SOLID-STATE PHYSICS

http://www2.phys.uniroma1.it/doc/mauri/ssp/

1 Introduction

1.1 Measuring electronic bands in solids with Arpes: quasiparticles and signature of interaction as lifetime broadening and kinks in the dispersion. Examples of experiments on neutral and doped graphene

1.2 Predictive power of theory: mean-field band structure comparison with experiments

2 Mean field description of electrons in solids: Hartree-Fock

2.1 Band structure in presence of spin-orbit interaction: spinor and Kramer's doublets

2.2 Ground-state of N-independent electron systems. Slater determinants and one-body density matrix

2.3 Ground-state of N-interacting electron systems. Energy in terms of the one-body density matrix and the two-body probability density.

2.4 Hartree-Fock (HF). General derivation non-collinear

2.2 HF collinear: magnetic and non magnetic cases

2.3 Self-consistent HF Hamiltonian

2.3 Interacting 3D Jellium: experimental realization, HF total energy and band structure, ferromagnetic instability, correlation energy, pair correlation function, impact of correlation on Kinetic energy

3 Mean field description of electrons in solids: Density functional theory

3.1 Hohenberg-Kohn (HK) and Kohn and Sham (KS) theorems

3.1 Thomas-Fermi approximated functional

3.3 HK and KS functionals and KS Hamiltonian

3.4 Approximated exchange and correlation functionals (LDA GGA)

4 Derivatives of total energy: physical observables

4.1 Introduction to IR and optical spectroscopy (dielectric tensor in IR and visible range) and Raman spectroscopy

4.2 First order derivatives: pressure, forces, and polarization

4.3 Second-order derivatives: electronic dielectric tensor, vibrational (phonon) frequencies, elastic constancies, IR vibrational activity (effective charges), and piezoelectric tensor

4.4 Third order derivatives: anharmonic vibrational broadening, Raman vibrational activity

5 Evaluation of derivatives of total energy: response theory for static perturbations with a mean field approach

5.1 Evaluation of first and second order derivatives within DFT: general expression from perturbation theory

5.2 Density-density response for a generic system (in real space and reciprocal space). Interacting and bare susceptibility in DFT and RPA.

5.3 Density-density response in Jellium. Lindhard functions in one two and three dimensions. Screened Coulomb potential in reciprocal and real space.

5.4 Response to a uniform static electric field in an insulator. Susceptibility, piezoelectric tensor and effective charges

6 Spontaneous electric polarization in solids as a Berry phase

6.1 Ferroelectric material: measurement of hysteresis cycles in the Polarization/electric field space. Spontaneous polarization (in zero electric field)

6.1 Polarization as average dipole per unit cell. Quantization of polarization for classical discrete charges and apparent paradox associated to the definition in a quantum mechanical context.

6.2 Definition of the Berry phase in the discrete and continuous case

6.3 Example of Berry phase: Aharonov-Bohm effect, molecular Aharonov-Bohm effect

6.4 Wannier functions. Definition and properties

6.5 Centroids of Wannier functions as a Berry phase in Bloch space

6.6 Demonstration that the spontaneous polarization is given by the centroids of Wannier functions

7 Exercise sessions (integral part of the program)

7.1 Graphene π-electron band structure and ARPES

7.2 Density matrix and pair correlation function in Jellium
7.3 Dissociation of the H_2 molecule with a 2-site Hubbard model: exact solution and approximated restricted and unrestricted HF solutions.
7.4 Calculation of the macroscopic susceptibility as long-wave limit of a sinusoidal modulated perturbation
7.5 Spontaneous polarization, Berry phase and Wannier functions of a linear 2-atom chain

Prerequisites: *Solid State Physics,* Ashcroft and Mermin*, Chapter 8 and 22 (with exercises), Appendix D, E, F*
For further reading:
Fundamentals of Condensed Matter Physics, Cohen and Louie, Cambridge University Press, *Chapters 5, 6, 7, 8, 10*
Solid State Physics (Second Edition), Grosso and Pastori-Parravicini*,* Accademic Press, *Chapters 4 and 8*
Quantum Theory of the electron liquid, Giuliani and Vignale, Cambridge University Press*, Chapters 1, 2, 3, 4 (selected parts).*