Spin-channel Keldysh field theory for weakly interacting quantum dots

Sergey Smirnov and Milena Grifoni
Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany
(Received 1 February 2012; revised manuscript received 7 March 2012; published 9 May 2012)

We develop a low-energy nonequilibrium field theory for weakly interacting quantum dots. The theory is based on the Keldysh field integral in the spin channel of the quantum dot described by the single-impurity Anderson Hamiltonian. The effective Keldysh action is a functional of the Hubbard-Stratonovich magnetization field decoupling the quantum dot spin channel. We expand this action up to the second order with respect to the magnetization field, which allows one to describe nonequilibrium interacting quantum dots at low temperatures and weak electron-electron interactions, up to the contacts-dot coupling energy. Besides its simplicity, an additional advantage of the theory is that it correctly describes the unitary limit, giving the correct result for the conductance maximum. Thus our theory establishes an alternative simple method relevant for investigation of weakly interacting nonequilibrium nanodevices.

DOI: 10.1103/PhysRevB.85.195310
PACS number(s): 72.15.Qm, 73.63.—b, 72.10.Fk

I. INTRODUCTION

Nonequilibrium nanoscopic systems having discrete electronic states currently attract unflagging attention of researchers from both experimental and theoretical sides because of practical applications in various electronic devices. Such systems also provide a unique platform for fundamental science since they represent a plexus of different fields of physics, leading to new complex and highly nontrivial physical scenario.

A particularly interesting physics arises when both electron-electron interactions and nonequilibrium significantly contribute to the state of a nanoscopic system. The system’s differential conductance, as is well known, may then enhance and exceed the value it would have without electronic correlations. This enhancement, taking place at low temperatures, signifies the appearance of new physics due to the system’s transition into a resonant many-particle Kondo regime discovered first in the context of magnetic alloys.

The single-impurity Anderson model (SIAM) is one of the main theoretical paradigms which is able to capture basic physics of nonequilibrium interacting nanoscopic systems. It describes a quantum dot (QD) with a single spin-degenerate level coupled to two fermionic contacts. The contacts have different chemical potentials with the difference specifying the voltage applied to the QD. This voltage is the source of nonequilibrium.

Quantum transport theories built upon SIAM can be divided into two classes: (1) operator-based theories and (2) field-integral-based theories. Within the first class one directly uses the second quantized operators while within the second class one transforms these operators into fields whose dynamics is governed by a certain effective action.

Among numerous examples of the first class of theories are perturbation theories in the electron-electron interaction as well as in the tunneling amplitude, noncrossing approximation, equations of motion, mean-field approximation, and renormalization group theories. At the same time the relatively new second class is not so wide, since field-integral concepts in physics of nonequilibrium interacting nanoscopic systems are just on the way of growing emergence. Here examples are given by analytical and numerical Keldysh field-integral theories.

The Anderson impurity model has two distinct fixed points—the weak-coupling fixed point and the strong-coupling or Kondo fixed point, each one being a Fermi liquid. Analytical field-integral-oriented theories are mainly based on slave-particle strong-coupling fixed-point approaches. For example, in Ref. 22 the saddle point analysis is applicable at temperatures below the Kondo temperature $T_K$ and thus the unitary limit is within its temperature range. However, being a $1/N$ expansion it gives an incorrect value of the conductance maximum for spin $1/2$. In Refs. 23 and 24 the effective Keldysh action is expanded around the zero slave-bosonic field configuration up to the second order in the slave-bosonic fields, and this restricts those theories to a temperature range close to and above $T_K$. These examples show that either the unitary limit is incorrectly described quantitatively or it cannot be reached at all due to temperature limitations of theories. However, it is desirable to have a field-integral theory treating the unitary limit properly since this limit gets more and more feasible in modern experiments, both for the strong-coupling and weak-coupling fixed-point regimes.

A practical guide for developing a second class theory having a proper treatment of the unitary limit in the weak-coupling fixed-point regime is given by the first-class theories, namely, perturbation theories being expansions in powers of the electron-electron interaction. Indeed, these theories are applicable at zero temperature and reproduce the correct value of the conductance maximum, $2e^2/h$. This gives one the cue that in the context of the field integration, a theory valid at zero temperature and having the correct unitary limit might be obtained through the expansion of its effective action in powers of the electron-electron interaction. Of course, such an expansion of the effective action also means an expansion in powers of a certain field. This field turns out to be nonuniquie and its choice is not obvious a priori. At this stage one usually relies upon various physical motivations which could simplify mathematical formulation and achieve physical clarity.

