basque center for applied mathematics

EXCELENCIA SEVERO OCHOA

EUSKO JAURLARITZA GOBIERNO VASCO
HEZKUNTZA, UNIBERTSITATE ETA IKERKETA SAILA
DEPARTAMENTO DE EDUCACIÓN, UNIVERSIDADES E INVESTIGACIÓN

Courses 2015-16

November 2, 4, 5, 6 & 11, 2015 (Nov. 2 11:30 - 13:30 ; Nov. 4-6 9:30 to 11:30; Nov. 11 15:00-17:00)

BCAM-Basque Center for Applied Mathematics, Bilbao, Basque Country, Spain www.bcamath.org

Carlos GARCÍA-CERVERA, University of California, Santa Barbara, USA

INTRODUCTION TO QUANTUM MECHANICS AND DENSITY FUNCTIONAL THEORY

The quantum many-body problem and its various approximations lie at the foundation of chemistry and condensed matter physics. In the non-relativistic case, in principle, all the equilibrium and non-equilibrium properties of the condensed matter can be derived by solving the many-body Schroedinger's equation. This equation has proven to be quite formidable, in many respects. There seems to be an, apparently, endless sequence of qualitatively different classes of solutions. Depending on the initial conditions and on the atoms involved, the solutions can display, for example, insulating, metallic, (electronic) super-conducting, highly correlated or topological character. Although there exists a handful of exactly solvable model quantum systems, which are of great importance for the theory of condensed matter, the Schroedinger equation in its general form remains unsolvable even with the present day computer revolution.

Equilibrium and non-equilibrium Density Functional Theories (DFT) are rigorous and formally exact theories which map the interacting N-electron problem into a non-interacting N-electron problem. The non-interacting electrons move in an effective potential that has a universal functional dependence on the electron density. As a result, the problem is reduced to a problem in dimension 3, amenable for computation. The development of the theory has had tremendous impact in a number of areas. So much so that Walter Kohn was awarded the Nobel Prize in Chemistry in 1998 for his development of this theory.

In this course we will provide a brief introduction to Quantum Mechanics and the Schroedinger equation, paying special attention to its spectral properties. In particular, we will explicitly solve some classical examples, such as the structure of the Hydrogen atom, and the cases of a delta-mass, step function, and harmonic potentials. These example illustrate not only some of the techniques, but also the fundamental differences between quantum and classical mechanics. After this introduction, we will focus on the mathematical foundations of density functional theory, covering some of the recent results in this area, and some of the challenges that remain.

REFERENTES

The teacher will extract material from "Quantum Mechanics" by Messiah (although other introductory texts on quantum mechanics can be used as well), "Density Functional Theory" by Parr and Yang, "Density Functional Theory" by Engel and Dreizler, and from published articles.

*Inscription is required: So as to inscribe send an e-mail to roldan@bcamath.org