Conference Booklet

Mathematical and Numerical Analysis of Electronic Structure Models

September 16-20, 2024

Welcome to the Manuel-conference!

Dear participant,
welcome to the fifth edition on the Mathematical and Numerical Analysis for Electronic Structure Models (MANUEL) conference. Previous editions in this conference were held in China, France and Germany:

- 2012: Beijing, China
- 2014: Berlin, Germany
- 2016: Roscoff, France
- 2019: Suzhou, China

The purpose of the conference is to bring together applied and computational mathematicians working on various aspects of electronic structure calculation which is subject to finding the state of the electrons for molecular systems.

Electronic structure calculation has many applications in computational chemistry, condensed matter physics, and material science and is related to many challenges of the 21st century, e.g., drug design, energy materials, and quantum computing. Electronic structure calculation comprises different methods, such as wave-function-based methods, Density Functional Theory (DFT), or Quantum Monte Carlo methods which are all derived from the electronic Schrödinger equation.

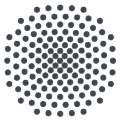
This conference addresses the mathematical community working on such problems which involves mathematical physics, analysis of PDEs, numerical analysis, numerical methods, and scientific computing but is also open to practitioners with a mathematical focus. The conference will be a platform to discuss the recent progress in the field and also intends to foster interactions between these different branches of Mathematics.
This booklet contains, for your convenience:

- a schedule with all the planned activities, academic or otherwise;
- many practical information;
- maps that will help you, reach the University of Stuttgart-Campus Vaihingen, navigate the campus itself and move around the city center of Stuttgart;
- and a detailed description of all the planned tutorials and talks.

Have a good time and enjoy the conference!

The local organizers

We kindly acknowledge financial support from:



Universität Stuttgart

SFB 1481
Sparsity and
Singular Structures

RWTH AACHEN
UNIVERSITY

DFG Deutsche
Forschungsgemeinschaft

SimTech

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Practical information

Wifi

The University of Stuttgart offers access to the Eduroam-network as well as the "uni-stuttgart-open"-network for the conference participants.

Public transportation

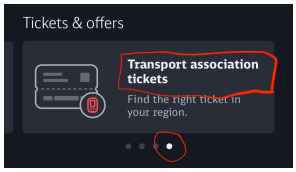
Important connections:

- Train station (Hauptbahnhof) to hotel: short walk. The hotel is next to the station. See also the maps below.
- Stuttgart airport to hotel: Take the tramway number U6 direction to "Gerlingen". Take the exit "Hauptbahnhof (Arnulf-Klett-Platz)".
- Hotel to University: S-Bahn lines 1,2,3 direction to Stuttgart-Vaihingen. Start at "Stuttgart Hbf (tief)" and take the exit "Universität".
- Stuttgart airport to university: Due to constructions, this is a bit trickier than usual. There are two options:
  - Take the bus X60 direction to "Bahnhof, Leonberg" with non-stop service to "Stuttgart, Universität". Runs only once an hour.
  - Take the tramway number U6 direction to "Gerlingen" and exit on "Hauptbahnhof (Arnulf-Klett-Platz)". Then, change to S-Bahn lines 1,2,3 (as above).
  - Take the bus replacement service "Bus S2E" to "Vaihingen, Stuttgart". Then change to the S-Bahn lines 1,2,3 (direction to Kirchheim, Schorndorf, Backnang).

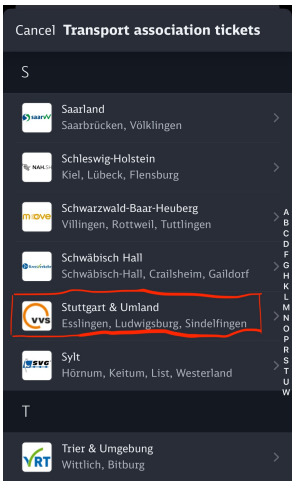
Tickets:

- Downloading the "DB Navigator App" is an easy solution to inform yourself about connections and to purchase electronic tickets.
- For navigating within Stuttgart and commuting to the university (does not include travel from and to the airport): buy a "1 zone ticket" of "Zone 1"
- For navigating within Stuttgart, commuting to the university and travel from and to the airport: buy a "2 zone ticket" of "Zones 1,2"
- Note that also a weekly pass is available for 30.00 and 35.80 Euro for "Zone 1" and "Zones 1,2' respectively, which might be worth if you stay the entire week. To purchase this ticket, select "Transport Association Tickets" under "Tickets & Offers" in the DB Navigator App and select the weekly ticket. Make sure you select the number of zones and the specific choice of zones correctly. The expressions might be called different if the default language in your mobile phone is different than English.

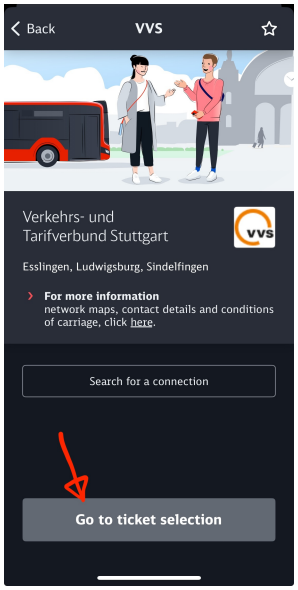
See Figure 1 for a graphical illustration.



