## TRAINING IN ADVANCED LOW ENERGY NUCLEAR THEORY

# **Course 4 -** Density Functional Theory and Self-Consistent Methods

### **Detailed Course Outline**

The program of the course has been designed so that students can start working on their computational projects and hands-on exercises as quickly as possible. For each lecture, the teaching team will release a set of slides (in LaTeX format) containing (i) the objective of the lecture, (ii) a condensed list of basic equations, theorems, results forming the backbone of the lecture and (iii) one or several take-away messages.

Week 1 - Basic techniques of quantum many-body physics		
Monday	General Introduction and Tools: Reminder of advanced quantum mechanics: Coordinate and momentum representations of the Hilbert space, discrete bases, operators, Schrödinger equation, spin, isospin	
Tuesday	Density functional theory (DFT): Existence theorems, Kohn-Sham schemes, local density approximation, exchange-correlation, self-interaction	
Wednesday	Second quantization: Fermions and bosons, Fock space, Wick theorem, equiva- lence between representations	
Thursday	Hartree-Fock (HF) theory: product states, density matrices, variational principle, Thouless theorem, Koopmans theorem	
Friday	Spontaneous symmetry breaking I: <i>Pairing correlations</i> . BCS theory, pairing tensor, Hartree-Fock-Bogoliubov (HFB) theory	

Week 2 - Structure and dynamics		
Monday	Spontaneous symmetry breaking II: <i>Nuclear deformation</i> . Symmetries, symmetry restoration	
Tuesday	Random Phase Approximation (RPA): Introduction to time-dependent Hartree-Fock (TDHF) theory, linear response, stability matrix	
Wednesday	Nuclear collective motion I: <i>Configuration mixing</i> . Multi-reference DFT, transition densities, generator coordinate method (GCM)	
Thursday	Nuclear collective motion II: <i>Adiabatic approximation</i> . Adiabatic approximation to time-dependent DFT, collective variables, residual interactions	
Friday	Phenomenological nuclear functionals I: <i>Energy density functional</i> . Invariance properties, effective pseudopotentials, Skyrme and Gogny forces, pairing forces	

Week 3 - Phenomenology and applications		
Monday	Phenomenological nuclear functionals II: <i>Practical implementation</i> . Nuclear matter, experimental constraints	
Tuesday	Nuclear phenomenology: Nilsson orbitals, experimental observables (multipole moments, gamma spectroscopy, moments of inertia, etc.)	
Wednesday	Realistic DFT solvers: theoretical models and code complexity, high- performance computing, numerical uncertainties	
Thursday	Open questions in nuclear DFT: non-empirical functionals, inclusion of collective correlations, symmetries	
Friday	Course summary, discussions	

#### Local info

The course will be held from July 17 to August 6 in 2016 at the University of York, UK. Lodging and food will be provided through a contract signed with the York Conferences. Students will be lodged in single rooms of the Alcuin College, where breakfasts and dinners will be provided, whereas lunches and coffees will be served in the Physics Department, which offers access to the lecture rooms and computer laboratory.

#### Teaching

The course will take the form of an intensive program of three weeks, with a total time of 45 h of lectures and directed exercises, about 75 h devoted to a computational project and a final assignment worth approximately 2 weeks of work. The total workload will amount to 150 hours, corresponding to **6 ECTS** in Europe. The final assignment will be graded with marks A, B, C, D, E and failed for Master students and passed/not passed for PhD students.

The proposed organization of the day is follows:

Organization of the day			
9:00am - 10:30am	Lectures		
10:30am - 11:00am	Coffee		
11:00am - 11:45am	Lectures		
11:45am - 12:30pm	Directed exercises		
12:30pm - 1:30pm	Lunch		
1:30pm - 3:30pm	Hands-on sessions, computational projects		
3:30pm - 4:00pm	Coffee		
4:00pm - 6:00pm	Hands-on sessions, computational projects		
6:00pm - 7:00pm	Discussions, Wrap-up of the day		