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Keldysh effective action theory for universal physics in spin-$\frac{1}{2}$ Kondo dots

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We present a theory for the Kondo spin-$\frac{1}{2}$ effect in strongly correlated quantum dots. The theory is applicable at any temperature and voltage. It is based on a quadratic Keldysh effective action parametrized by a universal function. We provide a general analytical form for the tunneling density of states through this universal function for which we propose a simple microscopic model. We apply our theory to the highly asymmetric Anderson model with $U = \infty$ and describe its strong-coupling limit, weak-coupling limit, and crossover region within a single analytical expression. We compare our results with a numerical renormalization group in equilibrium and with a real-time renormalization group out of equilibrium and show that the universal shapes of the linear and differential conductance obtained in our theory and in these theories are very close to each other in a wide range of temperatures and voltages. In particular, as in the real-time renormalization group, we predict that at the Kondo voltage the differential conductance is equal to 2/3 of its maximum.

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The Kondo state of a quantum dot (QD) continues to attract significant interest from both experiment and theory. The zero-dimensional platform available in modern nanotechnology provides a great advantage over bulk metals with magnetic impurities where the Kondo effect was originally observed.[1] Indeed, the possibility to enrich the physics with nonequilibrium as well as to independently tune various parameters of QD structures allows one to access different aspects of the Kondo physics predicted theoretically. One of these aspects is the universality of the zero bias anomaly or Kondo resonance in the differential conductance which, as has also been confirmed in experiments,[2,3] turns out to be a universal function of the temperature and voltage with the energy scale given by the Kondo temperature T_{K}. Another advantage of the QD framework is the possibility to study the fate of the many-particle Kondo resonance in the presence of external fields or when the QD is coupled to contacts with nontrivial ground states. Recent experiments have demonstrated the universality of the Kondo effect also within these advanced setups, e.g., with ferromagnetic contacts[4] and external magnetic fields.[5] Other aspects of the Kondo state, such as its use for spin manipulations[6] or ferromagnetic-superconducting correlations,[7] have been addressed in modern experiments.

The whole diversity of the Kondo physics in QDs can be well captured within the single-impurity Anderson model (SIAM).[8] Many theoretical concepts have been developed to solve SIAM for QDs in the Kondo state in equilibrium and nonequilibrium. All these theories can be, in general, classified with respect to their applicability to two possible regimes of the Kondo state: the weak-coupling regime, when the temperature is higher than the Kondo temperature, $T > T_{\mathrm{K}}$, and the strong-coupling regime, when $T < T_{\mathrm{K}}$. Among the theories which can access only the weak-coupling regime are, e.g., semianalytical perturbation theories[9] well above T_{K}, or advanced analytical slave-bosonic Keldysh field integral theories[10,11] which extend the applicability range close to T_{K}. In the strong-coupling regime for temperatures $T \ll T_{\mathrm{K}}$ there are slave-bosonic numerical mean field theories.[12,13] From high temperatures to temperatures not too much below T_{K} the noncrossing approximation (NCA)[14,15] is a numerical tool which, however, predicts a wrong scaling, $T_{\mathrm{NCA}} \neq T_{\mathrm{K}}$. A less quantitatively reliable theory, based on the method of equations of motion, may be used for a qualitative description in the whole temperature range. It has been applied, e.g., to QDs in an external magnetic field.[16] The whole temperature range can be comprehensively numerically described in equilibrium by the numerical renormalization group (NRG) method,[17] which is quite flexible with respect to different physical setups and has been used, e.g., for QDs coupled to ferromagnetic contacts.[18] In nonequilibrium the recently developed semianalytical real-time renormalization group (RTRG) method[19] is a promising theory.

The whole spectrum of modern theoretical methods is, in principle, enough to describe many fundamental properties of the Kondo state in spin-$\frac{1}{2}$ QDs in different regimes. However, a simple single analytical theory which could provide a reliable quantitative description of the Kondo physics at any temperature and voltage and which would elucidate its universality is highly desirable.

Here we make a fundamental step towards such a theory using the Keldysh field integral formulation in the slave-bosonic representation. Namely, we provide the tunneling density of states (TDOS) in the Kondo regime, Eqs. (5) and (6), and reduce the problem to finding a universal function of the temperature and voltage which enters this general form of the TDOS.

