$$T_{\mathrm{W}}(\rho) = \frac{1}{2}\int_{\mathbb{R}^3}\left|\nabla\sqrt{\rho(\mathbf{x})}\right|^2\mathrm{d}\mathbf{x}$$

$$\hat{H} = -\frac{\hbar^2}{2m_e}\sum_{i=1}^{N}\nabla_{\mathbf{r}_i}^2 + \frac{1}{2}\sum_{i}^{N}\sum_{j\neq i}^{N}\frac{e^2/4\pi\epsilon_0}{|\mathbf{r}_i-\mathbf{r}_j|} + \sum_{i}^{N}V(\mathbf{r}_i)$$

$$\mathcal{F}^\varepsilon(\rho) = \inf_{\sigma}\left\{\mathcal{F}(\sigma) + \frac{1}{2\varepsilon}\|\sigma-\rho\|^2\right\}$$

$$\rho_\psi(\mathbf{x}) = N\int_{\mathbb{R}^{3(N-1)}}|\psi(\mathbf{x},\mathbf{x}_2,\ldots,\mathbf{x}_N)|^2\mathrm{d}\mathbf{x}_2\ldots\mathrm{d}\mathbf{x}_N$$

$$E^\varepsilon(v) = \inf_{\rho}\left\{\mathcal{F}^\varepsilon(\rho) + \langle v,\rho\rangle\right\}$$

$$F_{\mathrm{LL}}(\rho) = \inf_{|\psi\rangle\mapsto\rho}\langle\psi|\hat{H}_0|\psi\rangle$$

$$E(v) = E^\varepsilon(v) + \frac{\varepsilon}{2}\|v\|^2$$

Workshop on Quantum Theory:
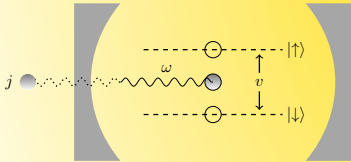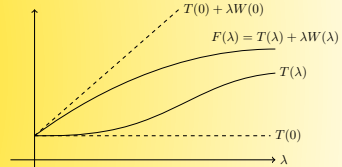## Foundations and Extensions of Density-Functional Theory

$$\mathcal{F}(\rho) = \sup_{v}\left\{E(v) - \langle v,\rho\rangle\right\}$$

$$E(v) = \inf_{\rho}\left\{\mathcal{F}(\rho) + \langle v,\rho\rangle\right\}$$

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = \hat{H}|\psi\rangle$$

CHUB

The OsloMet Quantum Hub

$T(0) + \lambda W(0)$

$F(\lambda) = T(\lambda) + \lambda W(\lambda)$

$T(\lambda)$

$T(0)$

λ

$|\uparrow\rangle$

ω

v

$|\downarrow\rangle$

j

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

RεGAL

Oslo
December 2nd – 6th, 2024

Workshop on Quantum Theory:
Extensions and Foundations of Density-Functional Theory

André Laestadius[*,†] and Vebjørn H. Bakkestuen[*,⊠]

Pilestredet 35, 0166 Oslo, Norway
02.12.2024 – 06.12.2024

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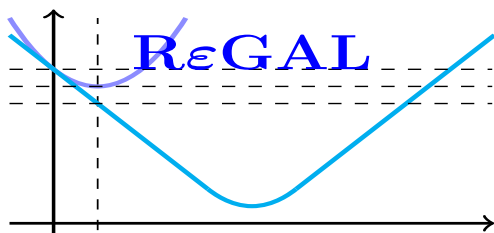*Department of Chemistry, University of Oslo*
⊠ `vebjorn.bakkestuen@oslomet.no`
⚭ `uni.oslomet.no/quantum/workshop-foundations-and-extensions-of-dft/`

The OsloMet Quantum Hub

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Abstract

The workshop will focus on the mathematical foundations and recent extensions of density-functional theory (DFT), a prime method for computational quantum-mechanical modelling. The increased use of DFT in physical situations where electrons couple to quantized electromagnetic fields requires a thorough revision of the foundations of the theory. Moreover, the application to model settings — commonly employed to describe light-matter interactions — revealed new properties of the theory that remain to be studied in detail. Furthermore, many practical uses of DFT rely heavily on approximations to the universal density functional. One avenue for evaluating new functional approximations is to solve the so-called inverse problem, that is the problem of retrieving the potential of a system given its electronic density. Such approaches are typically referred to as density-potential inversion schemes and are significantly less studied than the forward problems such as the Kohn–Sham scheme. Combined with the fact that efficient and stable implementations of density-potential inversion algorithms are largely lacking, this problem is of both fundamental and practical importance to DFT. All these topics pose interesting mathematical as well as numerical challenges that are of great relevance across multiple disciplines such as solid-state physics, quantum chemistry, and quantum optics. The workshop thus aims at bringing together researchers working on these and adjacent subjects in order to advance the applicability of DFT in both novel and established domains.