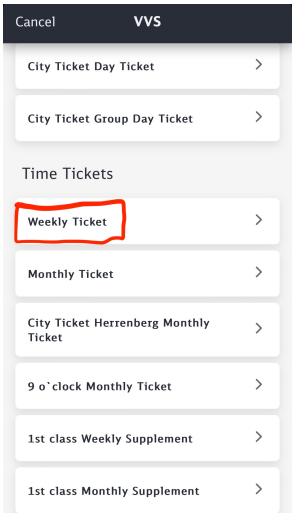
(a) Selection of local offers. Note, this is the forth tab under "Tickets & offers"



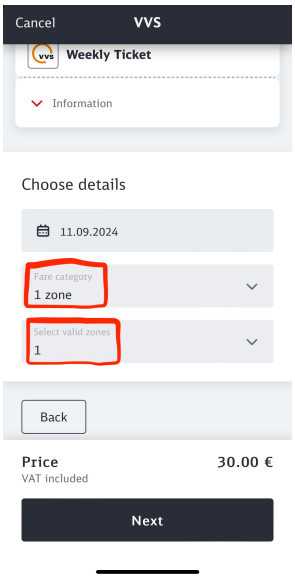
(b) Select "Stuttgart & Umland".



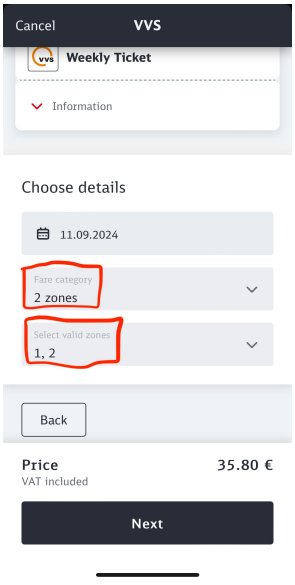
(c) Select "Go to ticket selection".



(d) Choose "Weekly Ticket" (or anything else if you want a single ticket or day pass for example).



(e) If you want 1 zone (Zone 1).



(f) If you want 2 zones (Zones 1,2)

Figure 1: Different steps to buy a weekly ticket for either zone 1 or zones 1,2 (inlcuding airport connections).

Eating

Lunch: With your conference-badge, you receive a free lunch at the canteen of the university (see map for its location). However, the organizers do not feel responsible for the quality of the food. Alternatives can be also found on Campus (see maps).

Dinner: Please find in the following a list of personal preferences of the organising committee for restaurants in the city of Stuttgart.

Swabian (local) food:

- Schellenturm, €€
- Sophie's brauhaus, brewery, €€
- Weinstube Kachelofen, €€
- Paulaner Stadtmitte, €€
- Gasthaus Bären: Swabian tacos (fusion), €€
- Alte Kanzlei, €€
- Stuttgarter Ratskeller, €€
- Goldener Adler, international and local food, reservation strongly recommended, €€€

Spanish:

- Jose y Josefina, reservation strongly recommended, €€€

Kebab:

- Alaturka, €
- Kebabhaus am Feuersee, €

Italian:

- Valle, €€
- Ristorante Goldoni, €€

Asian food:

- KuaiStyle, Authentic Chinese food & noodles, €€
- Tay Ho, Vietnamese, €
- Mikoto, Japanese/sushi, €€

Excursions:

There will be three groups guided by assistants that bring you to visit either

- Television-tower of Stuttgart (total elevation: 217 metres), price: 10.50€
- Mercedes-Benz museum, price: 16.00€
- Staatsgalerie (art), free entrance on Wednesdays

Unfortunately we can not cover any expenses occurring during the excursions.

Guided city tour:

There will be a free guided tour for us (shortly before the conference dinner) on Wednesday at 17:45. Please arrive on time. The meeting point is: Stuttgart Tourismus, Königstrasse 1a.

Conference dinner:

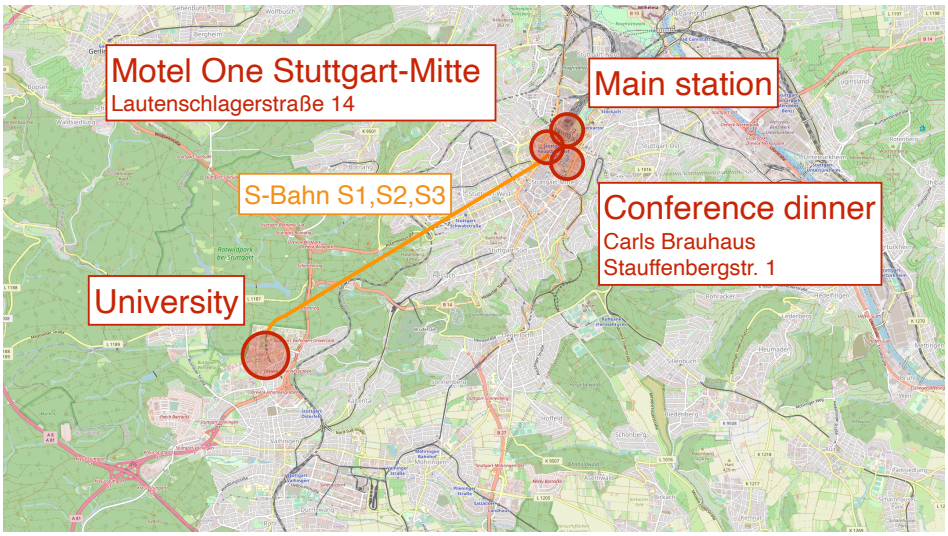
The conference dinner takes place on Wednesday 18.9. at Stauffenbergstraße 1 in Stuttgart, see the maps (below). The dinner starts at 19:00.

