HL 84: Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers VII

Time: Thursday 17:15–19:15 Location: TRE Phy

Topical Talk HL 84.1 Thu 17:15 TRE Phy

Continuum mechanics for quantum many-body systems: the anti-adiabatic approximation — •Giovanni Vignale[1], Xianlong Gao[2], Jianmin Tao[3], Stefano Pittalis[1], and Ilya Tokatly[4] — [1]Department of Physics, University of Missouri, Columbia, MO 65211, USA — [2]Department of Physics, Zhejiang Normal University, Jinhua, Zhejiang Province, 321004, China — [3]Department of Chemistry, Rice University, 6100 Main Street Houston, TX 77005, USA — [4]ETSF Scientific Development Centre, Dpto. Fisica de Materiales, Universidad del Pais Vasco, Centro de Fisica de Materiales CSIC-UPV/EHU-MPC, Av. Tolosa 72, E-20018 San Sebastian, Spain

Classical continuum mechanics is a theory of the dynamics of classical liquids and solids in which the state of the body is described by a small set of collective fields, such as the displacement field in elasticity theory; density, velocity, and temperature in hydrodynamics. A similar description is possible for quantum many-body systems. In this talk I show how the exact Heisenberg equation of motion for the current density of a many-body system can be closed by expressing the quantum stress tensor as a functional of the current density. I then introduce an "anti-adiabatic" approximation scheme for this functional. The anti-adiabatic scheme allows us to bypass the solution of the time-dependent Schroedinger equation, resulting in an equation of motion for the displacement field that requires only ground-state properties as an input. I illustrate the formalism by applying it to the calculation of excitation energies in a few model systems.

HL 84.2 Thu 17:45 TRE Phy

Discontinuities of the Exchange-Correlation Kernel and Charge-Transfer Excitations in TDDFT — •Maria Hellgren and Eberhard K.U. Gross — Max-Planck-Institute of Microstructure Physics, Weinberg 2, Halle, Germany

An intriguing consequence for density functional theory (DFT) arises when considering ensembles with densities integrating to fractional particle number. The total ground-state energy as a function of particle number consists of straight-line segments and, consequently, the corresponding exchange-correlation (XC) potential jumps discontinuously. This feature of the exact theory turns out to be a key property to incorporate in approximate functionals in order to obtain, e.g, accurate band-gaps of solids and correct molecular dissociation limits.

It has been demonstrated that the discontinuous nature of the static XC potential naturally carries over to the XC potential of time-dependent density functional theory (TDDFT) appearing in, e.g., time-resolved ionization processes. How the same property is reflected in the XC kernel, defined as the functional derivative of the XC potential with respect to the density, has, so far, not received any attention. The XC kernel is of fundamental importance in TDDFT as it gives access to the particle conserving excitation spectrum. In this work we have investigated the discontinuities of the XC kernel and found them to be crucial for the description of long-range charge-transfer excitations.

HL 84.3 Thu 18:00 TRE Phy

Insights in the T-matrix formalism — •Pina Romaniello[1,4], Friedhelm Bechstedt[2,4], and Lucia Reining[3,4] — [1]Université Paul Sabatier, Toulouse, France — [2]Friedrich-Schiller-Universitaet Jena, Jena, Germany — [3]École Polytechnique, Palaiseau, France — [4]European Theoretical Spectroscopy Facility

In many-body perturbation theory the self-energy $\Sigma = GW\Gamma$ plays a key role since it contains all the many body effects of the system. The exact self-energy is not known and approximations are needed. As first approximation one can neglect the vertex Γ and obtain the GW approximation. In some cases this is not sufficient, and one needs to go beyond this approximation. In this work we elucidate the concept of T-matrix [1] and its relation with Hedin's equations [2]. Starting from the exact definition of self-energy we illustrate several aspects of the T-matrix formalism: i) which approximations to the self-energy yield the T-matrix formulation, in comparison with those that, instead, yield GW and beyond; ii) the role of the particle-particle and electron-hole contributions to the T-matrix; iii) a screened version of the T-matrix; iv) an approximate vertex that produces the same self-energy as the screened T-matrix. Tests are done on the exactly solvable Hubbard molecule [3].

[1] L. P. Kadanoff and G. Baym, Quantum Statistical Mechanics, W. A. Benjamin, Inc. New York, (1962).

[2] L. Hedin, Phys. Rev. 139, A796 (1965).

[3] P. Romaniello, S. Guyot, and L. Reining, J. Chem. Phys. 131, 154111 (2009); P. Romaniello, F. Bechstedt, L. Reining, in preparation.