In this paper we choose this field as the Hubbard-Stratonovich field decoupling the electronic correlations in their spin channel. This means that such a magnetization field
is sensitive to the QD spin fluctuations induced by the electron-electron interaction. Since it has a magnetic origin, it is also susceptible to the QD magnetic properties. In particular, when the magnetic symmetry is violated, e.g., in the presence of a magnetic field, either directly applied to the QD or indirectly induced in the QD by the ferromagnetic contact proximity effect, the minimum of the effective Keldysh action moves from the zero magnetization field configuration and the new extremum provides the effective magnetic field experienced by the QD electron dynamics. On the contrary, in the absence of any magnetic structure the effective Keldysh action simplifies, admitting only even powers of the magnetization field.

In general, the effective Keldysh action is a nonlinear functional of the magnetization field. Here we expand it up to the second order in this field, which is also a second-order expansion in the electron-electron interaction. The quadratic model is an expansion about the weak-coupling fixed point, where the saddle-point magnetization vanishes. Thus such a theory must reproduce the unitary limit because it is an expansion about a Fermi liquid fixed point. Therefore, the goal of the present research is to develop a quadratic spin-channel Keldysh action as a functional of the Hubbard-Stratonovich framework and provides the general form of the effective spin channel in the single-impurity Anderson Hamiltonian, while Sec. IV converts it into the Keldysh field-integral formalism to provide an alternative theoretical tool for investigation of weakly correlated nonequilibrium nanosystems.

The paper is organized as follows. Section II introduces the spin channel in the single-impurity Anderson Hamiltonian, while Sec. III converts it into the Keldysh field-integral framework and provides the general form of the effective Keldysh action as a functional of the Hubbard-Stratonovich classical and quantum magnetization fields. In Sec. IV this action is expanded up to the second order in the magnetization fields and afterward it is used to obtain the QD tunneling density of states. Finally, the results are shown in Sec. V and with Sec. VI we conclude.

II. QUANTUM DOT SPIN CHANNEL

We first formulate the problem on the operator level and prepare at this stage for its subsequent field-integral formulation in the QD spin channel.

The single-impurity Anderson Hamiltonian reads

\[ \hat{H}_d = \sum_\sigma \epsilon_\sigma \hat{n}_{d,\sigma} + U \hat{n}_{d,\uparrow} \hat{n}_{d,\downarrow}, \]  

(1)

where \( \sigma = \uparrow, \downarrow \), \( \hat{n}_{d,\sigma} = \hat{d}_{d,\sigma}^\dagger \hat{d}_{d,\sigma} \), \( \{ \hat{d}_{d,\sigma}^\dagger, \hat{d}_{d,\sigma} \} \) are the QD creation and annihilation electronic operators, \( \epsilon_\sigma \) is the QD energy level, and \( U \) is the strength of the electron-electron interaction in the QD.

The contacts are fermionic noninteracting reservoirs described by the following Hamiltonian:

\[ \hat{H}_c = \sum_a \epsilon_a \hat{c}_a^\dagger \hat{c}_a, \]  

(2)

where \( a = \{ x, k, \sigma \} \) is the contact set of quantum numbers including the contacts label, \( x = L, R \) (left and right contacts), \( \{ \hat{c}_a^\dagger, \hat{c}_a \} \) are the contacts creation and annihilation operators, and \( \epsilon_a \) identifies the contact single-particle energies. The contacts are in equilibrium described by the Fermi-Dirac distributions, \( n(\epsilon) = \left[ \exp((\epsilon - \mu_x)/kT) + 1 \right]^{-1} \), where \( \mu_x \) are the contact chemical potentials, defining the voltage applied to the QD as \( V = (\mu_R - \mu_L)/e \), and \( T \) is the contact temperature which is assumed to be the same in the left and right contacts.