Contents

Schedule

	Time	Location	Event	Chair
Mon	13:00–13:45	PI460	Coffee & mingle	
	13:45–14:00	PI460	Welcome	
	14:00–16:45	PI460	Talks	E. Tellgren
Tue	09:00–12:00	PI460	Talks	M. Penz
	12:00–13:30		Lunch	
	13:30–16:45	PI460	Talks	S. Selstø
Wed	09:00–10:45	PI646	Talks	M. Matassa
	11:00–12:00	PI646	Public lecture	S. Denysov
	12:00–13:30		Lunch	
	13:30–		Discussions	
	19:30–	Grand Café	Dinner	
Thu	09:30–12:00	PI646	Talks	M. Ruggenthaler
	12:00–13:30		Lunch	
	13:30–16:50	PI460	Talks	T. Helgaker
Fri	09:00–12:15	PI460	Talks	P.F. Loos
	12:15–12:30	PI460	Closing	

Workshop on Quantum Theory:
Extensions and Foundations of Density-Functional Theory

Time	Monday	Tuesday *Chair:* M. Penz	Wednesday *Chair:* M. Matassa	Thursday *Chair:* M. Ruggenthaler	Friday *Chair:* P.F. Loos
9:00		M. Lotfigolian (20')			T. C. Corso (45')
9:30		O. Bohle (20')	S. Pittalis (45')	H. Koch (60')	
10:00		M. Herbst (45')	K. Li (45')		L. Garrigue (45')
10:30					
11:00		P. F. Loos (45')	*Chair:* S. Denysov F. Faulstich* (60')	T. Helgaker (60')	C. Jöns (20')
11:30		S. Sutter (20')			A. Davidov (20')
12:00		Lunch	Lunch	Lunch	V. Skogvoll (45')
12:30					
13:00	Coffee *P35, P1460*	*Chair:* S. Selstø		*Chair:* T. Helgaker	Closing
13:30	Welcome *Chair:* E. Tellgren M. Ruggenthaler (45')				
14:00		S. Kvaal (45')		M. Oster (45')	
14:30	M. A. Csirik (45')	T. Pedersen (45')		E. Polak (45')	
15:00					
15:30		S. E. Schrader (20')			
16:00	V. Falmår (20')	M. Penz (45')		E. Tellgren (45')	
16:30	V. Bakkestuen (20')			S. Giarrusso (45')	
17:00					

Workshop Dinner *Grand Café, 19:30—*

Location: *Auditorium P1646, P35*

Location: *Classroom P1460, P35*

Practicalities

Venue

The workshop will be held at the Pilestredet campus of OsloMet. All lectures, talks, and discussions will take place at *Ellen Gleditschs hus* (P35), Pilestredet 35, 0166 Oslo. Please use the rotating doors facing Holbergs plass as they are unlocked during the day, see Figure 2.1.

The most of the workshop will take place in the classroom PI460, located on the fourth floor in P35. Please see the Mazemap for directions.

The morning sessions on Wednesday and Thursday will take place in the auditorium PI646, which is located on the sixth floor in P35. Please see the Mazemap for directions.

Both rooms (PI460 and PI646) are located in the same part of P35, albeit on different floors. To access the rooms, please locate the glass elevators in the large open space directly inside the entrances to P35. Follow the stairs to the 4th or 6th floor, for PI460 or PI646 respectively. Both rooms are located on the left-hand side when coming up the stairs (right-hand side if you are taking the elevators).

Figure 2.1: View of the entrance to P35 form Holbergs plass.
(Photo: Benjamin A. Ward/OsloMet)

Directions

From the airport by train: Exit at *Nationaltheatret station*, the stop after Oslo
Central Station (Oslo S). Then P35 is only short walk away, < 10 min, see
Figure 2.2.