HL 84.4 Thu 18:15 TRE Phy

Stochastic current DFT for periodic systems — •Heiko Appel — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

Recently we have introduced stochastic current density functional theory (SCDFT) which is an approach that allows to describe decoherence and dissipation from first principles [1,2]. So far the method has been applied to finite systems only. In this talk I will present an extension of SCDFT to periodic systems. In particular I will discuss a scheme for the stochastic real-time propagation of the Kohn-Sham orbitals in extended systems and also address possible choices for the bath operators that appear in the SCDFT formalism. (Work supported in part by Lockheed Martin, DOE and MPG).

[1] Massimiliano Di Ventra and Roberto D'Agosta, Phys. Rev. Lett. 98, 226403 (2007).

[2] Heiko Appel and Massimiliano Di Ventra, Phys. Rev. B 80, 212303 (2009).

HL 84.5 Thu 18:30 TRE Phy

Wave function based treatment of electronic correlation in solids — •Andreas Grüneis[1], George H. Booth[2], James Spencer[3], Martijn Marsman[1], Ali Alavi[2], and Georg Kresse[1] — [1]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Vienna, Austria — [2]University of Cambridge, Chemistry Department, Lensfield Road, Cambridge CB2 1EQ, U.K. — [3]Department of Physics and Thomas Young Centre, Imperial College London, Exhibition Road, London SW7 2AZ, U.K.

The use of wave function based methods to treat electronic correlation, such as Møller-Plesset perturbation theory, coupled-cluster theory, and full configuration interaction (CI) is common practice in the field of computational quantum chemistry. Due to the computational cost involved, however, these methods have rarely been applied to extended systems. We have implemented the second-order Møller-Plesset perturbation theory and coupled-cluster singles and doubles (CCSD) theory within the framework of the Projector-Augmented-Wave method, using periodic boundary conditions and a plane wave basis set in VASP.[1] Moreover, an interface between VASP and the full CI quantum Monte Carlo (FCIQMC) code presented in Ref.[2] has been developed. We have tested our implementations on small molecules and solids. We outline techniques that reduce the computational effort of CCSD and FCIQMC calculations, such as the use of natural orbitals and progressive downsampling. [1] A. Grüneis et al. JCP 133, 074107 (2010). [2] G. H. Booth et al. JCP 131, 054106 (2009).

HL 84.6 Thu 18:45 TRE Phy

Finite temperature reduced density matrix functional theory (FT-RDMFT) A novel approach to the description of quantum systems in thermal equilibrium. — •Tim Baldsiefen and E.K.U. Gross — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Despite the big success of DFT for the description of groundstate properties of quantum mechanical systems, the finite temperature extension FT-DFT showed only little success in a restricted field of research. We develop the theoretical foundation for an alternative description of equilibrium properties, by employing the one-reduced density matrix (1RDM) rather than the density as central variable. The zero-temperature version of this theory proved to be quite successful in the last years, allowing for the description of groundstate properties of a wide class of systems (e.g. small molecules [1] and solids [2]). This sparks the hope, that a description of finite temperature ensembles by means of the 1RDM will succeed on fields of research formerly inaccessible by FT-DFT.

In this framework of FT-RDMFT we are able to employ methods from many body perturbation theory to develop approximate free-energy functionals. An application to the groundstate of the electron gas shows, that FT-RDMFT is able to significantly improve the groundstate energy compared to a strictly perturbative treatment.

[1] N. N. Lathiotakis et al., Phys. Rev. A, 79, 040501 (2009)

[2] S. Sharma et al., Phys. Rev. B 78, 201103(R) (2008)

HL 84.7 Thu 19:00 TRE Phy

Spin spirals in the uniform electron gas: Towards a new functional in SDFT

— •F. G. Eich[1,2] and E. K. U. Gross[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Freie Universität Berlin, Berlin, Germany

Based on our studies of the spin-spiral state of the uniform electron gas [1], we present a novel exchange-correlation functional for Spin-Density-Functional Theory (SDFT).

Much like in the well known local-density approximation (LDA) the local exchange-correlation energy is approximated by the exchange-correlation energy of the uniform electron gas. In contrast to the standard LDA the state of the electron gas is not only specified by its density but furthermore by its spin magnetization and spin-spiral wave vector. We show that, in order to determine a local spin-spiral wave vector, gradients of the spin magnetization have to be included in the functional.

As a first step towards application for real materials we obtain the energy of the spin-spiral electron gas using the random-phase approximation.

[1] F.G. Eich, S. Kurth, C. R. Proetto, S. Sharma, and E. K. U. Gross, Phys. Rev. B 81, 024430 (2010)