The QD and contacts interact through a tunneling coupling given by the tunneling Hamiltonian,

\[ \hat{H}_T = \sum_{\alpha \beta} (\epsilon_{a}^\dagger T_{\alpha \sigma}^0 \hat{d}_\sigma + \hat{d}_{\sigma}^\dagger T_{\alpha \sigma}^0 c_\alpha), \]  

(3)

where \( T_{\alpha \sigma}^0 \) are the tunneling matrix elements.

In order to construct a field integral in the QD spin channel, one has to rewrite the QD Hamiltonian in such a way that the

![FIG. 1. (Color online) Temperature dependence of the differential conductance maximum at the symmetric point obtained from the present spin-channel Keldysh field-integral theory for \( U = 0.9 \Gamma \), \( \epsilon_d = U/2 \). Here \( kT_0 \) is the zero-temperature QD TDOS half-width at half maximum. The red circles show the universal temperature dependence of the differential conductance maximum obtained in the numerical renormalization group theory (Refs. 35 and 36). In this case \( kT_0 \) is the Kondo temperature, which is approximately equal to the zero-temperature QD TDOS half-width at half maximum.](image1)

are the contact chemical potentials, defining the voltage applied to the QD as \( V = (\mu_R - \mu_L)/e \), and \( T \) is the contact temperature which is assumed to be the same in the left and right contacts.

![FIG. 2. (Color online) Equilibrium and nonequilibrium QD TDOS (17) at zero temperature, \( U = 0.8 \Gamma \), \( \epsilon_d = U/2 \). The effect of a finite voltage is to decrease and broaden the QD TDOS.](image2)
coupling to the QD electron spin variable becomes apparent. This can be achieved, e.g., using the following equality:
\[ \hat{h}_{d,\uparrow} \hat{h}_{d,\downarrow} = \frac{1}{2} (\hat{h}_{d,\uparrow} + \hat{h}_{d,\downarrow}) - \frac{1}{2} (\hat{h}_{d,\uparrow} - \hat{h}_{d,\downarrow})^2. \] (4)

As a result the QD Hamiltonian acquires the form explicitly involving the QD electron-spin degree of freedom,
\[ \hat{H}_d = \sum_{\sigma} \left( \varepsilon_{\sigma} + \frac{U}{2} \right) \hat{h}_{d,\sigma} - \frac{U}{2} \left( \sum_{\sigma} \sigma \hat{h}_{d,\sigma} \right)^2. \] (5)

The QD Hamiltonian in the form of Eq. (5) together with Eqs. (2) and (3) constitute a nonequilibrium interacting problem with the full Hamiltonian \( \hat{H} = \hat{H}_d + H_C + \hat{H}_T. \) The explicit presence of the QD electron spin in the operator formulation allows one to introduce within the Keldysh field-integral framework classical and quantum fields directly connected to the QD spin-channel dynamics, as it is shown in the next section.

III. SPIN CHANNEL KELDYSH FIELD INTEGRAL

An equality similar to Eq. (4) has been utilized\(^{27,34}\) to explore quantum critical phenomena, in particular, itinerant magnetic phases, using a field integral in the imaginary (or Matsubara) time formulation. The field integral in that approach is obtained by integrating out the fermionic degrees of freedom and obtaining an effective action as a functional of the Hubbard-Stratonovich field decoupling the spin channel. It turns out that such a Hubbard-Stratonovich field has a physical meaning of magnetization and it is sensitive to magnetic properties of systems.

In the same spirit, using real time and integrating out the fermionic degrees of freedom, one arrives at the Keldysh field integral\(^{27}\) for SIAM in the QD spin channel.

Here before integrating out the fermionic degrees of freedom the action is identical to the one in Eq. (6) of Ref. 25. However, after that stage we perform the Keldysh rotation\(^{27}\) and, instead of Ising-like discrete spin fields, we use a continuous Hubbard-Stratonovich field from Refs. 34 and 27.