Schedule

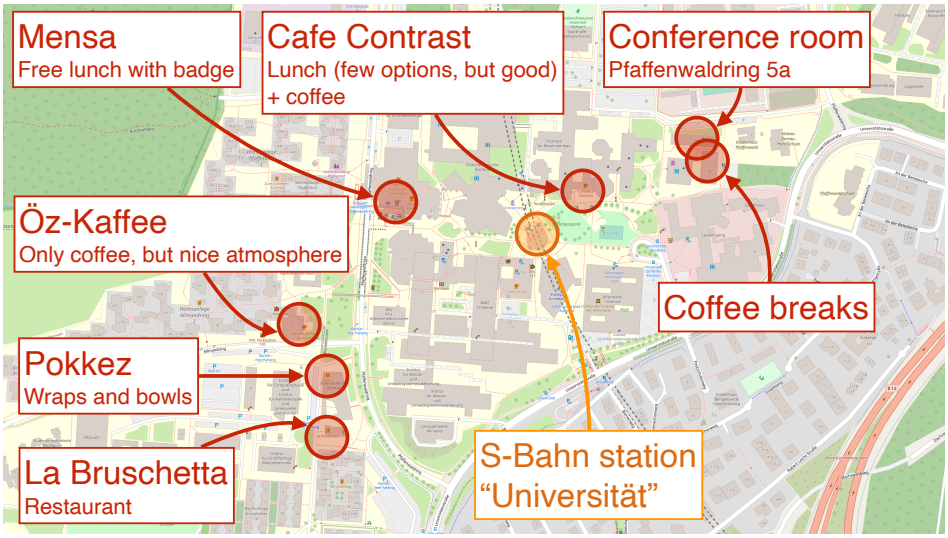
Conference Schedule: Mathematical and Numerical Analysis of Electronic Structure Models			
Date	**Time**	**Speaker**	**Title**
16.09.2024(Mo)		**Morning Session**	
	10:30-10:45	Opening	
	10:45-12:00	Antoine Levitt	Efficient Numerical Methods for Solving Eigenvalue Problems
	12:20-14:00	Lunch	
	14:00-15:15	Mi-Song Dupuy	Tensor (network) Methods in Electronic Structure
	15:15-15:45	Coffee Break	
	15:45-17:00	Agnieszka Miedlar and Paul Cazeaux	Fundamentals of Quantum Numerical Linear Algebra
17.09.2024 (Tu)		**Morning Session**	
	9:00-9:50	Filippo Lipparini	Grassmann Extrapolation as a Tool to Accelerate Ab-initio Molecular Dynamics
	9:50-10:20	Coffee Break	
	10:20-11:10	Salma Lahbabi	Density Functional Theory for Two Dimensional Homogeneous Materials
	11:10-12:00	Daniel Massatt	Momentum Space and Continuum Models of Incommensurate Bilayer 2D Materials
	12:00-13:30	Lunch	
	Afternoon Session		
	13:30-14:20	Huajie Chen	A Multilevel Method for Many-Electron Schrödinger Equations based on the Atomic Cluster Expansion
	14:20-15:10	Jürgen Dölz	On Uncertainty Quantification of Eigenvalue Problems
	15:10-15:40	Coffee Break	
	15:40-16:30	Virginie Ehrlacher	Numerical solution of eigenvalue Schrödinger problems using infinite-width two-layer networks
	16:30	Poster Session	
18.09.2024 (We)		**Morning Session**	
	9:00-9:50	Muhammad Hassan	On the Well-Posedness of the Discrete Coupled Cluster Equations
	9:50-10:40	Gero Friesecke	DMRG, New Post-DMRG-Methods, and Chemical Accuracy
	10:40-11:10	Coffee Break	
	11:10-12:00	Ali Alavi	Recent Progress with Transcorrelated Methodologies
	12:00-12:50	Fabian Faulstich	Exploring Ground and Excited States via Single Reference Coupled-Cluster Theory and Algebraic Geometry
	12:50-17:30	Excursions/Free	
	17:45-18:45	Guided City Tour	
	19:00	Social Dinner	
19.09.2024 (Th)		**Morning Session**	
	9:00-9:50	Michael Herbst	Reliable and Efficient Methods for Computing DFT Derivatives
	9:50-10:20	Coffee Break	
	10:20-11:10	Geneviève Dusson	Guaranteed Error Bounds for Electronic Structure Problems: Nonlinear Equations and Localized Basis Sets
	11:10-12:00	Xiaoying Dai	Mathematical Analysis and Numerical Approximations of Density Functional Theory Models for Metallic Systems
	12:00-14:00	Lunch	
	Afternoon Session		
	14:00-14:50	Paul Cazeaux	Ground State Preparation with Open Quantum System-inspired Algorithms
	14:50-15:40	Yingzhou Li	Optimal Orbital Selection for Ground States and Excited States Calculation on Classical and Quantum Computers
	15:40-16:10	Coffee Break	
	16:10-17:00	Di Fang	Time-dependent Hamiltonian Simulation: Quantum Algorithm and Superconvergence
20.09.2024 (Fr)		**Morning Session**	
	9:00-9:50	Tatjana Stykel	Riemannian Optimization Methods for Ground State Computations of Multicomponent Bose-Einstein Condensates
	9:50-10:40	Louis Garrigue	Coupling perturbation theory and the variational approximation
	10:40-11:10	Coffee Break	
	11:10-12:00	André Laestadius	Quantum-electrodynamical density-functional theory for the Dicke Hamiltonian
	12:00-12:50	Chao Yang	Numerical Methods for Simulating Non-equilibrium Quantum Dynamics
	12:50-15:00	Lunch	
	Afternoon Session		
	15:00-17:00	Individual Discussions and departure	

