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Leading temperature dependence of the conductance in Kondo-correlated quantum dots

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Abstract

Using renormalized perturbation theory in the Coulomb repulsion, we derive an analytical expression for the leading term in the temperature dependence of the conductance through a quantum dot described by the impurity Anderson model, in terms of the renormalized parameters of the model. Taking these parameters from the literature, we compare the results with published ones calculated using the numerical renormalization group obtaining a very good agreement. The approach is superior to alternative perturbative treatments. We compare in particular to the results of a simple interpolative perturbation approach.

Keywords: Kondo effect, quantum dots, Anderson model, renormalized perturbation theory

(Some figures may appear in colour only in the online journal)

1. Introduction

The manifestations of the Kondo effect in transport through semiconducting [1–6] and molecular [7–11] quantum dots (QDs) were a subject of great interest in recent years. The Kondo effect takes place when the occupancy of the isolated QD is such that its spin $S \neq 0$. For temperatures T below the Kondo temperature T_K this spin is totally or partially compensated by the conduction electrons of the leads leading to a many-body ground state with lower total spin. This implies a resonance at the Fermi energy in the spectral density of the dot state, that leads to an anomalous peak in the differential conductance $G(V) = \mathrm{d}I/\mathrm{d}V$ at zero bias voltage V, where I is the current through the QD. For the simplest systems with one relevant level and $S = 1/2$, these physical effects are usually well described by an impurity Anderson model (IAM), which contains the Kondo model as the limiting case in which valence fluctuations are absent [12]. The parameters of the IAM are the energy of the dot level E_d, the resonant level width Δ and the Coulomb repulsion U. The Kondo regime corresponds to $-E_d, U + E_d \gg \Delta$ [12].

In the Kondo limit, the properties of the IAM display universality. Physical observables are described by the same universal function, once the different physical magnitudes are scaled by T_K. For example, it has been shown that for $T \ll T_K$, the conductance $G(V, B)$ as a function of V and magnetic field B, as well as the magnetization are universal functions of $\mathrm{eV}/(k_B T_K)$ and $\mu_B B/(k_B T_K)$ for $\max(\mathrm{eV}, \mu_B B \gg k_B T_K)$ [13]. In the opposite limit of small V and T, Oguri [14, 15] has determined the scaling of $G(V, T)$ for $B = 0$ up to second order in T and V for the symmetric IAM (SIAM) in which $E_d = -U/2$ using a Fermi liquid approach, extending to finite V the renormalized perturbation theory (RPT) in U developed by Hewson [16] and using Ward identities. The result is given as an exact analytical expression in terms of renormalized parameters $\widetilde{\Delta} \sim k_B T_K$ and $\widetilde{U}$.

More recent experimental studies for the scaling properties of $G(V, T)$ for small V and T [5, 9] stimulated further theoretical work on the subject [17–24, 27–29, 31, 32][1] using different approximations, like RPT [17], $1/N$ expansion [18], non-crossing approximation [19], or decoupling of equations of motion [20]. While the results for the Kondo model have been extended to SU(N) symmetry [31], to fit experiment, calculations need to include some degree of valence

[1] The scaling with magnetic field in [24] was incorrect [25], corrected results for $U \leqslant 3\Delta$ were presented in [26][2].

fluctuations [17, 19] suggesting that one has to go beyond the Kondo model and use the IAM for a quantitative description. The effect of asymmetric coupling to the left and right leads and asymmetric drop in the bias voltage has been calculated up to second order in T and V using Fermi liquid approaches, for the SIAM [17, 21, 22]. The more general expression was given first by Sela and Malecki [21] and reproduced using RPT [22]. These results are exact up to terms of total second order in V and T.[2]

Some of these results of RPT were extended for $E_d \neq -U/2$ using two different approaches. One of them starts from renormalized parameters of the IAM, $\widetilde{\Delta}$, $\widetilde{U}$ and $\widetilde{E}_d$ [22, 28]. The other starts from $\widetilde{\Delta}$ and $\widetilde{U}$ for the symmetric case $E_d = -U/2$ (for which $\widetilde{E}_d = 0$) and performs another perturbation expansion around this point [23]. The authors call this approach renormalized superperturbation theory (rSPT) [29][3]. A controversy between the authors of both approaches exist for finite voltage V [28–30], but this does not affect equilibrium properties ($V = 0$) like the one discussed here. In the last years also higher-order Fermi-liquid corrections away from half filling were calculated [32].