From elsewhere in the city: The closest subway station (T-banen) is *Nation-
altheatret station*, see Figure 2.2. By bus or tram, the closest station is *Holbergs
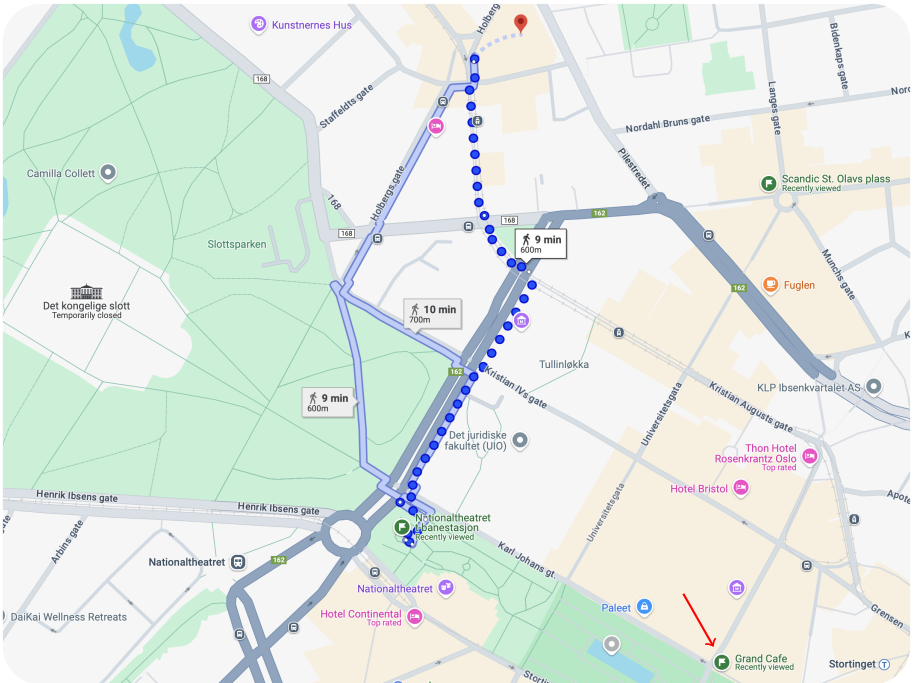plass* just outside P35.

Figure 2.2: Directions from *Nationaltheateret station* to *Ellen Gleditschs Hus
(P35)*. On foot it takes less than 10 minutes. The conference dinner will be
held at Grand Café, see red arrow. (Map by Google)

Lunches & Dinners

The Pilestredet campus is located centrally in Oslo and there is a variety of options for both lunch and dinner. During the workshop there will not be any organised lunches, and all participants are free to explore the local restaurants and cafeterias. Please note that restaurants in Norway generally close a bit earlier than in other countries in Europe. It is not uncommon that the kitchen closes as early as 21:00, but this might vary from restaurant to restaurant.

In addition to restaurants, there are a few options for lunch on campus. Some options are, the *SiO* cafeterias in P32, P35 (a smaller one), and P52 which offer a variety of warm dishes, salads, baguettes etc. Please note that most options are prised by weight, currently prised at 18.10 NOK per hg., about € 15.5 per kg. In addition, *Union167 Fyrhuset* offers a selection of baked goods, sandwiches and freshly baked pizzas, with pizzas raging from € 10 to € 13.

Workshop Dinner

The workshop dinner will be held on Wednesday the 4th of December. The dinner is included for all participants that have signed up using the Nettskjema. If you have any allergies or other restrictions, not declared in the Nettskjema, please let the organisers know prior to the dinner.

The dinner will be held at the historical *Grand Café*. Grand Café is situated on Karl Johans gate just next to Stortinget (the Norwegian parliament).

Figure 2.3: Grand Café, Stortinget (Arial by Apple)

Abstracts

Monday December 2nd

Ab initio quantum electrodynamics: from bare masses to modifications of thermodynamics
Michael Ruggenthaler

In this presentation I want to highlight the differences and opportunities for ab initio methodologies that arise when considering a quantum-electrodynamical description of atoms, molecules and solids. Based on a few analytical examples I will exemplify how the observable masses of charged particles arise, how they are changed when engineering the photon vacuum by optical cavities, and how such fundamental modifications can even influence the thermodynamic properties of matter. The latter is not a mere theory figment but there is plenty of experimental evidence. Then I will briefly sketch the basic mathematical framework of the Pauli-Fierz quantum field theory and highlight that it allows for a (at least formally) straightforward extension of ab initio methods such as density-functional theory to quantum electrodynamics.