One of the main QD physical observables is the tunneling density of states (TDOS), \( \nu_\sigma (\epsilon) = -(1/\hbar \pi) \text{Im}[G_{\sigma \sigma}^{\text{ret}} (\epsilon)] \) \( (G_{\sigma \sigma}^{\text{ret}} (\epsilon)) \) is the QD retarded Green’s function; below the upper indices \( + \) and \( - \) always denote, respectively, the retarded and advanced components of matrices in the Keldysh space, with the corresponding Keldysh field-integral representation.

\[ \nu_\sigma (\epsilon) = \frac{1}{2 \pi \hbar} \int dt \exp \left( \frac{i}{\hbar} \epsilon t \right) \int D[m(t)] \exp \left[ \frac{i}{\hbar} S_{\text{eff}} [m(t)] \right] (G^+ (\sigma t | \sigma 0) - G^- (\sigma t | \sigma 0)), \] (6)

\[ S_{\text{eff}} [m(t)] = - \int dt U m_s (t) m_q (t) - i \hbar \text{tr} [\text{ln} [G^{-1} (\sigma t | \sigma t')] - \text{ln} [G^{(0)-1} (\sigma t | \sigma t')]], \] (7)

\[ G^{-1} (\sigma t | \sigma t') = - \left( IG_{d}^{(0)-1} (\sigma t | \sigma t') - \frac{i}{\hbar} S_{\text{HS}} (\sigma t | \sigma t') \right) \frac{i}{\hbar} M_{T} (\sigma t | \sigma t'). \] (8)

Here \( m_s (t), m_q (t) \) are the classical and quantum magnetization fields being the Hubbard-Stratonovich fields decoupling the QD spin channel and \( G_{d}^{(0)-1} (\sigma t | \sigma t') \equiv G^{-1} (\sigma t | \sigma t') \) with \( U = 0. \) In Eq. (8) \( G_{d}^{(0)-1} (\sigma t | \sigma t'), G_{C}^{(0)-1} (\sigma t | \sigma t'), \) and \( M_{T} (\sigma t | \sigma t') \) are the following matrices in the Keldysh space:

\[ G_{d}^{(0)-1} (\sigma t | \sigma t') \equiv \delta_{\sigma \sigma} \left( \begin{array}{cc} \left\lceil \frac{\hbar}{2} - \frac{\hbar U/2}{\hbar} \right\rceil + i0^+ & \delta (t - t') \\ i \frac{\hbar}{2} - \omega + i0^+ & \delta (t - t') \end{array} \right), \] (9)

\[ G_{C}^{(0)-1} (\sigma t | \sigma t') \equiv \delta_{\sigma \sigma} \left( \begin{array}{cc} \left\lceil \frac{\hbar}{2} - \frac{\hbar U/2}{\hbar} \right\rceil + i0^+ & \delta (t - t') \\ i \frac{\hbar}{2} - \omega + i0^+ & \delta (t - t') \end{array} \right), \] (10)

\[ M_{T} (\sigma t | \sigma t') \equiv \delta_{\sigma \sigma} \left( \begin{array}{cc} m_s (t) & \frac{i}{2} m_q (t) \\ \frac{1}{2} m^\dagger q (t) & m_s (t) \end{array} \right), \] (11)

IV. SPIN CHANNEL EFFECTIVE KELDYSH ACTION AND TDOS

The effective Keldysh action, Eq. (7), is a nonlinear functional of the magnetization fields \( m_s (t) \) and \( m_q (t). \) In this section we want to investigate which kind of physics is described by this action when it is expanded up to the second order in the magnetization fields.

In this paper we are only interested in the effective field theory for QDs in the absence of any magnetic structure. It is easy to see that in this case Eq. (7) does not have odd powers in the magnetization fields. Indeed, the absence of any spin dependence just results in traces of the traceless Pauli operators \( \delta_\sigma, \) eliminating in this way all odd powers of the magnetization fields from...
where \( m_c(\omega) \) and \( m_q(\omega) \) are the Fourier transforms of the classical and quantum magnetization fields and \( \Sigma^+ V(\omega) \) are the retarded, advanced, and Keldysh components of the self-energy matrix. Assuming a symmetric energy-independent spin diagonal QD-contact coupling \( T_{\alpha\beta} = \delta_{\alpha\beta} T \) and an energy-independent contact density of states \( v_c \), we find the following analytical expressions for \( \Sigma^+ V(\omega) \) (\( \Sigma^0 V(\omega) = [\Sigma^+ V(\omega)]^* \)):