In [23] an analytical expression using rSTP was obtained for the coefficient c_T for the expansion for small T and $V = 0$ of the condunctance: $G(T) = G(0)[1 - c_T(T/T_K)^2]$. This result was compared with a fit of $G(T)$ for small T obtained using the numerical renormalization group (NRG) [24][1]. The comparison was poor, and rapidly deteriorates with increasing U. For $U = 3\Delta$ the rSPT expression for c_T increases as E_d increases from the symmetric point $E_d = -U/2$, while the NRG result decreases. Later the authors included ladder diagrams in their rSPT approach (at the cost of losing an analytical expression) obtaining a considerable improvement [29][3]. However still for $U = 3\Delta$ and $E_d > -0.6\Delta$ the comparison is rather poor. Furthermore, the fact that the rSPT results presented are limited to $U \leqslant \Delta$ is a shortcoming for two reasons. First, the Kondo regime $-E_d, U + E_d \gg \Delta$ is not reached. In the Kondo regime, the spectral density at the dot has in addition to the Kondo peak near the Fermi energy ϵ_F, two charge-transfer peaks at energies near $E_d - \epsilon_F$ and $E_d + U - \epsilon_F$ of total width 4Δ [33–36]. Then for $U = 3\Delta$ even in the symmetric case, the Kondo peak is merged with one charge-transfer peak and valence fluctuations are important. Second, for small U, simple ordinary (not renormalized) perturbation theory up to second order U [37–39] has been successful for different problems [40–42]. In particular, self-consistent interpolation schemes [40, 41, 43] permit to extend the validity of the results for U as large as a few Δ depending on the problem. The interpolative perturbation approach (IPA) proposed in [41], and extended to finite magnetic field in [43] has been applied to the coefficient c_B of the expansion of the conductance with magnetic field $G(B) = G(0)[1 - c_B(g\mu_B B/k_B T_K)^2]$ [27, 30] leading results superior to those of the rSPT including ladder diagrams [30]. This IPA requires to satisfy selfconsistently the Friedel sum rule [44] to each spin [43, 45]. While this rule cannot be extended to finite temperature T, we have explored a simple extension for $T \to 0$, as explained in section 3.

Table 1. Renormalized parameters $\widetilde{\Delta}/\Delta, \epsilon = \widetilde{E}_d/\widetilde{\Delta}$ and $u = \widetilde{U}/(\pi\widetilde{\Delta})$ obtained from NRG+RPT for several values of U/Δ and E_d/Δ [27].

U/Δ	E_d/Δ	$\widetilde{\Delta}/\Delta$	ϵ	u
3	−1.5	0.639	0	0.738
3	−1	0.671	0.196	0.732
3	−0.5	0.754	0.421	0.716
3	0	0.845	0.700	0.698
8	−4	0.120	0	0.985
8	−3	0.143	0.101	0.987
8	−2	0.235	0.247	1.004
8	−1	0.457	0.510	1.040
8	−0.5	0.609	0.715	1.060
8	0	0.746	0.977	1.081
$+\infty$	−6	2.51×10^{-4}	0.0937	1.009
$+\infty$	−5	1.21×10^{-3}	0.118	1.014
$+\infty$	−4	5.79×10^{-3}	0.160	1.025
$+\infty$	−34	0.0270	0.243	1.054
$+\infty$	−2	0.115	0.416	1.136
$+\infty$	−1	0.356	0.766	1.317
$+\infty$	0	0.640	1.338	1.594

In this work, using RPT we derive an analytical (although lengthy) expression of the coefficient c_T for the temperature expansion of the conductance, in terms of the renormalized parameters of the model $\widetilde{\Delta}$, $\widetilde{E}_d$ and $\widetilde{U}$. Taking tabulated values of these parameters from the literature for several values of the original parameters of the model, we obtain the corresponding c_T and compare them with published NRG results. The agreement is excellent for most of the calculated points. The results can be rather easily extended for other sets of parameters in comparison with NRG for dynamical quantities. We also calculated c_T within the IPA and compared with the other approaches.

In section 2, we explain briefly the RPT for the calculation of the Green functions and in particular the spectral density of impurity states and its expansion for $V = B = 0$ and small ω and T. The expression of c_T is given in section 2.4. The comparison with NRG and IPA results is presented in section 3. Section 4 contains a discussion.

