Program IWR School "Mathematical Methods for Quantum Chemistry"

time	So 1st Oct	Mo 2nd Oct	Tu 3rd Oct	We 4th Oct	Th 5th Oct	Fr 6th Oct
8:00		Registration				
9:00		Opening **Andreas Dreuw** Introduction to quantum chemistry	**Eric Cancès** An in-depth look at self-consistent field methods	**Andreas Dreuw** The Electron Correlation Problem	**Reinhold Schneider** Properties of coupled-cluster methods	**Guido Kanschat** Iterative eigensolver algorithms
10:00						
11:00		Coffee break **Eric Cancès** Mathematical structure of quantum mechanics	Coffee break Contributed talks	Coffee break **Reinhold Schneider** Mathematical structure of Post-HF methods	Coffee break Contributed talks	Coffee break Contributed talks
12:00			Lunch *Bräustadel*			Closing
13:00		Lunch *Bräustadel*	Excursion to **Frankfurt** guided city tour and afterwards **conference dinner**	Lunch *Bräustadel*	Lunch *Bräustadel*	
14:00		**Guido Kanschat** Numerical solution of operator eigenproblems		Contributed talks	Contributed talks	
15:00				Coffee break	Coffee break	
16:00		Coffee break Contributed talks		**Denis Davydov** **Katharina Kormann** Modelling simple quantum-mechanical systems	**Denis Davydov** **Katharina Kormann** Time-dependent problems	
17:00						
18:00	Registration					
19:00	Welcome reception and get-together			Get-together		
evening						

Lectures
Practical sessions
Contributed talks
Food, coffee, social

Monday 2nd October

Introduction to quantum chemistry (Dreuw)

- Basic physical principles and equations of quantum mechanics
- Born-Oppenheimer Approximation and the electronic Schrödinger Equation
- Introduction to Hartree-Fock
- Gaussian basis sets
- Koopmans' theorem
- Brillouin's theorem

Mathematical structure of quantum mechanics (Cancès)

- Hilbert spaces: Definition and properties
- Linear operators: Properties and examples in quantum mechanics
- Classification of spectra of self-adjoint operators and the physical interpretation
- Physical interpretation of the domain of an observable
- Structure of the spectra of typical Hamiltonians used in quantum-mechanical modelling

Numerical solution of operator eigenproblems (Kanschat)

- Min-max theorem for compact, self-adjoint eigenvalue problems in Hilbert spaces
- Galerkin approximation: Definition and concept
- Galerkin approximation for eigenvalue problems
- Error estimates for discretised eigenvalue problems

Contributed talks

- *Simon Etter:* Locality in Quantum Mechanics
- *Nguyen Ngoc Doanh:* Developing a framework for operation optimization of irrigation systems

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Tuesday 3rd October

An in-depth look at self-consistent field methods (Cancès)

- Mathematical derivation of the Hartree-Fock model
- Mathematical structure of the various formulations of Hartree-Fock
- Examples and properties of common self-consistent field algorithms for Hartree-Fock

Contributed talks

- *Yuki Yamamoto:* Molecular dynamics simulation and theoretical analysis of liquid pyrenes
- *Marlene Lund:* Large-Scale Semidefinite Programming in Computation of Many-Body Electronic Structures

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Wednesday 4th October

The Electron Correlation Problem (Dreuw)

- Issues with Hartree-Fock
- Electronic correlation
- Introduction to density-functional theory

Mathematical structure of Post-HF methods (Schneider)

- Slater determinants and Full CI
- Excitation and creation operators
- Second quantization
- Exponential ansatz and single reference coupled cluster

Contributed talks

- *Benjamin Kutschan:* Geometry of tensor decompositions
- *Prakash Lamichhae:* Dye Sensitized Solar Cell Using Fe/Co doped ZnO thin film and Organic Dye from Nactynthes Arbrotristics
- *Michael F. Herbst:* Employing lazy matrices for a flexible quantum-chemical simulation package

Practical session (Davydov, Kormann)

- Introduction to `deal.ii`
- Solving standard generalised hermitian eigenvalue problems with `deal.ii`

Thursday 5$^{\text{th}}$ October

Properties of coupled-cluster methods (Schneider)

- Projected coupled cluster equations (CC)
- Coupled cluster energy
- Convergence theory for CC
- Coupled Cluster Lagrangian and bivariational formulation

Contributed talks

- *Fabian Faulstich:* Mathematical Analysis of DMRG-TCC
- *Masahiko Taguchi:* QM/MM study on inhibitor of HIV-1 protease
- *Aynura Jafarova:* Qubit transfer with high fidelity in 1D fermion spin chains with nearest-neighbour interaction based on new recurrence relations for Racah polynomials
- *Ojo Gbenga:* Approximate solution of Eckhaus Equation Using Elzaki Decomposition Method
- *Aleena Alex:* Molecular Dynamic Studies of mineral water interfaces
- *Sabina Sadigova:* Frames, applications and abstract examples in Hardy classes

Practical session (Davydov, Kormann)

- Solving standard generalised hermitian eigenvalue problems with `deal.ii` (continued)
- Solving the Time-dependent Schrödinger equation

Friday 6$^{\text{th}}$ October

Iterative eigensolver algorithms (Kanschat)

- Power method and inverse power method with shift
- QR method as simultaneous power method
- Arnoldi and Krylov-subspace based methods

Contributed talks

- *Jan-Erik Oest:* n-dimensional Wave Packet Dynamics and Comparison with Approximate Methods
- *Tulika Gupta:* Analyzing reaction mechanism for selective CO_2 to HCHO conversion