Claudio Verdozzi's research profile

My research activity, started with the theoretical study of electron (Auger, Photoemission) spectroscopy. I i) introduced a supercell approach to deal with disorder and correlations in the late transition metal alloys [1], ii) provided a unitary description of the spectroscopical behavior of supported Pd transition metal clusters [2], iii) extended the theory of the Auger decay in solids to the case of long ranged final state interactions [3, 4] iv) proposed a scheme for a partial cancellation of self-energy and vertex corrections for short range interactions [5]. I then proposed a theoretical scheme to describe many-photon effects in inelastic light scattering phenomena [6], with the electron-photon coupling included to all orders. Model results showed the interesting effect of a dynamical Stark effect contribution to the second harmonic generation response. My interest in correlated systems led me to consider the adequacy of the GW approximation for strongly correlated systems [7] performing for the first time comparisons between exact and GW solutions. Later, I became interested in metal oxides surfaces and performed the first large-scale *ab-initio* Density-Functional studies for aluminum oxide-related systems [8, 9, 10]. I studied isolated La impurities in a sapphire matrix [8], and my theoretical predictions have been confirmed in several experiments. My work on the (0001) surface [9] characterized in detail for the first time the nature of the clean surface and the metal-sapphire interface and also qualified the nature of the ad-metal growth. I have also developed and implemented a temporal embedding scheme to switch on the fly between *ab-initio* and semi-empirical potentials, to reduce the computational effort in molecular dynamics [11]. In the past few years, I developed a general-purpose, exact diagonalization code and used it to study Kondo-type nanoclusters[12, 13], providing the first example of a Doniach phase diagram for a nanocluster with regions of prevailing Kondo or RKKY correlations. I used the same approach to perform the first study of entanglement in periodic Anderson clusters, obtaining an entanglement phase diagram and addressing the effect of charge fluctuations [14].

Since in Lund , my activity has been primarily devoted to the study of non equilibrium phenomena. In 2007, I introduced a Time-Dependent Density Functional Theory (TDDFT) description for strongly correlated finite systems in non equilibrium [15], which was then applied to cold fermion atoms in optical lattices [16]. Then, using Dynamical Mean Field Theory, I have introduced a new class of exchange-correlation potentials to describe via TDDFT the 3D Hubbard model out of equilibrium [17]. In the area of transport phenomena, I i) proposed an *ab-initio* quantum-classical mixed scheme to study nuclear dynamics in quantum transport [18]. With it, I provided the first example of current-induced molecular desorption as obtained from a full time-dependent approach and suggested the use of ac biases as a way to tailor electromigration. The results also showed the importance of nonadiabatic effects for ultrafast phenomena in nanodevices ii) I presented a time-dependent picture of Coulomb Blockade based on TDDFT, and investigated the relevance of a discontinuity in the exchange-correlation potential in molecular transport [19]. Another line of investigation I have recently pursued is the non equilibrium dynamics of strongly correlated clusters, in terms of many-body approximations within the framework of the Kadanoff-Baym equations [20]. This has provided insight into some basic shortcoming of many-body self-consistent approximations based on infinite partial summations, which remain also for clusters contacted to infinite reservoirs [21]. The NEGF approach has been recently applied to the dynamics of ultracold fermions in optical lattices [29], for opening-trap geometries.

I have also focussed on a description of the competing role of interactions and disorder in transport [22, 23] and in cold atom [26] phenomena, and used Density Functional Theory to provide an exact independent particle picture of such competition [24].

I have also performed a study on the use of ultrafast field to manipulate nuclear dynamics in molecular devices [27], and provide a general theory based on NEGF on how to descreibe molecular forces in molecular motors in the presence of interactions [25].

On a different direction, I have started a line of investigation for time-resolved spectroscopies at surfaces, in terms of explorative models solved exactly [28], via the Kadanoff-Baym equations [30, 31], and in terms of *ab-initio* GW treatments [32].

Finally, generalising previous work, I have studied the dynamical competition of Kondo and RKKY interactions, and how to proceed across different phases in a nonequilibrium Doniach-Phase Diagram [33].

These recent studies, clearly show the necessity of an appropriate treatment of correlations at the *ab initio* level, and for system out of equilibrium. Effort in this direction has just started, with a proposal from our group of an hybrid method which mixes the essential elements of NEGF and TDDFT [34].

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