2. Formalism

2.1. Hamiltonian

In the most general case, the model describes a QD interacting with two conducting leads, one at the left and one at the right, with chemical potentials μ_L and μ_R respectively, with μ_L-μ_R = eV. The system is at temperature T in presence of a magnetic field B. For the sake of completeness we begin discussing the general case, and later we take $V = B = 0$. The dot level has an on-site energy E_d controlled by a gate voltage and an on-site repulsion U. The Hamiltonian is that of the IAM

[2] There is a mistake in the ordinate axis in figure 2 of [26]: it should be c'_B and not c_B according to the notation of [24].

[3] The statements made in appendix A of [29] about [22] are simply not true, as shown in [30].

$$H = \sum_{k\nu\sigma} \varepsilon_{k\nu} c^\dagger_{k\nu\sigma} c_{k\nu\sigma} + \sum_\sigma E^\sigma_{\rm d} n_{{\rm d}\sigma} + \sum_{k\nu\sigma} (V_{k\nu} c^\dagger_{k\nu\sigma} d_\sigma + {\rm H.c.}) + U n_{d\uparrow} n_{d\downarrow}. \quad (1)$$

Here $\nu = L, R$ refers to the left and right leads and the operator $c^\dagger_{k\nu\sigma}$ creates an electron in the state with wave vector k and spin σ at the lead ν, Similarly $d^\dagger_\sigma$ creates an electron with spin σ at the QD. The number operator $n_{{\rm d}\sigma} = d^\dagger_\sigma d_\sigma$ and $E^\sigma_{\rm d} = E_{\rm d} - \sigma \mu_{\rm B} B$. We assume coupling to the leads $\Delta_\nu = \pi \sum_k |V_{k\nu}|^2 \delta(\omega - \varepsilon_{k\nu}) = \beta_\nu \Delta$ independent of energy, and define the total resonant level width $\Delta = \Delta_{\rm L} + \Delta_{\rm R}$.

2.2. Green function within renormalized perturbation theory

For a symmetric flat band of conduction states and constant Δ as we have assumed, the retarded Green function of the QD level for spin σ can in general be written as

$$G_{{\rm d}\sigma}(\omega) = \frac{1}{\omega - E^\sigma_{\rm d} + {\rm i}\Delta - \Sigma_\sigma(\omega)}, \quad (2)$$

where $\Sigma_\sigma(\omega)$ is the (unknown) retarded self energy.

The basic idea of RPT is to reorganize the perturbation expansion in terms of fully dressed quasiparticles in a Fermi liquid picture [16]. The parameters of the original model are renormalized and the renormalized values $\widetilde{\Delta}$, $\widetilde{U}$ and $\widetilde{E}^\sigma_{\rm d}$ can be calculated exactly from Bethe ansatz results [46–48], or accurately using NRG. One of the main advantages is that the renormalized expansion parameter $u = \widetilde{U}/(\pi\widetilde{\Delta})$ is small. In general $u \lesssim 1$. In the following we set the origin of one-particle energies at the Fermi level ($\epsilon_{\rm F} = 0$). Within RPT, the low-energy part of $G_{{\rm d}\sigma}(\omega)$ is approximated expanding the denominator around $\omega = \epsilon_{\rm F} = 0$, for $V = T = 0$. [16, 28]

$$G_{{\rm d}\sigma}(\omega) \simeq \frac{z}{\omega - \widetilde{E}^\sigma_{\rm d} + {\rm i}\widetilde{\Delta} - \widetilde{\Sigma}_\sigma(\omega)}, \quad (3)$$

where $z = [1 - \partial\Sigma_\sigma(\omega)/\partial\omega|_{\omega=0}]^{-1}$ is the quasiparticle weight, $\widetilde{\Delta} = z\Delta$ is the renormalized resonant level width, $\widetilde{E}_{\rm d} = z[E_{\rm d} + \Sigma_\sigma(0)]$ is the renormalized level energy and

$$\widetilde{\Sigma}_\sigma(\omega) = z[\Sigma_\sigma(\omega) - \Sigma_\sigma(0) - \omega\partial\Sigma_\sigma(\omega)/\partial\omega|_{\omega=0}]. \quad (4)$$

We emphasize that $\Sigma_\sigma(0)$ and $\partial\Sigma_\sigma(\omega)/\partial\omega|_{\omega=0}$ are calculated at $V = T = \omega = 0$ [30].

