

**WORKSHOP:**  
**Optimal Transport meets Density Functional Theory**  
University of Jyväskylä

Time-dependent DFT, 5th-7th June 2017

THE DENSITY-POTENTIAL MAPPING IN QUANTUM DYNAMICS I: BASICS

**Robert van Leeuwen**  
University of Jyväskylä

We will give an overview of the density-potential mapping in time-dependent density-functional theory (TDDFT). We give a discussion of the ideas that form the basis of TDDFT as well as the Kohn-Sham equations and initial state dependence of the density functionals. We further discuss the Runge-Gross mapping and issues of time-analyticity.

We finally outline the basic idea behind the fixed point formulation of the density potential mapping, as reviewed in recent work [1]. Different aspects of this idea will be developed further in more detail in a number of follow-up presentations in this workshop.

[1] *“Existence, uniqueness, and construction of the density-potential mapping in time-dependent density-functional theory”*, M. Ruggenthaler, M. Penz, R. van Leeuwen, J. Phys. Condens. Matter 27, 203202 (2015)

THE DENSITY-POTENTIAL MAPPING IN QUANTUM DYNAMICS II: STRUCTURES

**Michael Ruggenthaler**  
Max-Planck Institute for the Structure and Dynamics of Matter Theory

We will present a fixed-point approach to the density-potential mapping in time-dependent quantum mechanics. This approach is based on the continuity and the local force equation of quantum mechanics. First we will present under which conditions on the initial states and the external potentials these equations are well-defined. In a next step we will invert this equation, for which we need to show that a certain Sturm-Liouville operator is invertible. This will give us conditions on the allowed densities and boundary conditions and allows us to set up an iterative sequence that for a given time-dependent density should converge to the corresponding external potential. In our quest to guarantee that this iterative sequence converges, we show that the internal forces are functionally differentiable or at least Lipschitz continuous with respect to the external potentials. Implications are discussed.

THE DENSITY-POTENTIAL MAPPING IN QUANTUM DYNAMICS III: ISSUES

**Markus Penz**  
Department of Theoretical Physics, University of Innsbruck

The theoretical layout of a fully rigorous density-potential mapping in time-dependent quantum mechanics is scrutinized further in this talk. The two main ingredients for a supposed contraction mapping leading to a fixed point representing the unique external potential belonging to a given density are two inequalities. One is a bound for the inverse of a Sturm-Liouville operator and the other an estimate for the internal forces term with respect to the potential. At this stage the different pieces of the fixed-point scheme are brought into contact and one sees if they fit (spoiler alert: they don't). We want to highlight such issues and also describe possible ways to avoid them from the beginning.

# THE DENSITY-POTENTIAL MAPPING IN QUANTUM DYNAMICS IV: CONTROL THEORY AND NUMERICS

**Soeren Ersbak Bang Nielsen**

Max-Planck Institute for the Structure and Dynamics of Matter Theory

We present a local control theory method to construct the external potential  $v$  that, for a given initial state, produces a prescribed time-dependent density in an interacting quantum many-body system. This allows us to compute any property as a functional of the initial state and density, including the exact Hxc potential, and hence provides a powerful new tool to investigate the fundamental aspects of TDDFT. Additionally, it also provides multiple new density-based ways to do quantum control, complementing the usual potential-based methods. For example, it lets us do optimal control, but where we search over a set of densities instead of a set of potentials. This is mainly useful in the special cases where the objectives can be expressed in terms of the density only, in which case we can first simply find the optimal density, and then use our method, or when we can restrict the search to a small set of densities. Finally, the successful implementation reveals some interesting aspects of how to rigorously implement the time-dependent Schrödinger equation, which are not very well known.

# THE ROLE OF INTERACTIONS IN THE “RUNGE-GROSS THEOREM”

**Jonas Lampart**

CNRS & Universit Bourgogne ICB

Time-dependent density functional theory relies on a one-to-one correspondence between external potentials in the  $N$ -particle Schrödinger equation and the one-particle densities they generate. Runge and Gross argued that this correspondence holds (up to a time-dependent constant in the potential) for sufficiently “*nice*” external potentials. I will discuss a mathematical setting for this argument and explain when it can be made fully rigorous. The interaction potentials play an important role for this and I will discuss the problems that arise in the presence of singular interactions, like the Coulomb potential.