Maps

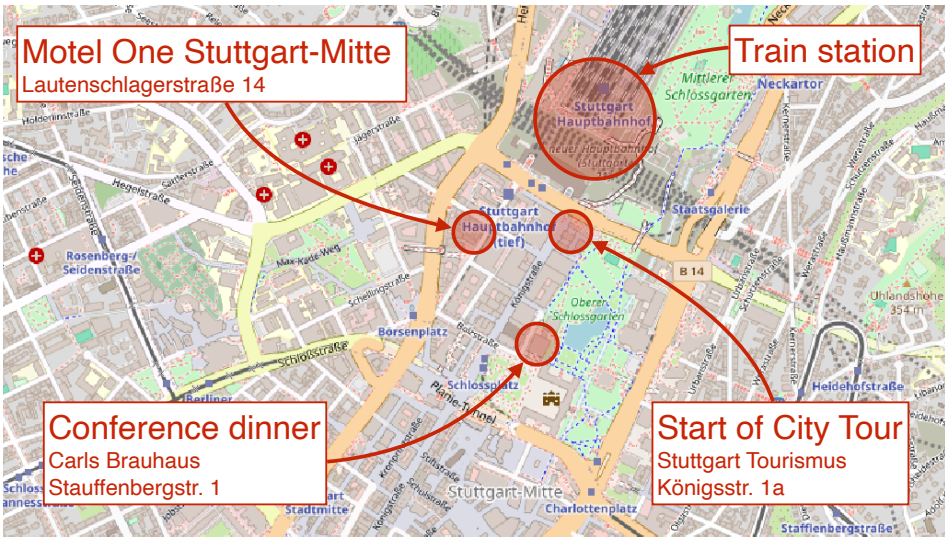
Global situation



University



Stuttgart City



Posters

First name	Family name	Poster title
Robert	Adam	A multidisciplinary undertaking: Challenges in the efficient implementation of internally contracted multireference coupled cluster methods
Vebjørn Hallberg	Bakkestuen	QEDFT: the Dicke Hamiltonian
Nibedita	Ghosh	Schwarz domain decomposition for COSMO models
Laura	Grazioli	Challenges in the Calculation of Molecular Energies and Properties in a Magnetic Field using Unitary Coupled-Cluster Theory
Clément	Guillot	A space-time variational formulation for the many-body electronic Schrödinger evolution equation
Johannes	Hauskrecht	Transcorrelated Embedding for Periodic Systems
Martin	Hermann	Riemannian Optimization for Multicomponent Bose-Einstein Condensates
Daniel	Kats	The mystery of the distinguishable cluster
Venera	Khoromskaia	Fast calculation of the excitation energies of molecules by using tensor-structured methods
Boris	Khoromski	Tensor methods for biomolecular modeling
Erwin	Lallinec	Benchmarking of numerical methods for density of states computation
Mathias	Oster	Coupled Cluster Theory: Towards an Algebraic Geometry Formulation
Anna	Paulish	Error propagation in statistical learning for data of heterogeneous quality
Elias	Polak	Learning correlation energy density functionals in real-space
Jonas	Püschel	An Energy-Adaptive Riemannian Conjugate Gradient Descent Method for the Kohn–Sham Model
Bonan	Sun	An inexact Krylov subspace methods for response calculations in density functional theory

Tutorials

16 Sept
10:45
PWR 5a

Efficient Numerical Methods for Solving Eigenvalue Problems

Antoine Levitt
Université Paris Saclay

I will review classical and more recent methods to solve eigenvalue problems, with an emphasis on those relevant for electronic structure computations.

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16 Sept
14:00
PWR 5a

Tensor (network) Methods in Electronic Structure

Mi-Song Dupuy
Sorbonne Université

This talk will begin with a brief overview of general tensor methods before delving into the specifics of tensor networks, with a particular emphasis on tensor trains (also known as matrix product states). These tensor trains have proven to be highly effective in addressing many-body ground-state problems. We will introduce the Density Matrix Renormalization Group (DMRG) algorithm, the primary practical tool in this context, and discuss key mathematical approximation results and the convergence properties of the DMRG algorithm.