The renormalized Coulomb repulsion $\widetilde{U}$ is given by a vertex function [14–16].

The spectral density of d electrons is

$$\rho_\sigma(\omega) = -{\rm Im} G_{{\rm d}\sigma}(\omega)/\pi. \quad (5)$$

The free quasiparticle spectral density of d electrons is given by

$$\widetilde{\rho}^\sigma_0(\omega) = \frac{\widetilde{\Delta}/\pi}{(\omega - \widetilde{E}^\sigma_{\rm d})^2 + \widetilde{\Delta}^2}. \quad (6)$$

Using Friedel sum rule [44, 45] one has

$$\pi\Delta\rho_\sigma(0) = \pi\widetilde{\Delta}\widetilde{\rho}^\sigma_0(0) = \sin^2(\pi\langle n_{{\rm d}\sigma}\rangle). \quad (7)$$

Thus, knowing the occupancies $\langle n_{{\rm d}\sigma}\rangle$ experimentally or by a Bette ansatz calculation for example, one can determine the ratios $\widetilde{E}^\sigma_{\rm d}/\widetilde{\Delta} = \cot(\pi\langle n_{{\rm d}\sigma}\rangle)$. The ratio $\widetilde{U}/\widetilde{\Delta}$ can be obtained from the expression of the impurity contribution to magnetic susceptibility at zero temperature [16]

$$\chi = (g\mu_{\rm B})^2 \widetilde{\rho}_0(0)(1 + \widetilde{U}\widetilde{\rho}_0(0))/2, \quad (8)$$

where $\widetilde{\rho}_0(\omega) = \widetilde{\rho}^\uparrow_0(\omega) = \widetilde{\rho}^\downarrow_0(\omega)$ for $B = 0$ and $\widetilde{\Delta}$ can be obtained either from the linear term γ_C in the impurity contribution to the specific heat [16]

$$\widetilde{\Delta} = \frac{2\pi k_{\rm B}^2}{3\gamma_C} \sum_\sigma \sin^2(\pi\langle n_{{\rm d}\sigma}\rangle), \quad (9)$$

or approximately in RPT from the half-width at half maximum of the Kondo peak in $\rho_\sigma(\omega)$ [27].

To obtain the spectral density $\rho_\sigma(\omega)$ out of the point $\omega = T = V = 0$, we need an approximation for $\widetilde{\Sigma}_\sigma(\omega)$. As in previous works [17, 27, 28] we use

$$\widetilde{\Sigma}_\sigma(\omega) = \widetilde{\Sigma}^2_\sigma(\omega) - \widetilde{\Sigma}^2_\sigma(0) - \omega\partial\widetilde{\Sigma}^2_\sigma/\partial\omega|_{\omega=0}, \quad (10)$$

where $\widetilde{\Sigma}^2_\sigma(\omega)$ is obtained using perturbation theory up to second order in $\widetilde{U}$, using the free quasiparticle spectral density $\widetilde{\rho}^\sigma_0(\omega)$ (or the corresponding Green function $1/(\omega - \widetilde{E}^\sigma_{\rm d} + {\rm i}\widetilde{\Delta})$). Since the constant first-order term vanishes in equation (10), a possible expression for $\widetilde{\Sigma}^2_\sigma(\omega)$ is [43]

$$\Sigma^2_\uparrow(\omega) = \widetilde{U}^2 \int {\rm d}\epsilon_1 {\rm d}\epsilon_2 {\rm d}\epsilon_3 \frac{\widetilde{\rho}^\uparrow_0(\epsilon_1)\widetilde{\rho}^\downarrow_0(\epsilon_2)\widetilde{\rho}^\downarrow_0(\epsilon_3)}{\omega + \epsilon_3 - \epsilon_1 - \epsilon_2 + {\rm i}\eta} \times [(1 - \tilde{f}(\epsilon_1))(1 - \tilde{f}(\epsilon_2))\tilde{f}(\epsilon_3) + \tilde{f}(\epsilon_1)\tilde{f}(\epsilon_2)(1 - \tilde{f}(\epsilon_3))], \quad (11)$$

where $\tilde{f}(\omega) = \sum_\nu \beta_\nu f(\omega - \mu_\nu)$, with $f(\omega)$ the Fermi function, and the same interchanging spin up and down.