# DISORDERED AND INTERACTING NONEQUILIBRIUM OPEN SYSTEMS: THE EXACT INDEPENDENT-PARTICLE PICTURE FROM DENSITY FUNCTIONAL THEORY

**Daniel Karlsson**

Department of Physics, Nanoscience center, University of Jyväskylä

Density-functional theories often make use of a constructed independent-particle system that reproduces exact quantities of the original interacting system. In systems out of equilibrium, we reverse engineer the true independent-particle potential and bias which reproduces the density and current of an interacting and disordered system. Such potentials can then be used to gain insight into how to non-ambiguously interpret interacting and disordered systems using single-particle potentials. We find that interactions always smoothen the effective disordered energy landscape. The increased smoothness does not always, however, lead to an increase in the current, due to strong interaction effects. We interpret the interplay between disorder and interaction, in an independent-particle picture, by a competition between the smoothness of the effective energy landscape and the reduced effective bias.

# FOUNDATIONS OF DENSITY-FUNCTIONAL THEORY FOR ELECTRON-PHOTON SYSTEMS

**Vasil Rokaj**

Max Planck Institute, Hamburg

In this presentation we study quantum particles interacting with a quantized electromagnetic field. More specifically, we focus on the system of one electron interacting with one photon mode through the minimal coupling prescription in dipole approximation. In the minimal coupling prescription except from the interaction

between the electron and the photon mode, there exists a self-interaction term for the electron. We discuss the importance of this self-interaction, which is a harmonic oscillator interaction, and we show that without this self-interaction our system becomes unbounded from below. In the last part we show how we can introduce such a system in the framework of density-functional theory.

# TIME-DEPENDENT DENSITY-FUNCTIONAL THEORY FOR STRONGLY INTERACTING ELECTRONS

**Luis Cort Barrada**

Department of Physics, Nanoscience center, University of Jyväskylä

We consider an analytically solvable model of two interacting electrons that allows for the calculation of the exact exchange-correlation kernel of time-dependent density functional theory. This kernel, as well as the corresponding density response function, is studied in the limit of large repulsive interactions between the electrons and we give analytical results for these quantities as an asymptotic expansion in powers of the square root of the interaction strength. We find that in the strong interaction limit the three leading terms in the expansion of the kernel act instantaneously while memory terms only appear in the next orders. We further derive an alternative expansion for the kernel in the strong interaction limit on the basis of the theory developed in [Phys. Chem. Chem. Phys. 18, 21092 (2016)] using the formalism of strictly correlated electrons in the adiabatic approximation. We find that the first two leading terms in this series, corresponding to the strictly correlated limit and its zero-point vibration correction, coincide with the two leading terms of the exact expansion. We finally analyze the spatial non-locality of these terms and the limitations of the adiabatic approximation. The ability to reproduce exact quantities in the strong interaction limit indicates that the adiabatic strictly correlated electron formalism is a useful formalism to study the density response and excitation properties for a wide range of systems with strong electronic interactions.

# SOME THOUGHTS FOR GOING BEYOND THE USUAL SCENE

**Klaas Giesbertz**

Vrije Universiteit Amsterdam

In my presentation I intend to discuss two possible directions to extend the strictly correlated electron (SCE) framework beyond its usual arena of applications. Currently, the SCE framework is applied exclusively to the density functional theory (DFT) setting. However, other choices than the density are possible. For example, we could also aim to reproduce the exact current or the exact one- / two-body reduced density matrix. I will discuss some of the advantages / disadvantages of using other quantities than the density.

In the second part of my talk, I would like to share some thoughts on extending the SCE framework to time-dependent DFT. It seems that we only need to recast the fixed point approach (discussed by M. Ruggenthaler, M. Penz and S. Nielsen) into a more suitable form for SCE.