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16 Sept
15:45
PWR 5a

Fundamentals of Quantum Numerical Linear Algebra

Agnieszka Miedlar and Paul Cazeaux
Virginia Tech

In this tutorial, we will present fundamental concepts of Quantum Numerical Linear Algebra for Scientific Computing. We will start with basic notions of quantum states, unitary operators, no-cloning theorem and measurements. After introducing block-encoding and Linear Combination of Unitaries (LCU), we will discuss solving quantum counterparts of classical numerical linear algebra problems, i.e., Quantum Linear System Problem (QLSP), Quantum Singular Value (eigenvalue) Transformation (QSVT), Hamiltonian Simulation and Trotterization. If time permits, we will talk about Adiabatic Quantum Computation (AQC) and Variational Quantum Eigensolver (VQE).

Talks

Grassmann Extrapolation as a Tool to Accelerate Ab-initio Molecular Dynamics

17 Sept
9:00
PWR 5a

Filippo Lipparini
Università di Pisa

Born-Oppenheimer ab-initio molecular dynamics (BOMD) simulations are a powerful tool to study complex molecular systems and phenomena. However, they are also computationally very demanding, as the require the solution to the quantum mechanical (usually, density functional theory, DFT) equations at each step of the trajectory propagation. It is therefore paramount to reduce as much as possible the cost of each energy calculation, which can be achieved by providing an accurate guess to the self-consistent field (SCF) solver. This is, however, not straightforward, as the density matrix must satisfy non-linear constraints to ensure its idempotency. Therefore, a linear combination of idempotent density matrices is not idempotent, which makes interpolating and extrapolating densities a complex and cumbersome task. Recently[1], we have used tools from differential geometry to map the manifold to which the density belongs onto its tangent space, which is indeed a vector space, and viceversa: this allows us to perform an extrapolation in a vector space and then map the extrapolated density back to the manifold, ensuring that it satisfies the correct physical requirements. Using these tools, we propose a strategy to compute an idempotent guess density for the SCF procedure starting from few densities available from the previous steps of MD[2]. The extrapolation coefficients are computed on-the-fly by solving a least square problem. To ensure good energy conservation, we have further refined our scheme to make it quasi time-reversible[3]. The proposed strategy is compared to Niklasson's extended Lagrangian Born-Oppenheimer (XLBO) scheme[4] on several multiscale BOMD simulation, showing very good performances and excellent stability.

[1] É. Polack, A. Mikhalev, G. Dusson, B. Stamm, F. Lipparini, Mol. Phys. 2020, 118, e1779834

[2] É. Polack, G. Dusson, B. Stamm, F. Lipparini, J. Chem. Theory Comput. 2021, 17, 6965-6973

[3] F. Pes, É. Polack, P. Mazzeo, G. Dusson, B. Stamm, F. Lipparini, J. Phys. Chem. Lett. 2023, 14, 9720-9726

[4] A. M. N. Niklasson, P. Steneteg, A. Odell, N. Bock, M. Challacombe, C. J. Tymczak, E. Holmström, G. Zheng, V. Wever, J. Chem. Phys. 2009, 130, 214109

Density Functional Theory for Two Dimensional Homogeneous Materials

17 Sept
10:20
PWR 5a

Salma Lahbabi
ENSEM-Université Hassan II de Casablanca

We study Density Functional Theory models for 2D materials in the 3D space. Our interest comes from the recent developments of two-dimensional materials, such as graphene and phosphorene, in the physics community [2]. In this work, we focus on homogeneous systems. We first show that a homogeneous material can be seen as a limit of periodic systems [1]. Next, we derive reduced models in the remaining orthogonal direction, for DFT models with and with- out magnetic fields [3, 4]. We show how the different terms of the energy are modified and we derive reduced equations in the remaining direction. We prove some properties of the ground state, such as perfect screening and precise decay estimates in the Thomas-Fermi model, and in Kohn-Sham models, we prove that the Pauli principle is replaced by a penalization term in the energy.

[1] S. Benjelloun, S. Lahbabi, and A. Moussa, Homogenization of 2D materials in the Thomas-Fermi-von Weizsacker theory, arXiv preprint arXiv:2312.08067, (2023).

[2] A. Geim and I. Grigorieva, Van der Waals heterostructures, Nature, 499(2013), pp. 419-425.

[3] D. Gontier, S. Lahbabi, and M. A., Density functional theory for homogeneous two dimensional materials, Comm. Math. Phys., 388 (2021), pp. 1475-1505.

[4] D. Gontier, S. Lahbabi, and A. Maichine, Density functional theory for two-dimensional homogeneous materials with magnetic fields, Journal of Functional Analysis, 285 (2023), p. 110100.

Momentum Space and Continuum Models of Incommensurate Bilayer 2D Materials

17 Sept
11:10
PWR 5a

Daniel Massatt

Louisina State University

Electronic structure of incommensurate 2D materials is well approximated by Wannierized tight-binding models, but these models do not immediately realize the critical relationship between momenta and energy vital for applications such as the construction of a many-body basis. Continuum models have become excellent tools for describing the low energy physics such as the Bistritzer-MacDonald model, but much is yet to be understood about the accuracy of these models.