We apply our theory to the highly asymmetric spin-$\frac{1}{2}$ SIAM with a strong electron-electron interaction, $U = \infty$ (extension to finite U is straightforward), and finite $\mu_0 - \epsilon_{\mathrm{d}}$ (ϵ_{d} is the single-particle QD energy level, μ_0 is the equilibrium chemical potential) at any temperature and voltage. The knowledge on this model up to now has been restricted by slave-bosonic mean field theories[12,13] deeply below T_{K} or, above T_{K}, by NCA (Refs. 14 and 15) and the Keldysh field theory.[10]

An exact description of the universal linear conductance can be accessed within NRG. However, little attention has been paid to its prediction for the linear conductance in the highly asymmetric SIAM. But what is more important is that NRG fails out of equilibrium and the only nonequilibrium theory able to cover the whole voltage range, RTRG,[19] is applicable only to the s-d model. Thus, out of equilibrium the situation with the highly asymmetric SIAM with $U = \infty$ is even worse.

Within the present work we eliminate this lack of knowledge on the Kondo regime of the highly asymmetric spin-$\frac{1}{2}$ SIAM with $U = \infty$ by deriving an analytical expression for the TDOS which provides (1) linear and differential conductance in the whole range of temperatures and voltages with the correct scaling T_K; (2) Fermi-liquid theory (quadratic temperature and voltage dependence of the differential conductance) at low energies; (3) analytical ratio between the corresponding Fermi-liquid coefficients. This ratio has been intensively discussed in the literature[20,21] for the symmetric spin-$\frac{1}{2}$ SIAM. However, little is known on this ratio for the highly asymmetric spin-$\frac{1}{2}$ SIAM with $U = \infty$; (4) a prediction identical to the one made in the RTRG[19] for the s-d model that in the deep nonequilibrium crossover region, at the Kondo voltage, the differential conductance is equal to $2/3$ of its maximum; and (5) excellent agreement with Hamann's analytical theory[22] for the s-d model at high temperatures.

Let us briefly recall the slave-bosonic approach used in Ref. 10. The original QD spin-$\frac{1}{2}$ fermionic operators of the Anderson Hamiltonian, d_σ, $d_\sigma^\dagger$ ($\sigma = \uparrow, \downarrow$), are expressed in terms of new spin-$\frac{1}{2}$ fermionic, $f_\sigma, f_\sigma^\dagger$, and slave-bosonic, $b, b^\dagger$, operators. Since the double occupancy is forbidden, these operators satisfy the constraint, $\hat{Q} = \hat{I}$ with $\hat{Q} \equiv b^\dagger b + \sum_\sigma f_\sigma^\dagger f_\sigma$. In practical calculations of observables this restriction is taken into account in the Keldysh field integral[23] representation of a given QD observable $\hat{O} = \mathcal{F}(d_\sigma^\dagger, d_\sigma)$ via the replacement of the QD Hamiltonian $\hat{H}_{\rm QD}$ with $\hat{H}_{\rm QD} + \mu\hat{Q}$, where μ is a positive real parameter with respect to which one takes the limit $\mu \to \infty$ at the end of the calculation,

$$\langle\hat{O}\rangle(t) = \frac{1}{\mathcal{N}_0}\lim_{\mu\to\infty} e^{\beta\mu}\int \mathcal{D}[\bar{\chi},\chi]e^{(i/\hbar)S_{\rm eff}[\bar{\chi}^{\rm cl,q}(\tilde{t});\chi^{\rm cl,q}(\tilde{t})]} \times\mathcal{F}[\bar{\chi}^{\rm cl}(t),\bar{\chi}^{\rm q}(t);\chi^{\rm cl}(t),\chi^{\rm q}(t)]. \tag{1}$$

Here $\chi^{\rm cl}(t)$ and $\chi^{\rm q}(t)$ [and $\bar{\chi}^{\rm cl}(t)$, $\bar{\chi}^{\rm q}(t)$] are the classical and quantum components (and their conjugate partners) of the QD slave-bosonic field which is the coherent state field of the slave-boson annihilation operator b, $S_{\rm eff}$ is the Keldysh effective action which depends on μ and governs the dynamics of the QD coupled to the contacts, $\beta \equiv 1/kT$ is the inverse temperature, and $\mathcal{N}_0$ is the normalization constant given in Ref. 10.

