TOPICS IN FUNDAMENTAL PHYSICS

[Michele Modugno, Asier Eiguren]

I. Introduction to the Physics of Ultracold Atoms (2 ECTS)

Introduction. General overview of the field. Historical perspective and current directions.

Condensation of bosons in harmonic traps. Condensates of non-interacting bosons. Trapped bosons at finite temperature. Critical temperature. Density of thermal particles. Finite size effects. Role of dimensionality. Effects of interactions.

Gross-Pitaevskii (GP) theory. Many-body Hamiltonian. GP equation. Thomas-Fermi regime. Hydrodynamic formulation. Scaling solutions. Free expansion. Small oscillations. Dipole mode. Scaling of a thermal gas. Momentum distribution.

Collective excitations. Bogoliubov theory. Quasi-particle thermal distribution. Uniform system. Landau criterion for superfluidity. Energetic and dynamical instabilities.

Ultracold atoms in optical lattices. General results for periodic systems. Semiclassical equation of motion. Bloch oscillations. Tight binding regime. Wannier functions. Discrete non-linear Schrödinger equation. Momentum distribution. Bose-Hubbard Hamiltonian. Mott insulator.

Bibliography

M. Modugno, *An introduction to the theory of Bose-Einstein condensation in trapped gases*, lecture notes.
F. Dalfovo et al., *Theory of Bose-Einstein condensation in trapped gases*, Rev. Mod. Phys. **71**, 463 (1999).
C. J. Pethick & H. Smith, *Bose-Einstein Condensation in Dilute Gases,* Cambridge, (2008).
I. Bloch et al., *Many-body physics with ultracold gases*, Rev. Mod. Phys. **80**, 885 (2008).
L. Pitaevskii & S. Stringari, *Bose-Einstein Condensation and Superfluidity*, Oxford (2016).

II. Topics in Computational Techniques in Condensed Matter (2 ECTS)

Introduction to Density Functional Theory. Historical background and importance of DFT. Basic principles and the Hohenberg-Kohn theorems. The Kohn-Sham equations. Exchange-correlation functionals: Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA).

Introduction to Plane Wave Expansion. Fourier transformation and the plane wave basis. Concept of cutoff and relation to space resolution. Periodic boundary conditions and reciprocal space. Introduction to QUANTUM ESPRESSO software.

Pseudopotentials. Role of pseudopotentials in plane wave calculations. Norm-conserving vs. ultrasoft pseudopotentials.

Linear Combination of Atomic Orbitals (LCAO). Fundamentals of LCAO. Comparison with plane wave methods. Introduction to SIESTA software.

Introduction to Wannier Functions. Definition and basic properties of Wannier functions. Comparison with Bloch functions. The Wannier function transformation.

Construction of Wannier Functions. Maximally localized Wannier functions (MLWFs). Methods to construct Wannier functions: Marzari-Vanderbilt method. Hands-on session: Constructing Wannier functions using Wannier90.

Applications of Wannier Functions. Band structure interpolation. Calculating Berry phases and Berry curvatures. Wannier functions in tight-binding models. Hands-on session: Band structure interpolation using Wannier functions.

Bibliography

D. Sholl, J. A. Steckel, *Density Functional Theory: A Practical Introduction*, Wiley, 2009.
J.M. Soler *et al.*, *The SIESTA Method for Ab Initio Order-N Materials Simulation*, J. Phys. Condens. Matter. **14**, 2745 (2002).
S. Baroni, S. de Gironcoli, A. Dal Corso, *Phonons and Related Crystal Properties from Density-Functional Perturbation Theory*, Rev. Mod. Phys. **73**, 515 (2001).
N. Marzari and D. Vanderbilt, *Wannier Functions and Their Applications,* Rev. Mod. Phys. **84**, 1419 (2012).

Assessment by **continuous evaluation** (homeworks, class activities).