The lesser and greater Green functions are defined similarly [28].

2.3. Expansion of the renormalized retarded self energy

In the following, we take $V = B = 0$. Then $\widetilde{E}^\sigma_{\rm d} = \widetilde{E}_{\rm d}$ independent of σ. Borrowing results from [38] for the expansion of $\widetilde{\Sigma}^2_\sigma(\omega)$ up to total second order in ω and T, and inserting them in equation (10) we obtain

$$\widetilde{\Sigma}_\sigma(\omega) = -u^2 \frac{\alpha\omega^2 + \beta(\pi k_{\rm B} T)^2 + {\rm i}\gamma[\omega^2 + (\pi k_{\rm B} T)^2]}{\widetilde{\Delta}}, \quad (12)$$

where we define

$$u = \frac{\widetilde{U}}{\pi\widetilde{\Delta}}, \epsilon = \frac{\widetilde{E}_{\rm d}}{\widetilde{\Delta}}, \quad s = \sin(\pi\langle n_{{\rm d}\sigma}\rangle) = \frac{\widetilde{\Delta}}{\sqrt{\widetilde{E}^2_{\rm d} + \widetilde{\Delta}^2}}, \quad c = \cos(\pi\langle n_{{\rm d}\sigma}\rangle), \quad (13)$$

and the coefficients α, β, and γ are given by

$$\alpha = s^4(t_1 + t_2),$$
$$t_1 = \frac{\arctan(\epsilon)/\epsilon - s^2}{4\epsilon},$$
$$t_2 = \arctan(\epsilon)[9/4 + 2\epsilon \arctan(\epsilon)] + \epsilon s^2[\frac{13 - 3\pi^2 + (\pi\epsilon)^2}{4} + (1 - 3\epsilon^2)g(\epsilon)],$$
$$g(\epsilon) = \frac{1}{\epsilon}\int_0^\epsilon dt[\arctan^2(t) + \frac{2}{t}\arctan^2(t)], \quad (14)$$

$$\beta = \frac{s^2}{3}[t_1(1 + 5\epsilon^2) - \frac{\epsilon s^2}{2}], \quad (15)$$

$$\gamma = \frac{s^4}{2}. \quad (16)$$

2.4. Conductance as a function of temperature

In linear response ($V \to 0$) and for $B = 0$, the conductance is given by [49]

$$G(T) = C\int d\omega \rho_\sigma(\omega, T)\left(-\frac{\partial f(\omega)}{\partial \omega}\right), \quad (17)$$

where C is a constant that depends on the couplings Δ_L and Δ_R.

Up to second order in the temperature T, using the Sommerfeld expansion one has

$$G(T) \simeq C[\rho_\sigma(0, T) + \frac{(\pi k_B T)^2}{6}\frac{\partial^2 \rho_\sigma(\omega, 0)}{\partial \omega^2}|_{\omega=0}. \quad (18)$$

Using equations (3), (5), (12)–(16) and (18) we obtain after some algebra the desired expression for the leading temperature dependence of the equilibrium conductance

$$\frac{G(T)}{G(0)} = 1 + \left(\frac{\pi k_B T}{\tilde{\Delta}}\right)^2[\frac{s^2}{3}(4c^2 - 1) + u^2\{2\left(\frac{\alpha}{3} + \beta\right)sc + \frac{4\gamma}{3}(1 - 2s^2)\}]. \quad (19)$$

3. Comparison with NRG for dynamical quantities and IPA

In [24][1], the coefficient c_T was defined as

$$\frac{G(T)}{G(0)} = 1 - c_T\left(\frac{T}{T_0}\right)^2, \quad (20)$$

where T_0 is of the order of the Kondo temperature and defined in terms of the magnetic susceptibility χ by