The Keldysh effective action is a nonlinear functional of the slave-bosonic fields. It represents the sum of the standard quadratic free slave-bosonic action $S_0[\bar{\chi}^{\rm cl}(t),\bar{\chi}^{\rm q}(t);\chi^{\rm cl}(t),\chi^{\rm q}(t)]$ and the complex nonlinear tunneling action $S_{\rm T}[\bar{\chi}^{\rm cl}(t),\bar{\chi}^{\rm q}(t);\chi^{\rm cl}(t),\chi^{\rm q}(t)] = -i\hbar\,{\rm tr}\ln[-iG^{(0)-1} - i\mathcal{T}]$, where the matrix $G^{(0)}$ and the matrix $\mathcal{T}$ are defined in Ref. 10: The matrix $G^{(0)}$ describes the isolated QD and contacts, while $\mathcal{T}$ accounts for the QD-contacts tunneling coupling. The dependence of the tunneling action on the slave-bosonic fields $\chi^{\rm cl}(t)$ and $\chi^{\rm q}(t)$ comes through the matrix $\mathcal{T}$.

We now perform a time-independent shift of the classical components of the slave-bosonic field in the matrix $\mathcal{T}$, $\chi^{\rm cl}(t) \to \chi^{\rm cl}(t) - \delta\sqrt{2}$, $\bar{\chi}^{\rm cl}(t) \to \bar{\chi}^{\rm cl}(t) - \gamma\sqrt{2}$, while leaving the quantum components $\chi^{\rm q}(t)$, $\bar{\chi}^{\rm q}(t)$ unchanged. Note that in general $\gamma \neq \bar{\delta}$ since $\chi^{\rm cl}(t)$ and $\bar{\chi}^{\rm cl}(t)$ are independent integration variables. This results in the appearance of nondiagonal blocks in the matrix $G^{(0)-1}$ which now takes the form

$$G^{(0)-1} = \begin{pmatrix} G_{\rm d}^{(0)-1}(\sigma t|\sigma' t') & M_{\rm T}^{(0)\dagger}(\sigma t|a' t') \\ M_{\rm T}^{(0)}(at|\sigma' t') & G_{\rm C}^{(0)-1}(at|a' t')\end{pmatrix}, \tag{2}$$

where the inverse of the diagonal blocks, $G_{\rm d,C}^{(0)}$, are the same as in Ref. 10 and the nondiagonal blocks are given as follows (for $M_{\rm T}^{(0)\dagger}$ γ is replaced with δ):

$$M_{\rm T}^{(0)}(at|\sigma t') = \frac{1}{\hbar}\delta(t-t')\gamma T_{a\sigma}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \tag{3}$$

where a is the set of quantum numbers describing the contact states and $T_{a\sigma}$ are the matrix elements of the tunneling Hamiltonian of SIAM. It is further assumed that $a = \{q,\sigma\}$, where q describes the contacts orbital degrees of freedom, σ is the contact spin, and $T_{q\sigma'\sigma} = \delta_{\sigma'\sigma}\tau$. The matrix $\mathcal{T}$ remains, as in Ref. 10, of diagonal but the off-diagonal blocks change (for $M_{\rm T}^\dagger$ γ is replaced with δ):

$$M_{\rm T} = \frac{\delta(t-t')T_{a\sigma}}{\sqrt{2}\hbar}\begin{pmatrix}\bar{\chi}^{\rm cl}(t) - \gamma\sqrt{2} & \bar{\chi}^{\rm q}(t)\\ \bar{\chi}^{\rm q}(t) & \bar{\chi}^{\rm cl}(t) - \gamma\sqrt{2}\end{pmatrix}. \tag{4}$$

Up to this point the theory is formally exact but obviously cannot be solved. To make it tractable we expand the tunneling action $S_{\rm T}$. The crucial difference with respect to Ref. 10 is that now we do not use the second-order expansion in the variables $\chi^{\rm cl,q}(t)$ (and their conjugates) but instead we expand up to the second order in the variables $\chi^{\rm cl}(t) - \delta\sqrt{2}$, $\bar{\chi}^{\rm cl}(t) - \gamma\sqrt{2}$ and $\chi^{\rm q}(t)$, $\bar{\chi}^{\rm q}(t)$.

At first sight the second-order expansion of the tunneling action in the variables $\chi^{\rm cl}(t) - \delta\sqrt{2}$, $\bar{\chi}^{\rm cl}(t) - \gamma\sqrt{2}$ and $\chi^{\rm q}(t)$, $\bar{\chi}^{\rm q}(t)$ may appear inadequate with respect to the Kondo physics. Indeed, this expansion contains linear terms in the original slave-bosonic fields $\chi^{\rm cl}(t)$, $\bar{\chi}^{\rm cl}(t)$ and $\chi^{\rm q}(t)$, $\bar{\chi}^{\rm q}(t)$. These terms shift the minimum of the effective action from the zero slave-bosonic field configuration to a finite one. Thus the symmetry is broken and the effective action of this type cannot describe the Kondo state having, as is well known, no symmetry breaking.

