Title: Excited States and Optical Response Theory

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ECTS: 2.5

Place: Skjernvej 4

Time: Each day from 9.00 – 12.00 and 13.00 to 15.30

In this PhD course, the focus in on excited states and their role in the optical response. We discuss general features of excitations induced by electromagnetic fields. The theoretical calculation of excited states in quantum mechanics is complicated because most methods are designed for ground-state calculation. This goes for conventional Hartree-Fock theory and density-functional theory (DFT). However, with suitable modification excited states can be computed with reasonable accuracy.

In the course, we will our way up from the simple case of an isolated atom, in particular, helium. Here, the lowest excitations are discrete states. We the turn to metallic nanoparticles and study the collective excitations, i.e. plasmons. Finally, we will investigate the optical response of crystalline semiconductor and look at many-body excitations here too.

The contents are listed below. Course material is "Electric, Optical and magnetic Properties of Nanostructures" 2014 version. Chapters 1, 2, 15, and 24 are background material.

1. 17/2 Optical response theory (Ch. 1+2)
2. 18/2 Optical response of simple atoms (Ch. 27)
3. 19/2 Hartree-Fock (HF) theory and DFT (App. 3+4)
4. 20/2 Computer implementation of Hartree-Fock theory in Gauss basis
5. 21/2 Configuration interaction and application to Helium (App. 4)
6. 24/2 Time-dependent density-functional theory (TDDFT) (Ch. 28)
7. 25/2 The jellium model of metallic nanoparticles (App. 5)
8. 26/2 Plasmons and properties of metallic nanoparticles (App. 5)
9. 27/2 Electronic and optical properties of semiconductors (Ch. 15)
10. 28/2 Excitons in semiconductors (Ch. 18+19).