Here we discuss the momentum space model, and provide a procedure for producing continuum models with controlled accuracy. We show the momentum space model is a direct transformation of the tight binding model, and is exponentially accurate with respect to truncation. We then construct a method for producing continuum models realized as Taylor expansions of the momentum space model. As a case study, we show the Bistritzer-MacDonald model is a Taylor expansion of the Wannier tight-binding model for twisted bilayer graphene, and illustrate how to improve accuracy of the model with additional terms. The procedure can be applied to a large class of tight-binding models such as TMDC bilayers, and error can be tuned by parameter choices.

A Multilevel Method for Many-Electron Schrödinger Equations based on the Atomic Cluster Expansion

17 Sept
13:30
PWR 5a

Huajie Chen

Beijing National University

The atomic cluster expansion (ACE) yields a highly efficient and interpretable parameterization of symmetric polynomials that has achieved great success in modeling properties of many-particle systems. In this talk, we extend the practical applicability of the ACE framework to the computation of many-electron wave functions. To that end, we develop a customized variational Monte Carlo algorithm that exploits the sparsity and hierarchical properties of ACE wave functions. We demonstrate the feasibility through the simulations of some typical molecular systems.

On Uncertainty Quantification of Eigenvalue Problems

17 Sept
14:20
PWR 5a

Jürgen Dölz

Institute for Numerical Simulation
University of Bonn

We consider generalized symmetric operator eigenvalue problems with random symmetric perturbations of the operators. This implies that the eigenpairs of the eigenvalue problem are also random. We investigate stochastic quantities of interest of eigenpairs of higher but finite multiplicity and discuss why for multiplicity larger than one, only the stochastic quantities of interest of the eigenspaces are meaningful. To do so, we characterize the Fréchet derivatives of the eigenpairs with respect to the perturbation and provide a new linear characterization for eigenpairs of higher multiplicity. As a side result, we prove local analyticity of the eigenspaces. Based on the Fréchet derivatives of the eigenpairs we discuss a meaningful Monte Carlo sampling strategy for multiple eigenvalues and develop an uncertainty quantification perturbation approach. We present numerical examples to illustrate the theoretical results.

Numerical solution of eigenvalue Schrödinger problems using infinite-width two-layer networks

17 Sept
15:40
PWR 5a

Virginie Ehrlacher

École des ponts ParisTech

The aim of this talk is to present recent results concerning the analysis of numerical schemes using two-layer neural networks with infinite width for the resolution of high-dimensional Schrödinger eigenvalue problems. Using Barron's representation of the solution with a measure of probability, the Rayleigh quotient associated to the eigenvalue problem is minimized thanks to a constrained gradient curve dynamic on the 2-Wasserstein space of parameters defining the neural network. Inspired by the work from Bach and Chizat, we prove that if the gradient curve converges, then the represented function is a solution of the eigenvalue problems considered, but not necessarily the lowest one. At least up to our knowledge, this is the first theoretical result of this type concerning the minimization of non-convex functionals. Numerical experiments are given to illustrate the advantages and drawbacks of the method. Open questions related to the interest of such approaches for the resolution of many-body electronic Schrödinger equations will be discussed.

This is joint work with Mathias Dus.

On the Well-Posedness of the Discrete Coupled Cluster Equations

18 Sept
9:00
PWR 5a

Muhammad Hassan

Ècole Polytechnique Fédérale de Lausanne

Coupled cluster methods are widely regarded as among the most effective algorithms for high precision resolution of the ground state energy of the electronic Schrödinger equation in the dynamical correlation regime. In this talk, I will discuss some recent results on the well-posedness of the discrete coupled cluster equations. The approach I describe is based on establishing a discrete inf-sup condition on the coupled cluster Fréchet derivative, which presents a challenge due to the non-symmetric nature of the underlying linear operator, and the fact that the Laplace operator has an essential spectrum on the unbounded domain $\mathbb{R}^n$. The main novelty of our approach is that it results in a sharper description of the local well-posedness regime of the discrete coupled cluster equations than the previous state-of-the-art. This is joint-work with Yvon Maday and Yipeng Wang (Laboratoire Jacques-Louis Lions, Paris).

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18 Sept
9:50
PWR 5a

DMRG, new post-DMRG-methods, and chemical accuracy

Gero Friesecke

Technical University of Munich

Achieving "chemical accuracy", 1 kcal/mole, which allows to reliably extract chemical behavior, is a longstanding dream of electronic structure simulations. Even the best methods such as coupled cluster or DMRG do not directly achieve this for molecules with a dozen electrons unless refined further (or unless already requiring supercomputing resources for tiny systems in a manner which lacks scalability to larger systems). A recent refinement of DMRG is the restricted active space density matrix renormalization group (DMRG-RAS) method. While a significant improvement of DMRG with similar computational cost, it is still a little bit short of chemical accuracy.