Mathematical ideas for DFT
Mihaly A. Csirik

I explore various generalizations of DFT, such as Spin DFT, CDFT and QEDFT, and the technical difficulties that lie in their analysis.

Quantum-Electrodynamical Density-Functional Theory for the Quantum Rabi Model

Vegard Falmår

Within a minimal implementation of quantum electrodynamics several key features of density-functional theory (DFT) are demonstrated, thus allowing the study of elementary properties of quantum-electrodynamical density-functional theory (QEDFT). I will employ the quantum Rabi model, which describes a two-level system coupled to a single photon mode. In this setting, the density variables of the system are the polarization and the displacement of the photon field. I will give analytical expressions for the constrained-search functional and the exchange-correlation potential and compare this to established results from QEDFT. I will further discuss a form for the adiabatic connection that is almost explicit in the density variables, up to only a non-explicit correlation term that gets bounded both analytically and numerically. This allows several key features of DFT to be studied without approximations.

Quantum-Electrodynamical Density-Functional Theory Exemplified by the Multimode Dicke Model

Vebjørn H. Bakkestuen

Several key features of density-functional theory (DFT) can be demonstrated within minimal models of quantum electrodynamics such as the multi-mode Dicke model [1], or its simplifications—the quantum Rabi and Dicke models [2]. These models allows the study elementary properties of quantum-electrodynamical density-functional theory (QEDFT), but also the explicit construction of many results from standard DFT. The multi-mode Dicke model— a fundamental model of quantum optics—describes light-matter interactions by simplifying the description of light to M quantum harmonic oscillators and the description of matter to N two-level systems. Within this model, the density variables of the system becomes the displacement of the photon field and the polarization of the matter. Focusing mainly on the multi-mode Dicke model, I will present some selected results for this QEDFT formulation. In particular, I will demonstrate a Hohenberg–Kohn theorem by the introduction of the notion of *regular densities*, introduce a Levy–Lieb type functional and give some of its analytical properties. This model allows several key features of DFT to be studied without approximations in an orbital free manner.

[1] Bakkestuen, V. H. *et al.* *Quantum-electrodynamical density-functional theory for the Dicke Hamiltonian* 2024. arXiv: 2409.13767 [math-ph].

[2] Bakkestuen, V. H. *et al.* *Quantum-Electrodynamical Density-Functional Theory Exemplified by the Quantum Rabi Model* 2024. arXiv: 2411.15256 [quant-ph]

Tuesday December 3rd

Moreau–Yosida Density-Potential Inversion
Maryam Lotfigolian

In this talk, I present the mathematical framework for density-potential inversion in density functional theory (DFT) using the Moreau–Yosida (MY) regulariztion. The methodology makes use of a "simpler" functional for an auxiliary system, typically the standard Kohn-Sham approach, and the proximal mapping of the MY transform. I will give analytical and numerical examples to illustrate the framework, including the derivation of effective potentials for a simple choice of function modelling kinetic energy for densities on the real line.

1D periodic Hartree-Fock as a proof-of-concept for regularised density-potential inversion
Oliver Bohle

TBA

Moreau–Yosida regularisation meets DFTK: How to do Kohn–Sham forward and inverse
Michael Herbst

In this hands-on presentation I will present the density-functional toolkit (DFTK [1]) an accessible toolbox for numerical simulations based on Kohn–Sham (KS) density functional theory. I will give an overview of its general capabilities (1D models, parallelisation, integration with materials modelling environments) and present on our recent addition, an inverse KS scheme based on the MY-regularised formulation of DFT.

[1] `https://github.com/JuliaMolSim/DFTK.jl/`

Excited-State Specific Functionals
of the Asymmetric Hubbard Dimer
Pierre-François Loos

