**PhD course in Physics, Astrophysics, and Applied Physics - Università degli Studi di Milano**
**PhD cicle 40 (2024-2025)**

**All lectures will be given in English.**

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| **Course title** | Quantum Theory of Matter |
| **Teacher in charge of the course** | Manini Nicola |
| **List of the teachers of the course** *[surname/name; affiliation; e-mail]* | Manini Nicola, UNIMI, nicola.manini@unimi.it<br>Onida Giovanni, UNIMI, giovanni.onida@unimi.it<br>Parola Alberto UNINSUBRIA alberto.parola@uninsubria.it<br>Achilli Simona, UNIMI, simona.achilli@unimi.it |
| **Training objectives** | Familiarizing the student with the main theoretical concepts and state-of-the-art methods for the calculation of structural and spectroscopic properties of molecules and solids. |
| **Prerequisites** *[please insert details and also **state whether the course has advanced contents** suitable for students with prior knowledge of the topics or is also suitable for students without prior knowledge]* | Practical quantum mechanics (Schrodinger equation, and its solutions in standard problems such as a free particle, the quantum harmonic oscillator, the one electron atom; canonical interpretation of the wave function; perturbation theory); basic concepts of electromagnetism and structure of solids. |
| **Detailed course program** | **General methods and concepts.**<br>- Symmetries in physics and group theory. Subgroups. Group representations. Examples. Product groups. Representation reducibility. Fundamental theorems of the group representation theory. Representation characters.<br>- Examples and applications to problems in condensed matter and solid-state physics.<br>- Born Oppenheimer separation. Adiabatic-diabatic transformation. Examples and applications. Ehrenfest dynamics.<br>**The many-electrons problem**<br>- Many-body Hamiltonian for N electrons and M nuclei.<br>- Summary on the variational principle and its application within the Hartree-Fock method.<br>- Matrix elements of 1 body and 2 body operators on determinantal states.<br>- Electron density and density matrix, and their functional derivatives.<br>- Total energy and double counting.<br>- Excitation energies and Koopman's theorem.<br>- Density Functional Theory: Hohenberg-Kohn, Thomas-Fermi, Kohn-Sham.<br>- Similarities and differences wrt HF. Local and semi-local density functionals.<br>- Theoretical tools: self-consistent ab-initio methods. Choice of the basis set. The pseudopotential description of core states. Periodic boundary conditions.<br>- Spectral functions. Self energy. Equation for the poles of the one-electron Green's function.<br>- Hedin's equations. The GWGamma scheme. The GW approximation. One-shot G0W0.<br>- GW implementation in open-source codes.<br>- Hybrid functionals.<br>- Excitonic effects in optical absorption spectra. Bethe-Salpeter equation. Local fields.<br>- Examples.<br>**Strongly-correlated electron systems**<br>- Role of the electron-electron interaction in the electronic structure of solids. Introduction to the second-quantization method. Fock |

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| | space, creation and annihilation operators, second-quantized Hamiltonian for the electron gas.<br>- Electronic structure of transition metals. Hubbard model. Mott transition. Strong and small coupling limits of the Hubbard model. Origin of antiferromagetism in condensed matter. The Heisenberg model.<br>- Metal-insulator transition in the Hubbard model: mean-field theory. Hubbard model with attractive interactions: superconductivity. Analogies with the BCS theory.<br><br>**Final hands-on**<br>Computational-lab with examples of application of an open-source DFT ab initio code for the calculation of electronic properties of molecular and cristal systems. |
| **Examination modalities** | The student can opt between (i) a traditional interview covering all course contents, (ii) a seminar presenting a focused topic studied through a few journal papers, or (iii) the discussion of an original calculation. |
| **Preliminary schedule**<br>*[please indicate the weeks when the lectures will be given]* | March 2025-May 2025 |