In [1] we introduced a further refinement, DMRG-RAS-X, where X stands for extrapolation. This method is based on the theoretical derivation and numerical validation of a remarkably accurate power law scaling of the errors of DMRG-RAS with the size of the underlying orbital spaces. The new method, DMRG-RAS-X, is found to reach chemical accuracy for strongly correlated systems such as the Chromium dimer, dicarbon up to a large cc-pVQZ basis, and even a large chemical complex like the FeMoco. The method is free of empirical parameters, performed robustly and reliably in all examples we tested, and has the potential to become a vital alternative method for electronic structure calculations in quantum chemistry, and more generally for the computation of strong correlations in nuclear and condensed matter physics.

[1] G.F., Gergely Barcza and Ors Legeza, J Chem Theory Comput. 20(1):87-102, 2024

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18 Sept
11:10
PWR 5a

Recent Progress with Transcorrelated Methodologies

Ali Alavi

Max Planck Institute for Solid State Research

Non-unitary similarity transformation of the many-electron Schrodinger equation using real-space Jastrow factors is a powerful, yet somewhat problematic, approach to simplifying the computational task of computing highly accurate energies for molecular and in-principle extended systems. It allows the use of sophisticated correlation factors, incorporating both universal features (such as cusp conditions) as well as system-specific features (such as shell effects), as well as long-range correlation (relevant in extended systems, especially metals), into the Jastrow factor, which is then transformed into an effective interaction in the Hamiltonian. The non-Hermitian character of the resulting transcorrelated Hamiltonian requires careful optimisation of the Jastrow parameters, but leads to compactifacation of the right-eigenvector of the TC Hamiltonian, which facilitates its calculation. The emergent three-body interactions can be handled quite accurately with suitable normal-ordering approximation, even in strongly correlated systems. We review the substantial progress in this field in the past few years, and give a perspective on upcoming developments and applications.

Exploring Ground and Excited States via Single Reference Coupled-Cluster Theory and Algebraic Geometry

18 Sept
12:00
PWR 5a

Fabian Faulstich

Rensselaer Polytechnic Institute

In this presentation, I will examine the intersection of algebraic geometry and coupled cluster theory within the context of quantum many-body systems. Although coupled cluster theory is a mature and well-established method that delivers high-accuracy results in quantum chemistry, the intricate mathematical structures underlying its governing equations – a high-dimensional polynomial system – remain a subject of ongoing mathematical inquiry. I will elucidate how algebraic geometry offers novel insights into the structure and solutions of these coupled cluster equations, particularly through the study of truncation varieties and their associated degrees, as well as the exploration of root structures via Newton polytopes and homotopy continuation methods. By presenting detailed examples and numerical simulations, I will demonstrate how these advanced mathematical techniques can further refine our understanding of the coupled cluster approach, especially in accurately predicting both ground and excited state energies.

Reliable and Efficient Methods for Computing DFT Derivatives

19 Sept
9:00
PWR 5a

Michael Herbst

Ècole Polytechnique Fédérale de Lausanne

High-throughput density-functional theory (DFT) simulation have become a central ingredient for the computational design of novel materials. For evaluating the suitability of a material to a technological applications, one needs to know its properties, i.e. how it responds to perturbations out of equilibrium. In DFT the required application of perturbation theory to simulate such properties is termed density-functional perturbation theory (DFPT) and leads to the Dyson equation. When solving this equation iteratively, each application of the involved operator (dielectric operator) in turn requires multiple linear systems to be solved (Sternheimer equations). For metals these linear systems can become ill-conditioned, making it challenging to propose efficient numerical schemes. We review some standard approaches in the literature and propose two new ingredients for an efficient algorithmic approach: (1) a Schur-complement trick to improve the conditioning of the inner Sternheimer equations and (2) a framework based on inexact Krylov methods to adaptively select looser convergence tolerances for the inner Sternheimer equations without compromising accuracy in the computed response quantities. Our schemes are implemented and tested using the Density-Functional Toolkit (https://dftk.org) and show a reduction of up to 80% computational time on non-trivial Heusler metal alloys.

This is joint work with E. Cancès, G. Kemlin, A. Levitt, B. Stamm and B. Sun.

Guaranteed Error Bounds for Electronic Structure Problems: Nonlinear Equations and Localized Basis Sets

19 Sept
10:20
PWR 5a

Geneviève Dusson

Université de Franche-Comté

In this talk, I will present recent results providing fully guaranteed and computable error bounds for the solutions to electronic structure problems. I will first present an a posteriori error estimation for Kohn-Sham equations with convex density functionals. I will then turn to the error estimation for linear eigenvalue problems discretized with localised basis sets.

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19 Sept
11:10
PWR 5a

Mathematical Analysis and Numerical Approximations of Density Functional Theory Models for Metallic Systems

Xiaoying Dai

Academy of Mathematics and Systems Science,CAS

In this talk, we will introduce our study on the energy minimization model arising in the ensemble Kohn-Sham density functional theory for metallic systems, in which a pseudo-eigenvalue matrix and a general smearing approach are involved. We investigate the invariance of the energy functional and the existence of the minimizer of the ensemble Kohn-Sham model. We propose an adaptive two-parameter step size strategy and the corresponding preconditioned conjugate gradient methods to solve the energy minimization model. Under some mild but reasonable assumptions, we prove the global convergence for the gradients of the energy functional produced by our algorithms. Numerical experiments show that our algorithms are efficient, especially for large scale metallic systems. In particular, our algorithms produce convergent numerical approximations for some metallic systems, for which the traditional self-consistent field iterations fail to converge. This is a joint work with Professor Stefano de Gironcoli, Dr. Bin Yang and Prof. Aihui Zhou.

