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The renormalized superperturbation theory (rSPT) approach to the Anderson model in and out of equilibrium

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Abstract. The properties of current-carrying steady states of strongly correlated systems away from the linear-response regime are of topical interest. In this article, we review the renormalized perturbation theory (rSPT), or renormalized SPT of reference [1] for the Anderson model. We present an extension to higher orders and compare the higher-order results with NRG calculations. Finally, we elucidate the role of Ward identities in calculating out-of-equilibrium properties and address claims made in the literature.

1. Introduction

Quantum dots as well as other artificial nanostructures, such as single-molecules attached to conducting leads, constitute very versatile devices, since their characteristic energy scales such as Fermi level, charging energy, level spacing can be tuned over a wide range [2, 3, 4]. The high degree of characterization of these systems has made it possible to investigate the properties of strongly-correlated electrons away from equilibrium in a well-defined setting [5, 6]. In particular, the low-temperature, low-bias differential conductance characteristics in these nanostructures often display a nearly universal conductance enhancement due to Kondo screening of the local, *i.e.*, localized on the quantum dot, dynamic degree of freedom by the lead electrons [7]. It is well established, that in equilibrium, i.e. within the linear response regime, the Kondo effect leads to an enhancement of the differential conductance $G = dI/dV|_{V=0}$ on the order of twice the quantum of conductance $2e^2/h$ in the limit $T \to 0$. These experimental results are usually interpreted within the context of the single-level Anderson model [8, 9]

$$H_{\rm AM} = \sum_{\lambda=L/R} H_0^{\lambda}(c_\lambda^\dagger, c_\lambda) + \sum_{\sigma=\pm} \epsilon_d d_\sigma^\dagger d_\sigma + U d_+^\dagger d_+ d_-^\dagger d_- + \sum_\lambda \sum_\sigma (V d_\sigma^\dagger c_{0\sigma\lambda} + \text{h.c.}) \qquad (1)$$

as the effective low-energy model. In Eq. (1), H_0^λ is a free electron Hamiltonian given in terms of $c_\lambda^\dagger$ and c_λ which describes the excitations of lead λ, $c_{0\sigma\lambda}^\dagger$ is the corresponding creation operator of lead λ at the quantum dot site $\mathbf{r} = 0$. V denotes the coupling strength between the lead states and the quantum dot states, described by d_σ and U is the charging energy of the dot.

Correspondingly, a large class of conductance experiments has been accurately fitted by an expression of the form [5, 6, 10, 11, 12]

$$\frac{G(0,0) - G(T,V)}{c_T G(0,0)} = \left(\frac{T}{T_K}\right)^2 + \alpha \left(\frac{eV}{k_B T_K}\right)^2 - \gamma c_T \left(\frac{eVT}{k_B T_K^2}\right)^2, \qquad (2)$$

where T_K is some characteristic energy scale which is obtained from the fit to the experimental results. When casting the low-temperature non-linear conductance of the Anderson model, Eq. (1) into the form (2), T_K becomes the Kondo temperature. The coefficients α and γ vary across different experimental systems [5, 6]. Already addressing how α and γ depend on the parameters of $H_{\rm AM}$ is a difficult task as it requires a proper description of the low-energy excitations of the Anderson model in a non-thermal steady state. While there is a rather complete picture of the equilibrium behavior of Eq. (1), such an understanding for the out-of-equilibrium properties is still lacking. This is largely due to the lack of reliable methods that can tackle the strongly correlated nature of the non-thermal steady state associated with $H_{\rm AM}$.

The equilibrium properties of the Anderson model have been studied extensively with the help of *e.g.* numerical renormalization group methods (NRG) [13], pseudoparticle [14] and Monte Carlo methods. Analytical methods have also been developed to study this problem, such as the bare perturbation theory of Yamada and Yosida [15, 16, 17]. An exact analytical solution has been obtained via Bethe Ansatz [18, 19, 20]. Unfortunately, fully reliable generalizations of these methods to the out-of-equilibrium problem are, at least at present, not available. However, a number of perturbative renormalization group (RG) methods have been proposed for non-equilibrium systems [21, 22], including functional perturbative RG [23]. Among the perturbative methods available, the renormalized perturbation theory (RPT) developed by Hewson [7, 24, 25, 26] provides a framework that can in principle be extended out of equilibrium, for instance by relying on exact Ward identities [27, 28]. The RPT provides an accurate description of the equilibrium Fermi-liquid regime in terms of quasi-particle excitations, characterized by effective interaction parameters [7, 24, 25].