$$T_0 = \frac{(g\mu_B)^2}{4k_B\chi}. \quad (21)$$

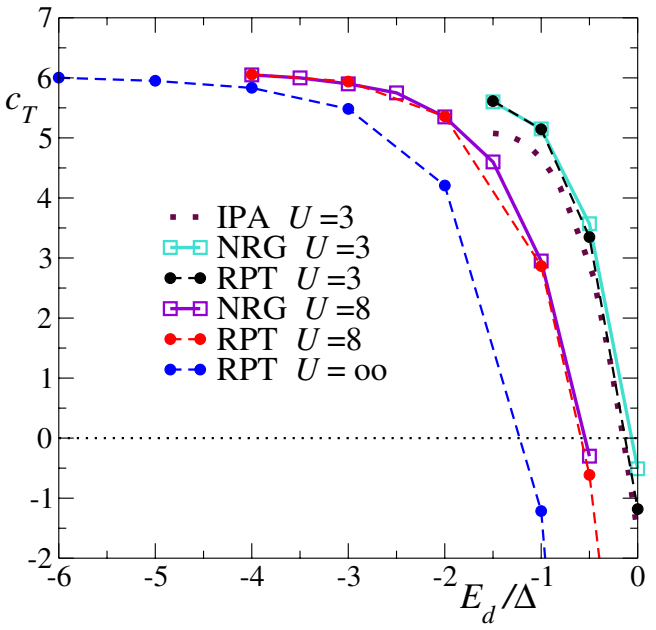

Figure 1. Coefficient c_T of equation (20) versus E_d for several values of U.

Equations (6) and (8) permit to express T_0 in terms of the renormalized parameters. For $-E_d = U/2 \to \infty$, $T_0 = \pi\tilde{\Delta}/(4k_B)$ [16] and $c_T = \pi^4/16 \approx 6.09$ [14, 15]. The values of the renormalized parameters parameters were calculated in [27] following the procedure explained by Hewson *et al* [50][4]. They are reproduced in table 1 for the ease of the reader. The original parameters include $U = 8\Delta$ (for which the system is in the Kondo regime near the symmetric point $E_d = -U/4$), and $U \to +\infty$ which is more realistic for several molecular QDs [11]. Using these renormalized parameters, we have calculated c_T using the expression of the previous section. The results are shown in figure 1.

We also show c_T for the same values of U as those in table 1 reported in figure 5 of [24][1]. In that work, c_T has been extracted from a fit to equation (20) of several low-temperature values (in the range $10^{-5}T_0 \leqslant T \leqslant 0.02T_0$) of the conductance $G(T)$ obtained using an NRG for dynamical quantities developed in [51]. In addition two values for z-averaging were used [24][1].

For a moderate value of $U = 3\Delta$, we also show the results of the IPA. These were obtained with the following procedure. First we used for the self-energy the result based on second-order perturbation theory at $T = V = 0$ and finite magnetic field B, as in [43]. The unperturbed Green functions

$$G^0_{d\sigma}(\omega) = \frac{1}{\omega - \varepsilon^\sigma_d + i\Delta}, \quad (22)$$

corresponding to the unperturbed Hamiltonian

$$H_0 = H - \sum_\sigma (E^\sigma_d - \varepsilon^\sigma_d)n_{d\sigma} - Un_{d\uparrow}n_{d\downarrow}, \quad (23)$$

[4] We interpret that in equation (42) of [50], the first member refers to $\tilde{\Delta}_\Lambda$ the renormalized Δ for $\Lambda \neq 1$, which is related to $\tilde{\Delta}$ by $\tilde{\Delta}_\Lambda = A_\Lambda\tilde{\Delta}$.

are calculated with effective on-site energies $\varepsilon_{\rm d}^{\sigma}$ determined self consistently to satisfy the Friedel sum rule for both spins [45]. From this calculations we extract $\varepsilon_{\rm d} = \varepsilon_{\rm d}^{\uparrow} = \varepsilon_{\rm d}^{\downarrow}$ for $B = 0$ and the magnetic susceptibility from numerical differentiation of the magnetization. Using equation (21) T_0 is obtained. Then, we calculate the IPA self-energy at finite temperature keeping $\varepsilon_{\rm d}$ fixed, and fit the low-T results to a quadratic dependence.

Since c_T has the same value replacing $E_{\rm d}$ by $U - E_{\rm d}$ we represent in figure 1 only $E_{\rm d} \geqslant -U/2$. It is apparent that c_T decreases monotonically showing a downward curvature with increasing (or decreasing) $E_{\rm d}$ starting from the symmetric point $E_{\rm d} = -U/2$, becoming negative for $E_{\rm d} \sim 0$.

