

Tentamen DIP, Maandag 23 januari 2017, 14:00-17:00 uur, Gorlaeus collegezaal 01

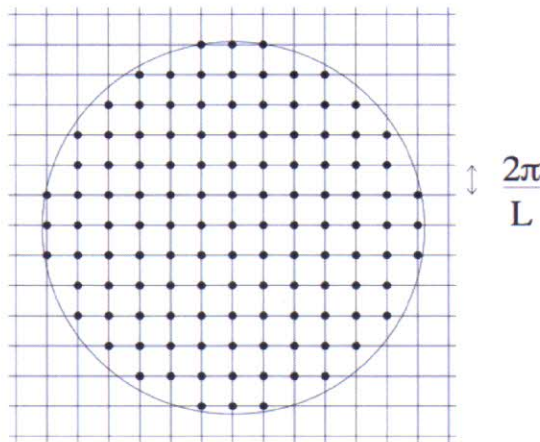
<p>Tentamen: Density Funtional Theory in Practice (DIP) (4423DFTP6-1617FWN)</p> <p>Datum: 23 januari 2017</p> <p>Tijd/tijdsduur: 14.00-17.00 (3 uur)</p> <p>Docent(en) en/of tweede lezer:</p> <p>Dr. J. Meyer</p> <p>Dit tentamen bestaat uit: (aantal opgaven en punten per opgave)</p> <ol style="list-style-type: none">1. Grondslagen van de DFT (30 punten)2. Basis sets en pseudopotentials (20 punten)3. DFT berekeningen in de praktijk (25 punten)4. Het von-Weizsäcker functioneel (25 punten) <p>Vermeld duidelijk op ieder vel: naam en studienummer</p> <p>Maak dit tentamen in blauwe of zwarte inkt. Geen potlood!</p> <p>Veel succes!</p>	<p>Exam: Density Funtional Theory in Practice (DIP) (4423DFTP6-1617FWN)</p> <p>Date: 23 January 2017</p> <p>Time/duration: 14.00-17.00 (3 hours)</p> <p>Lecturer(s) and/or second reader:</p> <p>Dr. J. Meyer</p> <p>This examination consists of: (number of items and points per item)</p> <ol style="list-style-type: none">1. Foundations of DFT (30 points)2. Basis sets and pseudopotentials (20 points)3. DFT in practical calculations (25 points)4. The von-Weizsäcker functional (25 points) <p>Please clearly indicate on each sheet: name and study number</p> <p>Please write with blue or black ink. Don't use a pencil!</p> <p>Good Luck!</p>
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1. Foundations of DFT (30 points)

- a) Why is the electron density of a molecule with N electrons a “more convenient” target variable than its wave function? (2 points)
- b) Explain what the Hohenberg-Kohn theorems state. (6 points)
- c) Which energy terms have Kohn and Sham introduced in attempt to reduce what is unknown about the Hohenberg-Kohn functional? (2 points)
- d) How are the Kohn-Sham equations coupled and why do they have to be solved iteratively? (4 points)
- e) How many different Kohn-Sham equations need to be solved for a spherical Ne atom in its ground state ($1s^2 3d^6 4s^2$), using non-relativistic LDA and LSDA? (2 points)
- f) For which system is the local density approximation (LDA) for the exchange-correlation functional exact? (2 points)
- g) Sketch Jacob's ladder for density functionals as introduced by John Perdew and give the name of one functional per rung of the ladder from the literature. (6 points)
- h) Which two fundamentally different paradigms are currently followed in order to improve exchange-correlation functionals? (2 points)
- i) In their very recent work discussed during the lecture (Science 355 (2017) 49), M.G. Medvedev *et al.* claim that “*Density functional theory is straying from the path toward the exact functional*”. Explain how they come to this statement. (4 points)

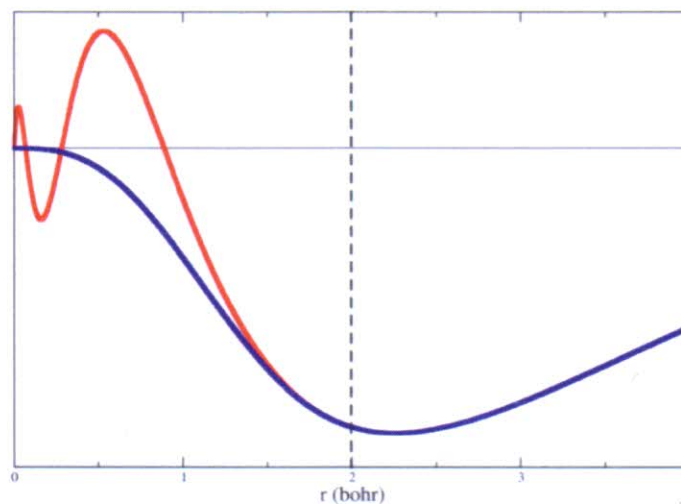
2. Basis sets and pseudopotentials (20 points)

- a) The Kohn-Sham equations are differential equations. However, after the introduction of a basis set, what kind of mathematical problem needs to be solved (on the computer) in order to obtain the Kohn-Sham single-particle energies? (2 points)
- b) Explain what Slater-type and Gaussian-type orbitals are and compare their advantages and disadvantages. (6 points)
- c) Explain what "STO-3G" stands for. (3 points)
- d) What does the picture below show in the context of the expansion of electronic states into plane waves?



What (else) determines the size of a plane wave basis set? (2 points)

- e) Which of the two colored lines in the picture below depicts a pseudo- and which depicts an all-electron wavefunction? What does the dashed line indicate? (2 points)



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f) Explain how pseudopotentials can reduce the size of a plane wave basis set in DFT calculations. (3 points)

g) Name one well-known DFT code using

- Gaussian atomic orbitals (GTOs)
- plane waves

as basis sets – either from the articles that were discussed during the lecture or used during the computer exercises. (2 points)

3. DFT in practical calculations (25 points)

- a) Name a common convergence criterion for a self-consistent field (SCF) cycle. (2 points)
- b) Explain what a density mixing scheme does and name one example for such a scheme. (4 points)
- c) (Bulk) Defects, surfaces and molecules break (three-dimensional) periodicity. Describe how these can be modeled within periodic boundary condition including sketches. What must be carefully checked in such calculations? (7 points)
- d) Explain how lattice constants are usually calculated with any given (periodic) DFT code. (4 points)
- e) What is the usual trend for the error of lattice constants calculated with LDA and GGAs, as e.g. observed by P. Haas *et al.* in their paper “*Calculation of the lattice constant of solids with semilocal functionals*” (Phys. Rev. B. 79 (2009) 85104) discussed during the lecture. (2 points)
- f) Together with many collaborators K. Lejaeghere *et al.* have investigated the “*Reproducibility in density functional theory calculations of solids*” in their article (Science 351 (2016) aad3000) discussed during the lecture. Describe what the authors distinguish as “precision” and “accuracy”. What kind of measure do the authors suggest for the former? What type of codes do generally yield results that are in very good agreement with each other? (6 points)

