters, the approach remains computationally feasible even in high dimension. While the derivation of a priori bounds for such approximations remains open, our least square functional naturally yields easily computable a posteriori error bounds. We also investigate the possibility of combining this space-time formulation with an adaptive scheme.