Ground State Preparation with Open Quantum System-inspired Algorithms

19 Sept
14:00
PWR 5a

Paul Cazeaux

Virginia Tech

An important subroutine in any quantum computing algorithm is the preparation of the initial useful and relevant quantum state of the machine, preferably efficiently and using a small number of ancilla qubits. In this talk, we will discuss a novel algorithm for the preparation of the ground state of a given Hamiltonian and its analysis, motivated by the novel approach [1] based on the approximation of Lindblad dynamics often used to model open quantum systems. Under certain assumptions on the eigenvalue distribution of the Hamiltonian and ability to apply certain random unitary operations, explicit mixing time estimates may be obtained showing polynomial scaling in the number of qubits.

[1] Z. Ding, C-F. Chen and L. Lin, Single-ancilla ground state preparation via Lindbladians, Phys. Rev. Research 6, 033147, 2024.

Optimal Orbital Selection for Ground States and Excited States Calculation on Classical and Quantum Computers

19 Sept
14:50
R104

Yingzhou Li

Fudan University

We propose incorporating an orbital optimization scheme into quantum eigensolvers to reduce the number of qubits required for a given problem. The optimal transformation is found by minimizing the ground state energy or excited state energies with respect to this partial unitary matrix. Through numerical simulations of small molecules up to 16 spin orbitals, we demonstrate that this method has the ability to greatly extend the capabilities of near-term quantum computers with regard to the electronic structure problem. We find that VQE paired with orbital optimization consistently achieves lower ground state energies than traditional VQE when using the same number of qubits and even frequently achieves lower ground state energies than VQE methods using more qubits.

Time-dependent Hamiltonian Simulation: Quantum Algorithm and Superconvergence

19 Sept
16:10
Online

Di Fang

Duke University

Hamiltonian simulation becomes more challenging as the underlying unitary becomes more oscillatory. In such cases, an algorithm with commutator scaling and a weak dependence, such as logarithmic, on the derivatives of the Hamiltonian is desired. We introduce a new time-dependent Hamiltonian simulation algorithm based on the Magnus series expansion that exhibits both features. Importantly, when applied to unbounded Hamiltonian simulation in the interaction picture, we prove that the commutator in the second-order algorithm leads to a surprising fourth-order superconvergence, with an error preconstant independent of the number of spatial grids. The proof of superconvergence is based on semiclassical analysis that is of independent interest.

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20 Sept
9:00
PWR 5a

Riemannian Optimization Methods for Ground State Computations of Multicomponent Bose-Einstein Condensates

Tatjana Stykel
Universität Ausburg

In this talk, we address the computation of ground states of multicomponent Bose-Einstein condensates by solving the underlying energy minimization problem on the infinite-dimensional generalized oblique manifold. First, we discuss the existence and uniqueness of a ground state with non-negative components and its connection to the coupled Gross-Pitaevskii eigenvalue problem. Then, we study the Riemannian structure of the generalized oblique manifold by introducing several Riemannian metrics and computing important geometric tools such as Riemannian gradients and Hessians. This allows us to develop the Riemannian gradient descent and Riemannian Newton methods based on different metrics. Exploiting first- and second-order information of the energy functional for the construction of appropriate metrics makes it possible to incorporate preconditioning into Riemannian optimization, which significantly improves the performance of the optimization schemes. A collection of numerical experiments demonstrates the computational efficiency of the proposed methods. (Joint work with R. Altmann, D. Peterseim and M. Hermann)

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20 Sept
9:50
PWR 5a

Coupling Perturbation Theory and the Variational Approximation

Louis Garrigue
CY Cergy Paris Université

Eigenvector continuation is a reduced basis method for eigenvalue problems, in which the reduced space is formed by the vectors extracted from perturbation theory. We give bounds for it and show that it is more competitive than perturbation theory.

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20 Sept
11:10
PWR 5a

Quantum-electrodynamical density-functional theory for the Dicke Hamiltonian

André Filip Johannes Carlzon Laestadius
University of Oslo

Abstract: We present a mathematical framework for density-type functions for a generalization of the Dicke model, which describes many two-level systems coupled to photonic modes. The density functions depend on the spin-matrix expectation value and the displacement, and we explore a formulation similar to standard density-functional theory.

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20 Sept
12:00
PWR 5a

Numerical Methods for Simulating Non-equilibrium Quantum Dynamics

Chao Yang
Lawrence Berkeley National Laboratory

A practical way to compute time-dependent observables of a non-equilibrium quantum many-body system is to focus on the single-particle Green's function defined on the Keldysh contour. The equation of motion satisfied by such a Green's function is a set of nonlinear integro-differential equations called the Kadanoff-Baym equations. We will describe numerical methods for solving this type of equations and show how to use dynamic mode decomposition and recurrent neural networks to reduce computational complexity.

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