It is clear that the comparison between RPT and NRG results are very good. For positive c_T the difference is of the order of the symbol size and increases as the on-site energy $E_{\rm d}$ is moved away from the symmetric point. For $U = 3\Delta$ the maximum difference between the values included in the figure is 0.67 for $E_{\rm d} = 0$ (12 % of the maximum value $c_T = 5.61$ for $E_{\rm d} = -U/2$).

In [24][1] also the coefficient c'_T was introduced which differs from c_T in the fact that the characteristic temperature T_0 was taken always as that of the symmetric point $T_0^{\rm sym} \leqslant T_0$. The relation between both coefficients is

$$\frac{c'_T}{c_T} = \left(\frac{T_0^{\rm sym}}{T_0}\right)^2 . \tag{24}$$

The above mentioned difference in c_T is reduced by a factor 0.18 ($k_{\rm B}T_0 = 1.3468\Delta$, $k_{\rm B}T_0^{\rm sym} = 0.5775\Delta$) in c'_T. Then, the maximum deviation in c'_T for $U = 3\Delta$ is below 0.1. In [29][3], a comparison between result of c'_T calculated with NRG and rSPT including ladder diagrams was presented for $U \leqslant 3\Delta$. From figure 1 of [29][3], it is clear that the deviation of both results is already larger than 0.8 for $U = 3\Delta$ and $E_{\rm d} = -0.3\Delta$. This indicates that our RPT results for $U = 3\Delta$ are nearly an order of magnitude more precise near $E_{\rm d} = 0$. Note that the rSPT results depend on two parameters, $\widetilde{\Delta}$, $\widetilde{U}$ for $E_{\rm d} = -U/2$, while in our RPT approach one has in addition $\widetilde{E}_{\rm d}$ and all parameters depend on $E_{\rm d}$.

For $U = 3\Delta$ we also show the results obtained using the IPA. In contrast to RPT and rSPT, the results do not depend on renormalized parameters. As a consequence, while RPT and rSPT give by construction the exact result at the symmetric point $E_{\rm d} = -U/2$ taking known values of $\widetilde{\Delta}$ and $\widetilde{U}$ with $\widetilde{E}_{\rm d} = 0$, IPA deviates from the correct result. This is due to its inaccuracy in the calculation of the magnetic susceptibility (which determines the energy scale T_0), underestimated by 8 % and also an underestimation of the curvature of $G(T)$. The accuracy of the IPA increases away from the symmetric point, and taking into accounts its simplicity, the IPA provides a rather good semiquantitative description for $U = 3\Delta$ (or lower), although c_T continues underestimated in the whole range of $E_{\rm d}$. The IPA seems to be better than the rSPT near the intermediate valence region.

The comparison between RPT and NRG for $U = 8\Delta$ shows that the agreement does not deteriorate with increasing U in contrast to the case of IPA [27] or rSPT [24, 29, 30][1]. For example, the underestimation of the magnetic susceptibility at the symmetric point by the IPA increases to 15 % for $U = 4\Delta$, while it is only 1.4 % for $U = 2\Delta$.

4. Summary and discussion

Using renormalized perturbation theory (RPT), we have provided an analytical expression for the coefficient of the leading temperature dependence of the conductance through a quantum dot, in terms of the renormalized parameters of the impurity Anderson model $\widetilde{\Delta}$, $\widetilde{E}_{\rm d}$ and $\widetilde{U}$. The expression is given by equation (19) where the different coefficients are defined by equations (13)–(16). Using equations (20) and (21) the coefficient c_T defined previously [24][1] is immediately obtained, and also c'_T (see equation (24)) which uses a fixed Kondo scale evaluated at $E_{\rm d} = -U/2$. Although the expression is lengthy it can be easily evaluated. The most difficult task is a 1D integration (last equation (14)). The renormalized parameters can be easily obtained from the spectrum of an NRG calculation [50][4] or from the calculation of static quantities with Bethe ansatz [46–48], or from experiment. Wiegmann and Tsvelick provide analytical expressions for the occupancy, magnetic susceptibility and specific heat, from which the renormalized parameters can be calculated using equations (5)–(9). Some tricks to evaluate integrals that enter these expressions are given in the appendix of [52].