\[
\Sigma^+ V(\omega) = \sum_{s,s'=\{+,-\}} I^+(s\omega,s'V), \quad \Sigma^0 V(\omega) = \sum_{s=\{+,-\}} [I^K_0(\omega,sV) + I^K_0(\omega,sV)].
\]

\[
I^+(\omega,V) = \frac{i}{4\pi} \frac{\Gamma}{\omega(2\Gamma - i\hbar\omega)} \left[ \frac{\hbar\omega}{2\Gamma\pi} \right] \left[ \frac{\hbar\omega}{\Gamma} \right] (\psi(x^+_2) + 2 \left( 1 - i\frac{\hbar\omega}{2\Gamma} \right) \psi(x^+_1) - 2 \psi(y^+_1)) - \frac{e^2 - 1 - \hbar}{4e^2 + 1 + 2\Gamma - i\hbar\omega},
\]

\[
I^K_0(\omega,V) = -i\text{Im} \left\{ \frac{1}{8\pi} \frac{\Gamma}{\omega(2\Gamma - i\hbar\omega)} \coth \left( \frac{\hbar\omega}{2\Gamma\pi} \right) \left[ \frac{\hbar\omega}{\pi} \left( \psi(x^+_2) - \psi(y^+_2) \right) - 2 \left( 1 + i\frac{\hbar\omega}{2\Gamma} \right) \left[ \psi(x^+_1) - \psi(y^+_1) \right] + 2 [\psi(y) - \psi(x^+_1)] \right] - \frac{e^2 + e^0}{4(e^2 + 1)(e^2 + 1) 2\Gamma + i\hbar\omega} \right\},
\]

where \( \Gamma = \pi v_c |T|^2 \), \( \psi(x) \) is the digamma function, and \( x^+_1, x^+_2, y^+_1, y^+_2, x^+_1, x^+_2, y^+_1, y^+_2, y^+_1, y^+_2, x^+_1 + i\hbar\omega/2\pi kT, y^+_1 + i\hbar\omega/2\pi kT, z \equiv (\epsilon_d + U/2 + eV/2)/kT + i\hbar\omega/kT, p \equiv -\hbar\omega/kT, q \equiv -\hbar\omega/kT - eV/kT \).

With the effective Keldysh action (12) one obtains the following expression for the QD TDOS:

\[
v_\alpha(\epsilon) = v_0(\epsilon) + \frac{iU^2}{4\pi^2\hbar^4} \left[ \frac{D^+ \left( \frac{\epsilon}{\hbar} \right)}{\hbar^2} \right]^2 \int d\omega \frac{2\pi}{\hbar} \left[ J^K_{\alpha} \left( \frac{\epsilon}{\hbar} - \omega \right) D^+(\omega) + \frac{1}{2} J^K_0 \left( \frac{\epsilon}{\hbar} - \omega \right) D^0_\alpha(\omega) \right] - \left[ \frac{D^- \left( \frac{\epsilon}{\hbar} \right)}{\hbar^2} \right] \int d\omega \frac{2\pi}{\hbar} \left[ J^K_0 \left( \frac{\epsilon}{\hbar} - \omega \right) D^-(\omega) + \frac{1}{2} J^K_\alpha \left( \frac{\epsilon}{\hbar} - \omega \right) D^0_\alpha(\omega) \right] + \frac{1}{2} D^0_\alpha \left( \frac{\epsilon}{\hbar} \right) D^+ \left( \frac{\epsilon}{\hbar} \right) \int d\omega \frac{2\pi}{\hbar} \left[ J^K_\alpha \left( \frac{\epsilon}{\hbar} - \omega \right) D^-(\omega) + J^K_0 \left( \frac{\epsilon}{\hbar} - \omega \right) D^+(\omega) \right],
\]

where

\[
v_0(\epsilon) = \frac{1}{\pi} \frac{\Gamma}{\sqrt{\epsilon^2 + (\epsilon_d + U/2)^2}}.
\]

\[
J^K_{\alpha}(\omega) = -i\hbar^2 \pi \frac{\Sigma^0_{\alpha}(\omega)}{[\hbar/2 - U \Sigma^0_{\alpha}(\omega)]/[\hbar/2 - U \Sigma^0_{\alpha}(\omega)]}, \quad J^K_0(\omega) = -i\pi U/\hbar^2 - U \Sigma^0_{\alpha}(\omega),
\]

\[
D^+(\omega) = \frac{\hbar}{\hbar\omega - (\epsilon_d + U/2) \pm i\Gamma}, \quad D^0_\alpha(\omega) = \frac{\hbar}{\hbar\omega - (\epsilon_d + U/2)^2 + i\Gamma},
\]

and \( F_{L,R}(\omega,V) \equiv \text{tanh}(\hbar\omega \pm eV/2)/2kT \).
V. RESULTS