However, the reasoning above misses one important aspect related to the Hilbert space on which the Keldysh effective action is defined. The point is that at fixed μ this Hilbert space is much wider than the QD Fock space having states only with zero and one electron. It is easy to show that when the Hilbert space is narrowed to the physical Fock space of the QD, i.e., when the limit $\mu \to \infty$ is taken, the linear terms in the Keldysh effective action do not generate any finite contribution to the physical observables of the QD. Thus they can be discarded from the outset and the symmetry of the Keldysh effective action is restored.

In this way one obtains a Keldysh effective action which is quadratic with respect to the original slave-bosonic variables $\chi^{\rm cl}(t)$, $\chi^{\rm q}(t)$ (and their conjugates) and where the shifts δ and γ have been absorbed into the kernel of the action. After this transformation the theory becomes formally identical to that in Ref. 10. The only difference is that now the self-energies in the quadratic action are parametrized by the shifts δ and γ.

Therefore, one can immediately write down the general form for the QD TDOS in the Kondo regime,

$$\nu_\sigma(\epsilon) = (\Gamma/2\pi)\{[\epsilon_{\rm d} - \epsilon + \Gamma\Sigma_{\rm R}(\epsilon)]^2 + [\Gamma\Sigma_{\rm I}(\epsilon)]^2\}^{-1}, \quad (5)$$

where $\Gamma \equiv 2\pi\nu_{\rm C}|\tau|^2$ ($\nu_{\rm C}$ is the contacts density of states).

The crucial change with respect to Ref. 10 concerns the retarded self-energy $\Sigma^+(\epsilon) = \Sigma_{\rm R}(\epsilon) + i\Sigma_{\rm I}(\epsilon)$ which now has a nontrivial dependence on $\alpha \equiv \delta\gamma$,

$$\Sigma^+(\epsilon) = \frac{1}{2\pi}\sum_x\left[\mathrm{Re}\,\psi\left(\frac{1}{2} + \frac{W}{2\pi kT}\right) - \psi\left(\frac{1}{2} + \frac{E_\alpha}{2\pi kT} - \frac{i\mu_x}{2\pi kT} + \frac{i\epsilon}{2\pi kT}\right) + i\frac{\pi}{2}\right], \quad (6)$$

where the sum is over the contacts ($x =$ L,R), $\psi(z)$ is the digamma function, $\mu_{\rm L,R} \equiv \mu_0 \mp eV/2$ (V is the bias voltage), W is the half-width of the contacts Lorentzian density of states ($W \gg kT, eV, \mu_0$) and $E_\alpha \equiv \alpha\Gamma/2$ is a complex energy.

A simple microscopic theory for $E_\alpha = E_\alpha^{\rm R} + iE_\alpha^{\rm I}$ is obtained using the fact that in the deep Kondo regime (which we estimate as $\mu_0 - \epsilon_{\rm d} \geqslant 4\Gamma$) in equilibrium and at zero temperature the TDOS has maximum at $\epsilon \approx \mu_0$ and this maximum is approximately equal to the unitary limit $2/\pi\Gamma$. This leads to the two equations $[\ln(2|E|/kT_{\rm K})]\sin\phi = (\pi/2 - \phi)\cos\phi$ and $[\ln(2|E|/kT_{\rm K})]^2 = \pi^2/4 - (\pi/2 - \phi)^2$, where $kT_{\rm K} \equiv 2W\,\exp[-\pi(\mu_0 - \epsilon_{\rm d})/\Gamma]$ is the Kondo temperature, $|E| \equiv \sqrt{(E_\alpha^{\rm R})^2 + (E_\alpha^{\rm I})^2}$, and $\phi \equiv \arctan(E_\alpha^{\rm I}/E_\alpha^{\rm R})$. These equations show that $\mathcal{E}_\alpha \equiv E_\alpha/kT_{\rm K}$ is a universal ratio which guarantees the correct scaling of the differential conductance. One gets $\mathcal{E}_\alpha^{\rm R} \approx 1.42$ and $\mathcal{E}_\alpha^{\rm I} \approx 1.05$. The universal ratio $\mathcal{E}_\alpha^{\rm I}/\mathcal{E}_\alpha^{\rm R}$ provides the universal phase $\phi \approx 2/\pi$. Using this model of $\mathcal{E}_\alpha$ we can calculate the differential conductance at any T and V.

