Investigation of the out of equilibrium Anderson impurity model with perturbative field theoretical methods

(Ph.D. thesis booklet)

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Introduction, overview

The physics of *strongly correlated* systems is a particularly relevant and actively researched field of condensed matter physics. Among others, the heavy fermion compounds, non-Fermi liquid materials are belonging to the family of strongly correlated systems, but the high temperature superconductors are also counted to here. For their description simplified models are used such as Hubbard model or Kondo lattice model, which are the lattice equivalents of the Anderson and Kondo models used for the description of quantum impurities.

The equilibrium properties of the strongly correlated systems are investigated both experimentally and theoretically for decades, but the investigation of their out of equilibrium properties has only become a particularly active field of research since the demonstration of the Kondo effect in quantum dots. By the development of microelectronics, it becomes possible to create a single artificial atom, i.e. correlated quantum impurity, and investigate the transport properties thereof among out of equilibrium circumstances. In most of the investigated systems, the quantum dot is arranged between two electrodes functioning as contacts for introducing and leading away electrons. Applying a third, capacitively contacted so-called gate electrode, a device called single electron transistor having three contacts can be obtained.

By the development of nanotechnology, smaller and smaller and more and more sophisticated devices can be produced: in the experiments, real atoms and molecules can be contacted in a controlled manner and extremely small temperatures (such as $\sim 10mK$) can be reached. The production of smaller and smaller circuits (miniaturization) is motivated by that the size of the classical transistors begins to reach its limit of applicability, by the same time, the single electron transistors realized by quantum dots can be realistic alternatives instead of them to reach even smaller sizes. Moreover, these microelectronic devices, because of their well controllable parameters, offer a good possibility for the experimental and theoretical physicists to investigate out of equilibrium strongly correlated systems and to compare the experiments with theories.

The purpose of my thesis is to investigate out of equilibrium Anderson model by means of field theoretical models. In my dissertation I combine the out of equilibrium Keldysh technique with mean field approximation, iterative perturbation theory, as well as the so-called fluctuation exchange approximation, and apply them for the description of multi-level quantum dots. Although, a number of theories has been developed for generalizing the solutions of the Anderson and Kondo model to out of equilibrium, so far none of them proved to be completely satisfying, and satisfying solutions for the single- or multi-level Anderson impurity model describing the strongly correlated quantum dot systems exists now only in equilibrium. Due this, as well as to the fact that many experimental systems are *truly* in the perturbative regime, the perturbation theory based techniques used by me which are applicable for the Anderson impurity model and carried out in the interaction parameter have an outstanding role. These techniques are not model specific, comparatively fast, and can be hopefully combined with molecular electronics calculations.

Purposes

The purpose of my thesis is to investigate on what parameter ranges are the out of equilibrium perturbation techniques achieved in the interaction parameter reliably applicable for the out of equilibrium Anderson impurity model, as well as to investigate whether these techniques are capable of describing the fine details of correlated behavior in the case of more general interactions, as well as more levels, and whether they are capable of reproducing the experimentally observed features. My further object is to develop and investigate a new method, which is more sophisticated than the single iterative perturbation theory and which is conserving, i.e. the out of equilibrium fluctuation exchange approximation.

After the introductory chapter of my thesis, firstly I investigate the out of equilibrium generalization of the mean-field theory and explore its limits in the simplest case, i.e. in case of the single level model. I take an emphasis on the basic failures of the mean-field theory, i.e. the prediction of development of a finite magnetic moment in certain parameter ranges.

After that, I generalize the iterative perturbation theory to the two-level nonequilibrium Anderson model, applying systematic perturbation theory in Coulomb interaction and the Hund's rule coupling. Eliminating the instabilities pertaining to the magnetic moment, I give the applicability range of this method, on which its convergence is stable, and I investigate the spectral and transport properties of the two-level Anderson model by means of this method.

By calculating transport properties, it is inevitably to satisfy the current conservation. This occurs as a problem in the iterative perturbation theory, at the same time, it is totally avoidable, if a *conserving* approximation is applied.

According to this, in the last chapter of my thesis I generalize the *conserving* fluctuation exchange (FLEX) approximation to out of equilibrium. This approximation sums up certain groups of the diagrams to infinite order in the interaction parameters. In my thesis, I sum up the so-called particle-hole diagrams, while these give the relevant component for the processes described by the Anderson impurity model. I investigate also the spectral- and transport properties of the model by means of this method.

New scientific results

I. I have solved the single level Anderson impurity model by means of out of equilibrium mean-field approximation. I have shown, that the out of equilibrium mean-field solution leads to unphysical features (hysteresis, phase transition, out of equilibrium magnetization) even in this simple system [1].

II. I have explored the ranges, where this method may lead to unphysical results (such as more than one stable solution, spontaneous development of a local magnetic moment, hysteresis) in such out of equilibrium, e.g. *ab initio* type, calculations, in which mean-field approximation is applied. I have shown, that by high bias voltage and strong correlation, there is a new out of equilibrium region where the mean field theory predicts spontaneous local moment formation [1].

III. I have investigated the transport properties of the single level Anderson impurity model using mean-field approximation. Besides, I have disclosed the coexistence regions appearing in the mean-field solution. I have shown, that the mean field solution predicts – as a failure – spin polarized transport in certain regions [1].

IV. I have generalized the iterative perturbation theory for the two-level Anderson impurity model, considering Hubbard on site interaction (U), as well as Hund's rule coupling (J) on the energy levels. I have described the behavior of a two-level quantum dot around singlet-triplet transition with this method, and I have investigated the equilibrium spectral functions, the linear conductance, as well as the differential conductance obtainable by numerical differentiation from the current. Comparing the obtained results to experimental data, I have experienced considerable similarity except that the applied approximation gives a slightly incorrect value for the Kondo scale. The iterative perturbation theory was capable of reproducing the main features observable in the out of equilibrium dI/dV curves, such as the two-stage Kondo effect, the development of a singlet-triplet gap, and the maximum observable in the linear conductance near the transition [2, 3].

V. I have generalized the conserving, i.e. conservation laws fulfilling fluctuation-exchange (FLEX) approximation to out of equilibrium circumstances for any number of energy levels, and I have applied it for the two-level Anderson impurity model. The method which was developed by me is capable of effective description of more complicated quantum dot systems [4].

VI. I have also investigated the behavior of two-level quantum dots around singlet-triplet transition in out of equilibrium fluctuation exchange approximation. I have compared the results to experimental results, I have obtained results for the spectral functions, the linear conductance and the differential conductance which essentially agree with them. This approximation – unlike the iterative perturbation theory – gives back the Kondo scale realistically [4].

VII. I have explored the applicability ranges of the developed iterative perturbation theory and fluctuation-exchange approximation as a function of the hybridization based level width normalized interaction parameters (U/Γ, J/Γ), and I have experienced that both perturbation theory based methods can be used below medium values of the normalized interaction parameters [3, 4].

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