Using Eq. (17) one can obtain the QD TDOS using a numerical frequency integration. Since the expansion (12) of the effective Keldysh action (7) in the classical $m_m(t)$ and quantum $m_q(t)$ magnetization fields is an expansion about the weak-coupling fixed point, our simple quadratic field-integral theory is valid only for weakly interacting QDs, $U \lesssim \Gamma$. Such a theory must reproduce at low temperatures the correct value $2e^2/h$ of the conductance maximum, known as the unitary limit. Let us recall that this is not the case in existing Keldysh field-integral strong-coupling fixed-point theories, both analytical and numerical. In the analytical theories the unitary limit is either incorrectly described quantitatively or it cannot be reached at all due to temperature limitations related to proliferation of slave-bosonic oscillations. In the numerical theories the unitary limit is difficult to reach because the memory time becomes infinite at zero temperature.

In Fig. 1 we show the temperature dependence of the differential conductance maximum. This figure confirms the consistency of the results obtained in the previous section. Indeed, at low temperatures they give the correct value of the differential conductance maximum $2e^2/h$, as it must be for the expansion about the weak-coupling Fermi liquid fixed point. Additionally, we plot the universal temperature dependence of the differential conductance maximum obtained in the numerical renormalization group theory. The comparison between the curves demonstrates that when $U$ increases so that at the symmetric point the system becomes closer to the Kondo regime, the low-temperature behavior of the differential conductance maximum obtained in the numerical renormalization group theory. The comparison between the curves demonstrates that when $U$ increases so that at the symmetric point the system becomes closer to the Kondo regime, the low-temperature behavior of the differential conductance maximum obtained in the numerical renormalization group theory.

The results of our spin-channel Keldysh field-integral theory show that in the weak-coupling fixed-point regime both finite voltages and finite temperatures have a similar impact on the QD TDOS, making it lower and broader in comparison with the zero temperature equilibrium QD TDOS, as one can see from Figs. 2 and 3. This behavior is different from the one in the strong-coupling fixed-point regime where the finite voltage splits the Kondo resonance as soon as it becomes bigger than its width.

Finally, the quadratic spin-channel Keldysh field-integral theory can also be used to calculate the QD differential conductance as a function of the applied voltage. In Fig. 4 the zero temperature differential conductance is shown for the noninteracting $U = 0$ and interacting, $U = 0.8\Gamma$, $U = 1.0\Gamma$ QDs. Once again, as in Fig. 1, the correct value of the maximum in Fig. 4 proves the consistency of the quadratic spin-channel Keldysh field-integral theory.

VI. CONCLUSION

We have developed a spin-channel Keldysh field-integral theory for nonequilibrium interacting QDs. To describe nonequilibrium interacting states of the QD, we have introduced a collective degree of freedom, a magnetization field, being the Hubbard-Stratonovich field decoupling the spin channel of the electron-electron interaction. The complex QD dynamics has been reduced to the magnetization field dynamics governed by the effective Keldysh action being a nonlinear functional of the magnetization field. We have expanded this action up to the second order in the magnetization field. This expansion represents an expansion about the weak-coupling fixed point and thus must reproduce the unitary limit of weakly correlated QDs. The QD TDOS has been derived and the differential conductance has been calculated as a function of the temperature and voltage. These calculations have correctly reproduced the conductance maximum and thus confirmed the consistency of our theory, establishing an alternative versatile and simple tool to explore nonequilibrium weakly interacting QDs, in particular, in the
unitary limit which becomes more and more relevant in modern experiments.

ACKNOWLEDGMENT
Support from the DFG SFB 689 is acknowledged.