Course Outline

Course outline, grading policy, resources etc.

Octave Tutorial

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es from the tutorial held on 13/11/2012

ecture Notes

nese lecture notes are for the use of PHYS741 students.
nters to references and additional reading material is given
below the links to lecture notes. The notes are being updated
stantly so make sure to check back often.

- Lecture 01 : Variational principle (updated 04/10/2012)
  - Micheal Springborg, Methods of Electronic Structure Calculation : Chapter 5
  - Octave codes for linear variation :
    - integral.m
    - second_der.m
    - delta_linear.m

- Lecture 02 : Fundamental concepts in solid states (updated 13/10/2012)
  - Charles Kittel, Introduction to Solid State Physics : Chapters 1 and 2
  - Richard Martin, Electronic Structure : Chapter 4
  - Micheal Springborg, Methods of Electronic Structure Calculation : Chapter 19
  - Otfried Madelung, Introduction to Solid State Theory : Chapter 2

- Lecture 03 : The many-body Hamiltonian and the functional derivative (updated 09/03/2009)
  - Kieron Burke : ABC of DFT (excellent book by Prof Burke) : Chapter 2
- Lecture 04 : Hartree-Fock theory (updated 15/03/2009)
  - Micheal Springborg, Methods of Electronic Structure Calculation : Chapter 9
  - Philip Phillips, Advanced Solid State Physics : Chapter 4
- Lecture 05 : Total energy in terms of density (old)
- Lecture 06 : The Hohenberg-Kohn theorem and Kohn-Sham equations (updated 06/04/2009)
  - Walter Kohn : Nobel Lecture
  - P. Hohenberg and . Kohn : Phys Rev 136 B864(1964)
  - W. Kohn and J. Sham : Phys Rev 140 A1133 (1965)
  - R. Stowasser and R. Hoffmann : What do Kohn-Sham Orbitals and Eigenvalues Mean?, Journal of the Americal Chemical Society, 121, 3414 (1999)
- Lecture 07 : Planewave expansion (old)
- Lecture 08 : The pseudopotential (updated 03/05/2009)

    - Efthimios Kaxiras, Atomic and Electronic Structure of Solids : Chapter 2.7
    - Hamann, Schluter and Chiang : Phys Rev Lett, 43, 1494 (1979)
    - Kleinman and Bylander : Phys Rev Lett 48 1425
    - D. Vanderbilt : Phys Rev B 41 7892 (1990)
- Lecture 09 : Brillioun zone integration (old)
- Lecture 10 : Self-consistent solution of the Kohn-Sham equations (old)
- Lecture 11 : Iterative diagonalization methods (old)
- Lecture 12 : Exchange and correlation (old)

Term paper topics and related reading material

- DFT and strongly correlated systems
    - What is the Hubbard U and how is it incorporated into a DFT calculation?
    - The LDA+U method
    - The LDA+U+V extension
    - Dynamical mean field method and DFT
- Relativity
    - How is relativity incorporated into the DFT Hamiltonian?
    - Spin-orbit coupling
    - Noncollinear spin
- The band gap problem
    - The band gap problem in DFT, Janak's theorem, the problem of discontinuous derivative
    - Many-body perturbation theory
    - The GW method and the Bethe-Salpeter ansatz
- TDDFT and current density functional theory
- Exchange-correlation functionals
    - Homogeneous electron gas
    - Local density approximation (LDA)
    - Generalized-gradient approximation (GGA)
    - Spin considerations
    - Hybrid functionals
    - Exact exchange
- Chemical methods
    - Hartree-Fock
    - Configuration interaction
    - Coupled clusters
- USPP, PAW, GIPAW
- Electric and magnetic fields in DFT
- Meaning of KS orbitals

Homework

- Homework 01 : Due on 8 Nov 2012
    - integrate.m
    - differentiate.m

- Homework 02 : Due on 22nd November Thursday
- Homework 03 : Due on 20th December Thursday