In this talk, we discuss the construction of the exact functionals for the (singlet) ground state and two singlet excited states of the asymmetric Hubbard dimer at half-filling [1] using both Levy's constrained search method and Lieb's convex formulation. While the ground-state functional is well-known to be convex with respect to the density, the functional corresponding to the doubly excited state is shown to be concave. For the first excited state, the density-potential mapping is noninvertible, leading to a "functional" that is partial and multivalued [2]. This functional consists of two branches—one concave and one convex—each associated with distinct domains of the external potential. Although the fully interacting first excited state is not adiabatically connected to a non-interacting Kohn–Sham state, we demonstrate how to analytically continue the energy as a function of the interaction strength to address this issue [3].
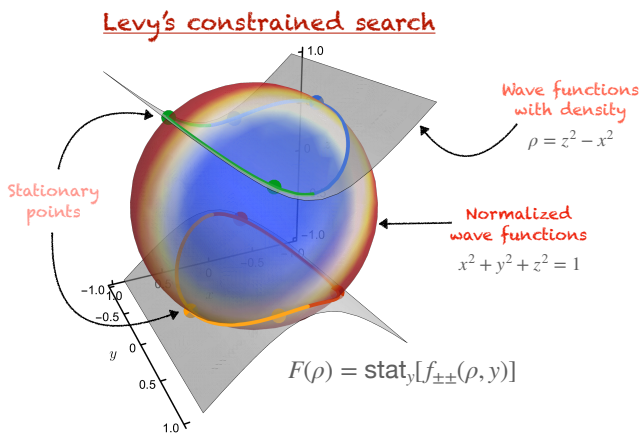
Figure 3.1: Illustration of the Levy constrained-search procedure in the asymmetric Hubbard dimer.

[1] D J Carrascal *et al.* "The Hubbard Dimer: A Density Functional Case Study of a Many-Body Problem". In: J. Phys. Condens. Matter 27 (2015), p. 393001.

[2] S. Giarrusso and P. F. Loos. "Exact Excited-State Functionals of the Asymmetric Hubbard Dimer". In: J. Phys. Chem. Lett. 14 (2023), p. 8780.

[3] S. Giarrusso and P. F. Loos. In: (in preparation).

v-Representability on Periodic Domains: a Sobolev Space Approach
Sarina Sutter

I will present our recent work about finding functional-analytic properties of the densities that allow v-representability. For particles on a ring, we can show that the density is contained in H^1. This space already arises naturally from the finite kinetic energy condition which guarantees that $\sqrt{\rho} \in H^1$. In this setting it is possible to show v-representability for a large class of densities if we allow for distributional potentials. The idea is to use standard techniques from convex analysis to find a suitable potential. Moreover, I will present the difficulties and the advantages of having non-zero temperature which includes an additional entropy term.

On coupled-cluster theory for bosons
Simen Kvaal

In this talk, I will outline a mathematical study of coupled-cluster (CC) theory for bosons. Such a theory is relevant for computational treatments of matter coupled to electromagnetic fields and for the vibrational Schrödinger equation, to name two applications. In fact, for benchmarking DFT methods that take into account quantized electromagnetic fields, methods like boson CC theory coupled to electronic CC is likely to be the only relevant choice. However, CC theory for bosons has certain mathematical problems, and the now-established mathematical framework for fermion (electron) CC does not work at all in this case.

Molecular structure and quantum dynamics without the Born-Oppenheimer approximation
Thomas Pedersen

TBA

Time evolution as an optimization problem - solving the time-dependent Schrödinger equation with Explicitly Correlated Gaussians

Simon Elias Schrader

I present Rothe's method as an approach for solving the time-dependent Schrödinger equation using Explicitly Correlated Gaussians (ECGs). A linear combination of ECGs provides a compact parameterization of multidimensional wave functions well-suited for accurate calculations of molecular properties [1]. While propagating ECGs using a time-dependent variational principle is challenging, Rothe's method addresses this issue by recasting time evolution as an optimization problem [2]. I will introduce Rothe's method with ECGs and show that it can be used to propagate linear combinations of ECGs, thereby obtaining a compact representation of time-dependent wave functions, illustrated by (1) calculating the High-Harmonic Generation (HHG) spectrum of the Hydrogen atom in a strong laser field, using only 50-180 Gaussians [3]; and (2) obtaining the spectrum of the multidimensional Henon–Heiles potential with only up to 40 Gaussians [4], illustrating the broad applicability of the method to various problems. I will also explain how the method can be adapted for the time evolution of orbitals in methods like time-dependent Hartree–Fock. I will conclude with an outlook on future applications and potential improvements.

[1] J. Mitroy *et al.* (2013). Rev. Mod. Phys. 85, 693.

[2] S. Kvaal *et al.* (2022). arXiv: `2207.00271v3 [quant-ph]`.

[3] S. E. Schrader *et al.* (2024). J. Chem. Phys. 161, 044105.

[4] S. E. Schrader, T. B. Pedersen and S. Kvaal (2024). arXiv: `2411.05459v1 [physics.chem-ph]`.