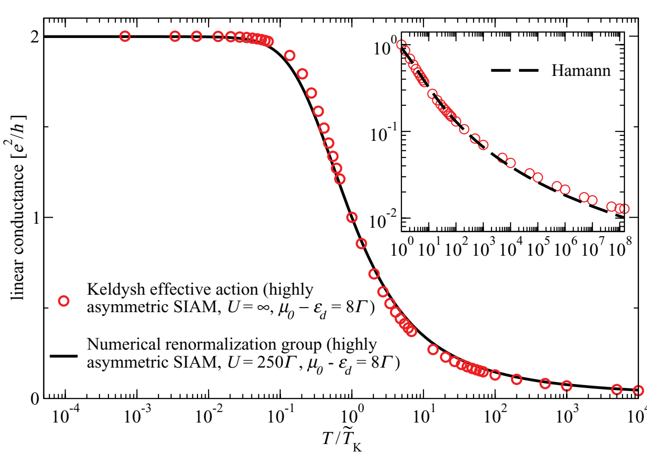

FIG. 1. (Color online) The quadratic slave-bosonic Keldysh field integral theory (circles) provides the universal equilibrium description of the Kondo spin-$\frac{1}{2}$ effect in the asymmetric SIAM with $U = \infty$ at any temperature, i.e., in the weak-coupling regime, strong-coupling regime, and in the crossover region. The NRG results (solid line) are provided by T. Costi and L. Merker (research center of Jülich). The inset compares our theory with that of Hamann (Ref. 22), which is known to describe well the high-temperature regime. In this plot $\widetilde{T}_{\rm K}$ is defined as the temperature at which the differential conductance maximum reaches half of its unitary limit value. One gets $\widetilde{T}_{\rm K} \approx 1.47T_{\rm K}$.

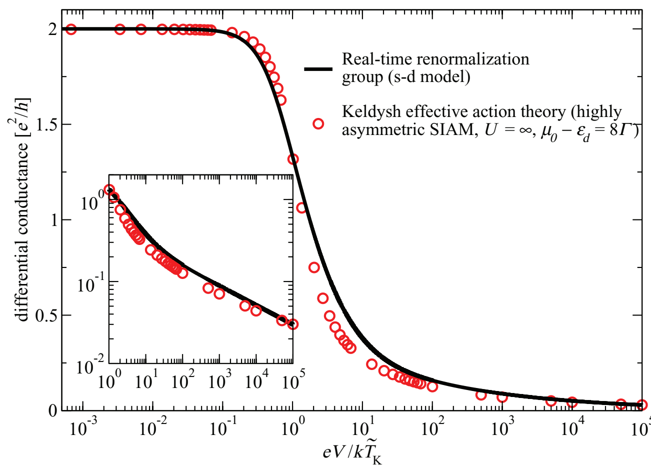

FIG. 2. (Color online) The universal differential conductance as a function of the bias voltage at $T = 0$ in the Keldysh field integral theory for the asymmetric SIAM with $U = \infty$ (circles) and in the RTRG theory for the *s-d* model (solid line). The RTRG data are provided by M. Pletyukhov and H. Schoeller (University of Aachen). The inset shows the high-voltage asymptotics of these two models. Although the asymmetric SIAM and *s-d* model are different, their universal shapes of the differential conductance are very close to each other in the whole range of the bias voltage. In particular, both models lead to an identical prediction: At the Kondo voltage $eV = k\widetilde{T}_{\rm K}$, the differential conductance is equal to 2/3 of its maximum.

In Fig. 1 we compare the equilibrium results of our theory and NRG for the highly asymmetric spin-$\frac{1}{2}$ SIAM. In our theory $U = \infty$. The NRG results have been obtained for $U = 250\Gamma$. Increasing U further in NRG does not produce any significant change in the universal characteristics. In both models $\mu_0 - \epsilon_{\rm d} = 8\Gamma$. The presence of the universal function in the QD TDOS leads to the universal temperature dependence of the differential conductance maximum (linear conductance) in the whole temperature range. As one can see from the figure, the universal shape of the linear conductance obtained in our theory is very close to the one in NRG.

