DOKTORAND:	Sarah Reimann
GRAD:	Philosophiae doctor
FAKULTET:	Det matematisk-naturvitenskapelige fakultet
INSTITUTT:	Kjemisk institutt
FAGOMRÅDE:	Teoretisk kjemi
VEILEDERE:	Trygve Helgaker, Ulf Ekström, Alex Borgoo
DISPUTASDATO:	02.11.2018

AVHANDLINGENS TITTEL: *Treatment of Magnetic Fields in Density-Functional Theory*

Necessity to improve the density of present approximate density functionals to fully benefit of a magnetic-field dependence

Density-functional theory (DFT) is the most widely used method for electronic structure calculations, including the computation of magnetic properties for molecular systems. However, standard DFT calculations utilize exchange-correlation density-functional approximations (DFAs) that have been developed in the absence of a magnetic field. It is still not understood how to include the magnetic in a rigorous way.
This work investigates the possibility to use the density and the magnetic field as basic variables, as opposed to current DFT (CDFT) where the electron density and the current density are used. The connection between both approaches is established.
From a more practical point of view, the effect of introducing a magnetic-field dependence into DFAs to improve the computation of magnetic properties is investigated. One important conclusion is that the present absence of this field dependence is a leading source of error for calculations of NMR shielding constants.
However, for another magnetic property, the magnetizability, the main error is due to the poor self-consistent density of the DFAs. This suggests that it is important to improve the density of existing DFAs, since otherwise the benefits of introducing a magnetic-field dependence get lost due to larger errors made by the poor density.
This work shows that the main error that is made in the density in the presence of a magnetic field is already present at zero field strength. Therefore, it is important to improve present DFAs even in the absence of a field.