Constrained Search in Imaginary Time

Markus Penz

A new optimization method for the constrained-search functional that is based on imaginary-time evolution is introduced. The constraints are generally given as fixed expectation values of self-adjoint and linearly independent operators, and only a finite number of such constraints is possible. The discussion includes an alternative Hohenberg–Kohn theorem and some insight into the connectedness of the constraint manifold within the Hilbert space of wavefunctions.

Wednesday December 4th

**Gauge symmetries of density functionals:
from first principles to practical approximations for magnetism**
Stefano Pittalis

Spin-current-density-functional theory (SCDFT) includes spin-orbit couplings and Zeeman fields on equal footing with electromagnetic scalar potentials and, thus, offers an appealing unified framework for noncollinear magnetism, spintronics, orbitronics, and topological states. The basic variables of SCDFT include the (paramagnetic) particle- and spin-currents besides the particle- and spin-densities. The characterizing property of the exchange-correlation (xc) energy in SCDFT is the invariance under $U(1) \times SU(2)$ local gauge transformations. Developing effective approximations, however, requires to go beyond generalized-gradient approximations (GGAs) by considering functional forms that depend on spinors explicitly. In Ref. [1], we thus extend ideas and procedures of the Generalized Kohn-Sham approach of DFT to SCDFT and verify its power to compute accurate induced/enhanced spin-orbit-coupling band splittings. In Ref. [2], by enforcing the $SU(2)$ gauge invariance, we add an explicit dependence on spin-currents to the SCAN functional — and similar Meta-GGAs — without resorting to empiricisms. Applications on time-reversal symmetric states of molecules and materials confirm the practical relevance of the extension. In Ref. [3], we enable the visualization of molecular bonds and atomic shells in spin-polarized non-collinear many-electron states by deriving a $U(1) \times SU(2)$ gauge invariant electron localization function. In Ref. [4], guided by gauge considerations, we put forward a modification of the SCAN functional that reduces the tendency towards over spin-polarized solutions.

[1] J.K. Desmarais, G. Ambrogio, G. Vignale, A. Erba, S. Pittalis "Generalized Kohn-Sham Approach for the Electronic Band Structure of Spin-Orbit Coupled Materials" Phys. Rev. Materials 8, 013802 (2024)

[2] J.K. Desmarais, J. Maul, B. Civalleri, A. Erba, G. Vignale, S. Pittalis "Spin-currents via the gauge-principle for meta-generalized-gradient exchange-correlation functionals" Phys. Rev. Lett. 132, 256401 (2024)

[3] J.K. Desmarais, G. Vignale, K. Bencheikh, A. Erba, S. Pittalis "Electron localization function for non-collinear spins" Phys. Rev. Lett. 133, 136401 (2024)

[4] J.K. Desmarais, A. Erba, G. Vignale, S. Pittalis "Meta-Generalized-Gradient Approximation made Magnetic", arXiv: 2409.15201 [cond-mat.mtrl-sci] (2024)

The Semantics of Second Quantization
Kangbo Li

The second quantization can often be a significant obstacle in developing novel ideas for electronic structure theories in terms of both derivation and implementation. In this talk, we aim to automate this process by modeling the second quantization as a language and defining its semantics. This approach addresses a reasonable class of problems expressible in the language instead of on a case by case basis. Using the semantics, we leverage compiler technologies to automate the derivation of the particle-hole formalism, the vacuum expectation, and symmetry factor counting. As a demo, we will walk through a mostly automated derivation and implementation of coupled cluster doubles theory (also know as coupled electron pair approximation). Lastly, we will discuss current limitations including reliability and performance issues.

A practical guide to quantum linear algebra
Fabian Faulstich

We provide an introductory and practical guide to quantum phase estimation algorithms. We begin with a concise overview of the principles of qubits, focusing on state visualization, measurement intricacies, and their relationship to the classical eigenvalue problem. We introduce the Hadamard test and quantum phase estimation (QPE) as methods for eigenvalue approximation. For both algorithms, we detail their mathematical foundations, implementation steps, and error analyses, demonstrating how precision improves with increased measurements or ancilla qubits. Example simulations are performed using hardware emulators and the IBM Eagle One quantum machine, comparing the two approaches. Finally, we highlight the practical significance of QPE by applying it to the Transverse Field Ising Model, illustrating its utility in quantum physical systems.