Moreover, the differential conductance as a function of the bias voltage turns out to be also universal. In Fig. 2 we show the nonequilibrium results of our theory for the same model as in Fig. 1 and the RTRG results.[19] One sees that the nonequilibrium universal shape of the differential conductance for the asymmetric spin-$\frac{1}{2}$ SIAM with $U = \infty$ is very close to that in the *s-d* model. In particular, in the deep nonequilibrium crossover both theories predict the same result for the value of the differential conductance at the Kondo voltage, namely, 2/3 of its unitary limit value. This universal result has been used[24] as a new experimental tool to measure $T_{\rm K}$.

At low energies we obtain[25] the differential conductance analytically, $G(T,V) = (2e^2/h)[1 - c_T(T/T_{\rm K})^2 - c_V(eV/kT_{\rm K})^2]$. The absence of linear terms in $G(T,V)$ proves that the low-energy sector of our theory is the Fermi liquid. It is known[20,21] that for the symmetric SIAM $c_V/c_T = 3/(2\pi^2)$. However, for the highly asymmetric spin-$\frac{1}{2}$ SIAM with $U = \infty$ and finite $\mu_0 - \epsilon_{\rm d}$ little is known on c_V/c_T. For this asymmetric model our theory predicts

$$c_T = \frac{4}{3}\frac{2\,\ln(2|\mathcal{E}_\alpha|)+1}{|\mathcal{E}_\alpha|^2}, \quad \frac{c_V}{c_T} = c_a\frac{3}{2\pi^2}, \tag{7}$$

where $c_a = [4\,\ln(2|\mathcal{E}_\alpha|)+1]/[4\,\ln(2|\mathcal{E}_\alpha|)+2] \approx 0.86$.

At $T > T_\mathrm{K}$ the linear conductance is well described by the analytical expression[25] obtained by Hamann.[22] Hamann's theory, based on the s-d model, neglects charge fluctuations present in the SIAM. Thus it underestimates the conductance.[26] Our theory agrees well (inset in Fig. 1) with Hamann's result until the asymmetry and charge fluctuations become important at high T.

The results above show that the nonequilibrium universal behaviors of the highly asymmetric spin-$\frac{1}{2}$ SIAM with $U = \infty$ and symmetric SIAM or s-d model are close to each other. The difference between them partly results from their fundamental physical difference [e.g., the Fermi-liquid coefficients, like c_V, are sensitive to the asymmetry of the SIAM (see Ref. 27)] and partly from the quality of our theory and the quality of RTRG. Within our theory the last point is equivalent to the question whether the theory with constant $\mathcal{E}_\alpha$ may be improved through a dependence of $\mathcal{E}_\alpha$ on the voltage and temperature. In Ref. 25 we show that a very simple dependence of $\mathcal{E}_\alpha^\mathrm{I}$ on the temperature and voltage may, indeed, notably change the equilibrium and nonequilibrium results, obtained using the constant model. Since the function $E_\alpha = (kT_\mathrm{K})\mathcal{E}_\alpha$ effectively takes into account higher-order terms in Γ, a microscopic model for the temperature and voltage dependence of $\mathcal{E}_\alpha$ may result from a proper renormalization group theory. In particular, taking into account the quartic terms in the Keldysh effective action and performing the one- and two-loop analysis may provide a renormalization of the quadratic term and, as a result, a function $\mathcal{E}_\alpha = f(T/T_\mathrm{K}, eV/kT_\mathrm{K})$.

In conclusion, we have proven the existence of a universal function $\mathcal{E}_\alpha$, rigorously appearing in the formalism, and demonstrated how it determines the QD TDOS. A simple microscopic model for $\mathcal{E}_\alpha$ has been proposed. This has allowed us to unify the strong-coupling regime, weak-coupling regime, and crossover region of the Kondo state in equilibrium and nonequilibrium within a single analytical expression for the TDOS. To demonstrate the practical importance of our theory we have applied it to the highly asymmetric spin-$\frac{1}{2}$ SIAM with $U = \infty$. Our theory has provided the differential conductance in the whole range of temperatures and voltages with the correct scaling T_K, its Fermi-liquid behavior at low energies, an analytical expression for the ratio between the Fermi-liquid coefficients, the prediction that at the Kondo voltage the differential conductance is equal to 2/3 of its maximum, and an excellent agreement with known theories at high energies. At the same time it has raised a challenge to develop a renormalization group method to improve the quality of the present theory.

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[25] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.87.121302 for the low- and high-energy behavior of our theory and how the results of the main text could change if the universal function had a dependence on the temperature or voltage.

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