Universität Rostock Traditio et Innovatio

INSTITUT FÜR PHYSIK

Promotionskolloquium

Am Freitag, dem 09. Dezember 2016, verteidigt um 15:00 Uhr
im Hörsaal I des Instituts für Physik

Herr M.Sc. Mārtiņš Brics
(Theoretische Physik)

seine Dissertation zum Thema:

"Benchmarking time-dependent renormalized natural orbital theory with exact solutions for a laser-driven model helium atom"

Abstract

Intense, ultra-short laser pulses interacting with atoms, molecules, clusters, and solids give rise to many new fascinating phenomena, not at all accessible to quantum mechanics textbook perturbation theory. A full numerical solution of the time-dependent Schrödinger equation (TDSE) for such strong-field problems is also impossible for more than two electrons. Hence, powerful time-dependent quantum many-body approaches need to be developed. Unfortunately, efficient methods such as time-dependent density functional theory (TDDFT) fail in reproducing experimental observations, in particular if strong correlations are involved. In TDDFT, the approximation not only lies in the so-called exchange correlation potential but also in the density functionals for the observables of interest. In fact, with just the single-particle density alone it is unclear how to calculate, e.g., multiple-ionization probabilities or photoelectron spectra, or, even worse, correlated photoelectron spectra, as measured in nowadays experiments.

In general, the simple structure of the time-dependent many-body Schrödinger equation for a highly-dimensional many-body wavefunction can only be traded for more complicated equations of motion for simpler quantities. In this thesis, a theory is examined that goes one step beyond TDDFT as far as the complexity of the propagated quantity is concerned. In time-dependent renormalized natural orbital theory (TDRNOT), the basic quantities that are propagated in time are the eigenvalues and eigenstates of the one-body reduced density matrix (1-RDM). The eigenstates are called natural orbitals (NOs), the eigenvalues are the corresponding occupation numbers (ONs). Compared to TDDFT, the knowledge of the NOs and the ONs relax the problem of calculating observables in practice because they can be used to construct the 1-RDM and the two-body reduced density matrix (2-RDM).

After the derivation of the equations of motion for a combination of NOs and ONs, the so-called renormalized natural orbitals (RNOs), TDRNOT is benchmarked with the help of a numerically exactly solvable model helium atom in laser fields. In the special case of time-dependent two-electron systems the two-particle density matrix in terms of ONs and NOs is known exactly. Hence, in this case TDRNOT is exact, apart from the unavoidable truncation of the number of RNOs per particle taken into account in the simulation.

It is shown that, unlike TDDFT, TDRNOT is able to describe doubly-excited states, Fano profiles in electron and absorption spectra, auto-ionization, Rabi oscillations, high harmonic generation, non-sequential ionization, and single-photon double ionization in excellent agreement with the corresponding TDSE results.

Interessenten sind herzlich eingeladen!

Prof. Dr. W. Vogel
Promotionsbeauftragter