Thursday December 5th

Ground state conical Intersections -
A challenge in electronic structure theory
Henrik Koch

I will give an overview of the state-of-the-art and discuss our recent insight into the problem.

Current-Density-Functional Theory in a Convex Treatment
Trygve Helgaker

In his seminal 1983 paper, Lieb gave an elegant and rigorous mathematical formulation of density-functional theory (DFT), in which the ground-state energy and the universal density functional are identified as each other's Legendre–Fenchel transforms [1]. Importantly, Lieb also demonstrated that his convex density functional is nothing but Levy's constrained-search functional expressed in its ensemble formulation [1, 2], a key result in modern DFT. Recent work has considered the relationship between minimizing densities in DFT and ground-state densities [3].

For electronic systems in an external magnetic potential, current-density functional theory (CDFT) was introduced by Vignale and Rasolt in 1987, who introduced the paramagnetic current density as a basic variable in addition to the density [4]. The rigorous mathematical development of CDFT began a decade ago [5–9] but the identification of the constrained-search functional with the Legendre–Fenchel transform was only made in 2021 [10].

At the same time, the last decade has seen significant progress in the application of CDFT to molecular systems in the presence of a magnetic field [11, 12]. CDFT is now routinely used to study the exotic chemistry of molecules in ultrastrong magnetic fields, for example [13].

In the talk, we review the convex formulation of CDFT, while also briefly discussing its applications to chemistry in strong magnetic fields.

[1] E. Lieb, Int. J. Quantum Chem. 1983, 14, 243.

[2] M. Levy, Proc. Natl. Acad. Sci. USA 1979, 76, 6062.

[3] S. Kvaal, T. Helgaker, J. Chem. Phys. 2015, 143, 184106.

[4] G. Vignale, M. Rasolt, Phys. Rev. Lett. 1987, 59, 2360.

[5] E. I. Tellgren *et al.* Phys. Rev. A 2012, 86, 062506.

[6] A. Laestadius, M. Benedicks, Int. J. Quantum Chem. 2014, 114, 782.

[7] A. Laestadius, Int. J. Quantum Chem. 2014, 114, 1445.

[8] A. Laestadius *et al.* J. Chem. Theory Comput. 2019, 15, 4003.

[9] A. Laestadius *et al.* J. Chem. Theory Comput. 2019, 15, 4003.

[10] S. Kvaal *et al.* J. Phys. Chem. Lett. 2021, 12, 1421.

[11] E. I. Tellgren *et al.* J. Chem. Phys. 2014, 140, 034101.

[12] J. W. Furness *et al.* J. Chem. Theory Comput. 2015, 11, 4169.

[13] M. J. Pemberton *et al.* J. Chem. Phys. 2022, 156, 204113.

Variationally Correct Neural Residual Regression for Parametric PDEs: On the Viability of Controlled Accuracy

Mathias Oster

This talk is about learning the parameter-to-solution map for systems of partial differential equations (PDEs) that depend on a potentially large number of parameters covering all PDE types for which a stable variational formulation (SVF) can be found. A central constituent is the notion of variationally correct residual loss function meaning that its value is always uniformly proportional to the squared solution error in the norm determined by the SVF, hence facilitating rigorous a posteriori accuracy control. It is based on a single variational problem, associated with the family of parameter dependent fiber problems, employing the notion of direct integrals of Hilbert spaces. Since in its original form the loss function is given as a dual test norm of the residual a central objective is to develop equivalent computable expressions. A first critical role is played by hybrid hypothesis classes, whose elements are piecewise polynomial in (low-dimensional) spatio-temporal variables with parameter-dependent coefficients that can be represented, e.g. by neural networks. Second, working with first order SVFs, we distinguish two scenarios: (i) the test space can be chosen as an L^2-space (e.g. for elliptic or parabolic problems) so that residuals live in L^2 and can be evaluated directly; (ii) when trial and test spaces for the fiber problems (e.g. for transport equations) depend on the parameters, we use ultraweak formulations. In combination with Discontinuous Petrov Galerkin concepts the hybrid format is then instrumental to arrive at variationally correct computable residual loss functions. Our findings are illustrated by numerical experiments representing (i) and (ii), namely elliptic boundary value problems with piecewise constant diffusion coefficients and pure transport equations with parameter dependent convection field.

