Technische Universität Berlin
Institut für Theoretische Physik
Lecture Course: Prof. Dr. Matthias Scheffler, Dr. Patrick Rinke, Dr. Alex Tkatchenko
Exercises: Dr. Volker Blum

April 25, 2012

http://www.itp.tu-berlin.de/menue/lehre/lv/ss12/wahlpflichtveranstaltungen/theoretische_festkoerperphysik_i_ii_theoretical_material_science/

Theoretical Material Science: Exercise Sheet 3

Please hand in solutions by: Wednesday, May 2, start of the exercise class

Exercise 7 (4 points): *Koopmans' theorem*
Inspect the chapter in the lecture notes, where the relation between Ionization energy I_k and Lagrange parameters ϵ_{oi} is shown, i.e. at the equation

$$I_k := \langle \Phi^{N-1} | H^{e,N-1} | \Phi^{N-1} \rangle - \langle \Phi^N | H^{e,N} | \Phi^N \rangle \approx -\epsilon_{o_k s_k}.$$

Write down and explain the calculation leading to this result. Which assumptions are needed?

Exercise 8 (8 points): *Numerical solution of free atoms, using an electronic structure code*
The following description is only a skeleton description of the task. A more detailed description of the tasks to be performed will be provided separately. The actual task will be performed using a general-purpose electronic structure code, installed at the "PC pool" of the Physics Department. We will begin the exercise together at the PC pool. Any remaining parts should be done as homework during the opening hours of the pool.

a) Using a so-called "minimal basis" (only one basis function, valid for hydrogen), perform a self-consistent Hartree-Fock calculation for the Hydrogen atom. What are the single-particle energies and total energies? How close are they to the result that you expect? What could be the origin of the difference?

b) Perform the same calculation, except using the "local-density approximation" of Kohn-Sham density functional theory. What do you obtain? Do the results match your expectations?

c) Repeat tasks a) and b), but this time with "basis sets" of increasing size. What are the eigenvalues and total energies, and at which point do you conclude "convergence"?

d) Plot the electron density of the (converged) free Hydrogen atom in three dimensions and visualize the result.

e) Plot the electron density of the (converged) free Hydrogen atom along the x axis (in one dimension), but integrated on a sphere (for a spherical atom, this means $4\pi r^2 n(r)$). At which distance from the nucleus do you find the major part of the electron density?

f) For the Si atom, compare the eigenvalues, total energy, one-dimensional and three-dimensional density in Hartree-Fock theory, and in the local-density approximation. What is the meaning of the order of the eigenlevels, and which differences for the different levels of theory do you observe? Do the results match your expectations? Can you interpret the shape of the 1d density?

Please turn over!⟶

- **Webpage of the lecture:**
  http://www.itp.tu-berlin.de/menue/lehre/lv/ss12/wahlpflichtveranstaltungen/theoretische_festkoerperphysik_i_ii_theoretical_material_science/
  http://th.fhi-berlin.mpg.de/sitesub/lectures/spring_2012/
- **Lecture:** Tue. & Wed., 10:00 h -12:00 h (sharp!) in room EW 203, TU Berlin
- **Exercise:** Wed., 14:00 h in room EW 229
- **Literature:**
  - Ashcroft, Mermin, David: Solid state physics, Saunders College, Philadelphia, 1981
  - Kittel: Quantum theory of solids,Wiley, New York, 1963
  - Ziman: Principles of the theory of solids, Cambridge University Press, Cambridge, 1964
  - Ibach, Lueth: Solid-state physics: an introduction to principles of materials science, Springer, Berlin, 1995
  - Madelung: Festkörpertheorie, Springer, Berlin, 1972
  - Scherz: Quantenmechanik, Teubner, Stuttgart, 1999
  - Dreizler, Gross: Density functional theory: an approach to the quantum many-body problem, Springer, Berlin, 1990
  - Parr, Yang: Density-functional theory of atoms and molecules, Oxford University Press, Oxford, 1994
  - Anderson: Basic notations of condensed matter physics, Benjamin/Cummings, London, 1984
  - Marder: Condensed matter physics, Wiley, New York, 2000
  - Martin: Electronic Structure, Cambridge University Press, Cambridge, 2004
  - Kohanoff: Electronic Structure Calculations for Solids and Molecules: Theory and Computational Methods, Cambridge University Press, Cambridge, 2006
- **"Übungsschein"-criteria:**
  - Regular and active participation in the exercises
  - Presentation of homework tasks and
  - 50% of the homework points.
  - Active participation in computational exercises
- **Consultation hours:**
  - Prof. Dr. Matthias Scheffler, Dr. Alex Tkatchenko, Dr. Patrick Rinke: by appointment
  - Dr. Volker Blum: Available Wed. 16:00 (after the exercise class) or by appointment