CONSIGLIO NAZIONALE DELLE RICERCHE
SHORT-TERM MOBILITY PROGRAMME (YEAR 2009)

Proponent: Dr. Nicola Mastronardi
Istituto per le Applicazioni del Calcolo "Mauro Picone" (Bari, Italy)
Recipient: Dr. Valerio Olevano
Institut Néel--CNRS (Grenoble, France)

FINAL REPORT

During the short visit, the recipient has contributed to achieve a relevant result on the investigation of the fundamentals of Condensed Matter systems for potentially wide applications (for instance in Nanoelectronics and Spintronics); it is also of broad interest to the general physics community, for all the following reasons.

Density-Functional Theory (DFT) revealed in the last thirty years a very successful ab initio Many-Body theory to calculate ground-state properties of Condensed Matter systems, ranging from three-dimensional bulk solids, to zero-dimensional atoms. The predictions of DFT on ground-state properties such as the total energy and the crystallographic structure are in very good agreement, normally within 4%-5% the experimental measured values. On the other hand, the theoretical prediction of Condensed Matter excited-state properties, *e.g.* the electronic structure and dielectric/optical spectra, still represents a challenge. Indeed, DFT is not an in principle exact theory to calculate excitations and other formalisms should be resorted to address such an issue. One of them is Time-Dependent Density-Functional Theory (TDDFT), an extension of DFT to account for the time-dependent external perturbations which excite the system. However, some work has still to be done to devise the right approximations to the unknown quantities of the theory such as the exchange-correlation functional. Indeed, it seems that the Local-Density Approximation (LDA), is not in the time-dependent case as successful as in the static DFT case.
Another possible ab initio approach to excited-state properties and spectroscopy is represented by the framework of Many-Body Quantum Field Theory (MBQFT), which is an approach settled on much more physical terms. Beyond the perturbative approaches to this theory which demonstrated unsuccessful, the functional approach has lead to the formulation of the Hedin's equations, a set of five integro-differential equations to be solved self-consistently; and the devise of the GW approximation, consisting in the neglection of Vertex corrections, to solve Hedin's equations in an approximate way. The GW approximation has demonstrated in the last twenty years a valid first-principle approach to predict electronic excitations measured in Photo-Emission Spectroscopy. Further approximations, such as those employed in the ab initio Bethe—Salpeter equation (BSE) approach, have demonstrated its ability to reproduce optical spectra.

During the short visit, the recipient has contributed to explore new approaches to MBQFT toward the formulation of an effective, phenomenological theory in such a way to simplify it by integrating out some of its degrees of freedom. So far Hedin's equations have been solved only for simple models like Hubbard's or jellium, while no realistic physical system has been solved yet due to the difficulties in spotting the effective degrees of freedom of the theory. An effective Lagrangian provides a reliable framework where a phenomenological full calculation of excited-state properties of realistic Condensed Matter systems can be performed. Such approach has been succesfully developed in Particle Physics (Standard Model, Heavy Quark Effective Theory, Chiral Perturbation Theory, etc.) in the past and it is still an active field of research (Heavy Density Effective Theory). Thank to this newly formulated effective/phenomenological MBQFT framework, a solution to the main problem is

viable: describing appropriately the Vertex corrections. Indeed within a phenomenological framework, Vertex corrections can be more easily introduced, and fully taken into account by solving the traditional BSE, a well known integro-differential equation describing the bound-states of several physical systems like quark-antiquark mesons in particle physics, or electron-hole excitons bound-states in Condensed Matter. Vertex corrections are both crucial in reproducing the optical and Auger spectra, and also in correctly reproducing the position of satellites in Angle Resolved Photo-Emission Spectroscopy (ARPES) measured spectral functions. Finally, Vertex correction seems at the base of a correct description of strongly correlated systems such as lanthanides, actinides, transition metals oxides and high-temperature superconductors.

The methodology is well known. Green's function theory, also called (improperly) Many-Body Perturbation Theory (MBPT), is a Quantum Field Theory (QFT) based on a formalism of second quantization of operators. The fundamental degree of freedom is the Green's function or propagator, which represents the probability amplitude for the propagation of an electron from x to y, being x/y two points in the Minkowskian space-time. The main advantages of this theory are that: 1) avoids indexes running on the many particles; 2) fermionic antisymmetrization is automatically imposed; 3) allows to treat systems with varying number of particles; 4) most importantly, condenses inside the Green's function all the Physics of the system.

As any other QFT (for example Quantum Electro-Dynamics, or QED) also the Many-Body can be expanded in Perturbation Theory (kind of Taylor expansion), the coupling being the Many-Body interaction term. The Green's function as well as any other quantity of the theory (the Self-Energy, the Polarization) can be calculated at a given order of Perturbation Theory. A Feynman diagrammatic analysis is hence possible. The theory at the first order is equivalent to the Hartree--Fock theory. However the coupling is not small (with respect to, for example, the interaction term with ions) and the Taylor expansion does not converge. The second order is not necessarily smaller than the first. Thus one needs to resort to more complicated methods to solve the theory, partial resummations of diagrams at all orders, or better, iterative methods. Indeed, MBPT can be solved thanks to a set of five integro-differential equations, called Hedin's equations, that have to be solved iteratively until self-consistence.

Of course further investigation is needed but the ground-breaking message of such a work is clear: any reliable picture is possible only by having at disposal a robust theoretical approach to the reconstruction of realistic systems. The present collaboration walks along with this creed: the Science to be the ground for both production processes and answers to individual/collective needs. In that respect this research activity meets the stringent criteria of the relevant 7th Framework Programme guidelines issued by the European Union.

In conclusion, the Short-Term Mobility Programme (year 2009) by CNR has supported a fruitful collaboration between two Institutions (CNR--CNRS) sharing the same mission. Such a collaboration has been already employed on 2007-2009 and it will continue in the future.

Both parts wish to keep it in the future in the framework of financed programmes dedicated to this purpouse.

Bari (Italy), July 20th 2009

Sincerely,
Dr. Nicola Mastronardi (proponent)