The calculation of dynamical quantities like the conductance is not possible with Bethe ansatz, and much more complicated within NRG [53, 54]. To calculate c_T directly within NRG for dynamical properties required several calculations at different temperatures within an optimized range of temperatures and for two different logarithmic discretizations (z-averaging) [24][1]. We would like to notice that even the calculation of the static magnetic susceptibility χ (which determines T_0, see equation (21)) within NRG is much easier determining first the renormalized parameters and then using equation (8), as done in [27]. A direct calculation of χ using standard NRG well inside the Kondo regime displays oscillations with temperature and even negative values [55, 56]. A full density-matrix NRG was required to solve this problem [55], but this is not necessary to calculate the renormalized parameters [50][4].

Our calculation with RPT is therefore much easier than direct evaluation of the conductance using NRG. It also has the advantage over ordinary (not renormalized) perturbation approaches [27, 30], or the so called renormalized superperturbation theory (rSPT) including ladder diagrams [29][3] that the results do not deteriorate rapidly with increasing U allowing us to reach the Kondo regime $-E_{\rm d}, U + E_{\rm d} \gg \Delta$.

Different approaches discussed here (RPT, rSPT, NRG, but not IPA) give the same correct value of c_T at the symmetric point $E_{\rm d} = -U/2$. Also by definition, c_T and c'_T coincide at this point (see equation (24)). Out of this point, since T_0 can be considerably larger than $T_0^{\rm sym}$, the magnitude of c'_T is smaller or much smaller than c_T. From this analysis, it is clear that plotting c_T instead of c'_T is more appropriate to see differences

between different approaches. Moreover T_0 is directly related with the width of the Kondo peak in the spectral density of states $2\Delta_\rho$ (the ratio Δ_ρ/T_0 has been calculated within RPT in [27]), which in turn is of the order of the width $2\Delta_G$ of the zero-bias anomaly in the conductance $G(V)$ [35], which is experimentally accessible. The ratio Δ_G/Δ_ρ depends on the ratio of the couplings between left and right leads Δ_L/Δ_R and has been calculated [35].

In the Kondo regime, an empirical formula that fits the NRG results for the temperature dependence of the conductance very well has been proposed [57]. It can be written in the form

$$G(T) = \frac{G(0)}{\left[1 + (2^{1/s} - 1)(T/T_K^G)^2\right]^s}, \tag{25}$$

where $s = 0.22$ and T_K^G (of the order of T_0) is the temperature at which the conductance falls to half of the zero temperature value: $G(T_K^G) = G(0)/2$. One may wonder to which extent the expansion of this expression for $T \to 0$

$$\frac{G(T)}{G(0)} \approx 1 - c_E \left(\frac{T}{T_K^G}\right)^2$$
$$c_E = s(2^{1/s} - 1) \approx 4.92, \tag{26}$$

gives the correct $c_T = \pi^4/16 \approx 6.09$ in the Kondo limit. Comparing equations (20) and (26), one realizes that to answer this question one needs to know the ratio T_K^G/T_0. We have calculated this ratio for two cases presented above: $U \to \infty$, $E_d/\Delta = -6$, and $U/\Delta = 8$, $E_d/\Delta = -4$. For the first case, equations (6) and (8) and the data of table 1 give $\chi = 0.99/(\pi\widetilde{\Delta})$ and then from equation (21) $k_B T_0 \approx 0.79\widetilde{\Delta}$. Taking $\widetilde{\Delta} = 2.51 \times 10^{-4}\Delta$ from table 1, one obtains $k_B T_0 = 1.99 \times 10^{-4}\Delta$, which almost coincides with the value $k_B T_K^G = 1.98 \times 10^{-4}\Delta$ obtained using NRG for dynamical quantities [58]. Since the value obtained by RPT for these parameters is $c_T = 6.00$ (see figure 1), c_E is an underestimation by 17 %. It is interesting to note that the RPT calculation of the half width at half maximum of the spectral density for these parameters is [27] $\Delta_\rho = 0.706\widetilde{\Delta} = 0.89 k_B T_0$. Similarly, for $U/\Delta = 8$, $E_d/\Delta = -4$, we obtain $c_T = 6.05$, $\Delta_\rho = 0.90 k_B T_0$ $k_B T_0 = 0.791\widetilde{\Delta} = 0.095\Delta$, while $k_B T_K^G = 0.101\Delta$ [58]. In this case, $c_E/c_T = 0.72$. The failure of equation (25) to accurately reproduce the low-T behavior in the Kondo regime is due to the fact that it was devised to fit the conductance in a wide temperature range and not just for small T.

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