PROJECT TITLE: **Nonequilibrium phenomena and dynamics in nanoscale systems**

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1. Research project objectives. The rapid progress in miniaturization of electronic devices inevitably brings the current technology closer to a certain natural limit, when the manipulation of individual molecules, atoms or spins will constitute the basis for processing and storing information. Regardless of how distant this perspective seems to be, comprehensive understanding of physics at the nanoscale will certainly be of vital importance. The theoretical studies of transport properties of nanoscale systems, such as molecules, quantum dots or nanowires, due to strong electron correlations, are not an easy task and the methods used are very often based on a series of approximations. Consequently, there are relatively few results that can be considered as benchmarks, and which can be directly compared to experiments. The aim of this project is thus to provide very accurate results and new predictions for problems that have not been studied so far. One of such open problems is undoubtedly the accurate quantitative calculation of transport characteristics in non-equilibrium conditions and the determination of dynamics with exact treatment of correlations. Therefore, the main goal of this project is to develop and adapt advanced numerical methods based on renormalization group techniques to study transport properties of correlated nanoscale systems, with particular emphasis on non-equilibrium and dynamical phenomena. Within this project we will in particular analyze the non-equilibrium transport characteristics of molecules, such as molecular magnets, and their artificial counterparts, which can exhibit the two-stage or underscreened Kondo effects. In addition, for molecular and quantum dot systems, we will investigate the non-equilibrium heat conductance and the Seebeck coefficient, as well as the spin Seebeck coefficient in the case of junctions with ferromagnetic contacts. The next goal of the project is to analyze the time-dependent transport and quantum quench dynamics of correlated nanostructures. In this context, we will determine the time-dependence of the local density of states, which will allow studying the formation and evolution of the Kondo resonance. In the first stage, we will consider the time-dependent transport for molecular junctions and then the analysis of transport dynamics will be extended to hybrid nanostructures with superconducting electrodes. This will shed new light on the time-dependence of interplay and competition between different types of correlations, including electron pairing, Andreev reflection and the Kondo screening. Last but not least, we will also analyze the time-dependent transport for complex nanoscale systems exhibiting exotic Kondo states, such the non-Fermi liquid two-channel Kondo state, and quantum critical phenomena.

2. Research project methodology. The aim of the project is to perform a comprehensive analysis of non-equilibrium phenomena and dynamics in nanostructures exhibiting strong electron correlations. Currently, one of the most accurate methods used to study the transport properties of the considered systems is the numerical renormalization group method. Unfortunately, this method works only at equilibrium and, therefore, it

cannot describe the systems under real nonequilibrium conditions. In order to carry out an accurate quantitative analysis of non-equilibrium transport with exact treatment of all correlations, a novel technique based on a combination of the numerical renormalization group method and the density matrix renormalization group with the thermofield approach will be implemented and developed within the project. Moreover, in order to examine the dynamics and determine the time-dependent transport properties of considered systems, the time-dependent numerical renormalization group method will be applied. These methods will be appropriately developed and adapted to describe the properties of the studied nanostructures.

3. Expected impact of the project on the development of science. The investigations of different transport phenomena, including the Kondo effect and quantum critical behavior, in complex, hybrid nanoscale systems are currently the subject of many investigations carried out in the leading scientific teams in the world. This is undoubtedly related to the fact that the studied nanostructures allow for a fully controllable analysis of fundamental interactions and processes at the atomic scale. Besides, such systems are extremely interesting due to potential applications, for example, in information storage and processing technologies, quantum information technology, nanoelectronics, as well as in quantum thermoelectrics. The goal of this project is to develop advanced numerical methods and to apply them to study the transport properties of correlated nanostructures, such as molecules and their artificial counterparts attached to external electrodes. This will allow for generating benchmark results and predictions about the dynamics and nonequilibrium transport in nanostructures, which could be directly compared with the current and future experiments. It can be expected that the results obtained during the execution of this project will, on the one hand, provide new and beyond the state of the art knowledge and understanding of transport properties of nanostructures, and, on the other hand, they will stimulate further experimental research and exploration of new phenomena. The project results will be disseminated to the scientific community by publications in prestigious international journals and by presentations at international conferences.