Real-space machine learning of correlation density functionals
Elias Polak

Machine learning (ML) is increasingly playing a pivotal role in extending the reach of quantum chemistry methods for both molecules and materials. However, in density functional theory—the primary workhorse for quantum simulations—using ML to address the limitations of human-designed density functional approximations (DFAs) remains elusive, as ML-based approximations suffer from severely limited transferability to unseen chemical systems. The talk will explore the application of real-space ML to DFAs to address this challenge, where energies are learned point-by-point in space through energy densities. This specialized training strategy optimizes the learning process of deep neural networks for energy model functions. Central to the real-space learning approach is the derivation and implementation of correlation energy densities from regularized perturbation theory, enabling two distinct directions for real-space ML of DFAs. First, the Local Energy Loss (LES) model trains energy densities against their implemented counterparts at each point in space. By expanding each system's single energy data point into thousands of spatial data points, LES dramatically enhances the transferability of ML DFAs compared to traditional global energy training. Second, the spin-resolved correlation energy density allows the derivation of real-space, ML-based, and regularized extensions of Spin-Component-Scaled second-order Møller-Plesset perturbation theory. The resulting model opens new avenues for constructing transferable ML DFAs.

Current density and kinetic energy density in density-functional theory
Erik Tellgren

TBA

Electronic Vector Potential from the Exact Factorization of a Complex Wavefunction

Sara Giarrusso

We generalize the definitions of local scalar potentials named kinetic potential and $(N-1)$ potential, which are relevant to properly describe phenomena such as molecular dissociation with density-functional theory, to the case in which the electronic wavefunction corresponds to a complex current-carrying state. In such a case, an extra term in the form of a vector potential appears which cannot be gauged away. Both scalar and vector potentials are introduced via the exact factorization formalism which allows us to express the given Schrödinger equation as two coupled equations, one for the marginal and one for the conditional amplitude. The electronic vector potential is directly related to the paramagnetic current density carried by the total wavefunction and to the diamagnetic current density in the equation for the marginal amplitude. An explicit example of this vector potential in a triplet state of two non-interacting electrons is showcased together with its associated circulation, giving rise to a non-vanishing geometric phase.

Friday December 6th

Mathematical aspects of the adiabatic Dyson equation in linear response time-dependent density functional theory
Thiago Carvalho Corso

In this talk, we present some rigorous results on the Dyson equation for the density-density response function (DDRF) that plays a central role in linear response time-dependent density functional theory (LR-TDDFT). More precisely, we first present a functional analytic setting that allows for a unified treatment of the Dyson equation with general adiabatic approximations for discrete (finite and infinite) and continuum systems. In this setting, we derive a representation formula for the solution of the Dyson equation in terms of an N-body operator version of the Casida matrix. We then present several consequences of this solution formula; in particular, we discuss the stability of the solution and characterize the maximal meromorphic extension of its Fourier transform. In addition, we show that for adiabatic approximations satisfying a suitable compactness condition, the maximal domains of meromorphic continuation of the initial density-density response function and the solution of the Dyson equation are the same. The results presented here apply to widely used adiabatic approximations such as (but not limited to) the random phase approximation (RPA) and the adiabatic local density approximation (ALDA). In particular, these results show that neither of these approximations can shift the ionization threshold of the Kohn-Sham system.

TBA
Louis Garrigue

TBA

Force-Based Density Functional Theories:
An Alternative Framework for Constructing Effective Potentials
Christian Jöns

We introduce an alternative framework for constructing effective potentials in density functional theory by leveraging the fundamental role of forces in determining the electronic structure. By reformulating the Hamiltonian description in terms of forces, we derive a new expression for the exchange potential that is directly related to the forces acting on the electrons. This force-based approach enables the development of more transferable and accurate exchange-correlation functionals, which can overcome limitations of traditional energy-based methods. As a concrete example, we demonstrate how the force-based static Hartree-exchange approximation transforms to a non-adiabatic approximation in time-dependent density-functional theory.

TBA
Alexandar Davidov

TBA

Numerical solutions to the Gross–Pitaevskii Equation using ComFiT
Vidar Skogvoll

The Gross-Pitaevskii equation (GPE) is a cornerstone in the modeling of Bose-Einstein condensates, describing macroscopic quantum phenomena through a nonlinear Schrödinger equation. In this talk, I will go through some of the background theory on the GPE, and present ComFiT, an easy-to-use computational framework for solving the partial differential equations efficiently. I will also talk about the role of vortices in such condensates, including how they can be modeled and visualized using ComFiT, and their importance in understanding the dynamics and topological structures within these quantum systems.

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Notes