Motivated by the above-mentioned experiments, following Refs. [25, 27], and in the spirit of Ref. [29], we recently developed the rSPT [1] - a renormalized superperturbation theory in terms

of dual fermions [30, 31] on the Keldysh contour. Using this method, we studied steady-state non-equilibrium transport in the single-level Anderson model beyond particle-hole symmetry, by constructing a perturbative scheme based on a particle-hole symmetric reference system [1]. We constructed the reference system non-equilibrium self-energy at finite bias by extending Oguri's Ward identity approach [27, 32], which has the advantage of providing a current conserving expansion by construction [33, 1, 32]. The dual fermion, an auxiliary fermionic degree of freedom, is used to construct a systematic expansion around the interacting reference system [30].

Within the rSPT, we have studied the role of level asymmetry (gate voltage) and local Coulomb repulsion (charging energy) on the non-linear conductance of the single-level Anderson model in the steady-state regime [1, 34]. A comparison of our analytic results for the linear response transport coefficients with NRG calculations demonstrated an excellent quantitative agreement, even at relatively large level asymmetry [34]. Moreover, our results have recently provided a theoretical framework to describe and interpret magneto-transport experiments in single-molecule transistors [35].

In this article, we review the rSPT and extend the calculation to higher order (in the renormalized interaction) than reported before. In section 5, we compare the higher order calculation with NRG calculations for the linear-response transport coefficients. In the appendix, we exemplify the proof of Oguri's Ward identity [36] and address claims made in the literature regarding the validity of this identity.

2. Path-Integral representation on the Keldysh contour

We consider the single-level Anderson model, Eq. (1), which can be represented by a non-equilibrium functional on the Keldysh contour [1],

$$Z = \int \mathcal{D}[\hat{\psi}^\dagger, \hat{\psi}]\, \mathcal{D}[\hat{\Phi}^\dagger, \hat{\Phi}] e^{iS[\hat{\psi}^\dagger, \hat{\psi}, \hat{\Phi}^\dagger, \hat{\Phi}]}, \tag{3}$$

where the action in the Schwinger-Keldysh matrix representation is

$$\begin{aligned} S[\hat{\psi}^\dagger, \hat{\psi}, \hat{\Phi}^\dagger, \hat{\Phi}] &= \int_{-\infty}^{+\infty} dt \left\{ \sum_{k,\lambda,\sigma} \hat{\psi}^\dagger_{k\lambda\sigma}(t) \left(i\partial_t - \epsilon_{k\lambda}\right) \hat{\sigma}_3 \hat{\psi}_{k\lambda\sigma}(t) + \sum_{\sigma} \hat{\Phi}^\dagger_\sigma(t) \left(i\partial_t - E_{d\sigma}\right) \hat{\sigma}_3 \hat{\Phi}_\sigma(t) \right. \\ &\left. + \sum_{k,\lambda,\sigma} \left[V_{k\lambda} \hat{\Phi}^\dagger_\sigma(t) \hat{\sigma}_3 \hat{\psi}_{k\lambda\sigma}(t) + h.c. \right] \right\} + i\, S^{int}[\hat{\Phi}^\dagger, \hat{\Phi}; U]. \end{aligned} \tag{4}$$

Here, the fields are two-component spinors in the index that distinguishes between the forward and backward branch of the Keldysh contour and σ_3 is the 3rd Pauli matrix in this space. The index $\lambda = L, R$ represents the left and right electrodes, U is the Coulomb interaction, and $E_{d\sigma} = \epsilon_{d\sigma} + U/2$ is the shift of the local resonance level with respect to the particle-hole symmetric condition $\epsilon_d = -U/2$. In the presence of a local magnetic field B, the local level has to be shifted by the Zeeman term, *i.e.*, $\epsilon_{d\sigma} = \epsilon_d - \sigma g \mu_B B/2$. The action defined by Eq.(4) is Gaussian in the Grassman fields $\hat{\psi}_{k\lambda\sigma}$ representing the lead electrons by virtue of their non-interacting nature. As a result, the $\hat{\psi}_{k\lambda\sigma}$ fields can be integrated out. This procedure yields an effective action for the localized electron states described by the Grassman fields $\hat{\Phi}_{\sigma\omega}$, which represent the d_σ of Eq. (1). In frequency-space this effective action is given by [1]

$$\begin{aligned} iS[\hat{\Phi}^\dagger, \hat{\Phi}; U, E_{d\sigma}, \Delta] &= i \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \sum_\sigma \hat{\Phi}^\dagger_{\sigma\omega} \left(\omega + i\Delta\right) \hat{\sigma}_3 \hat{\Phi}_{\sigma\omega} + iS^{int}[\hat{\Phi}^\dagger, \hat{\Phi}; U] \\ &\quad - i \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \sum_\sigma \hat{\Phi}^\dagger_{\sigma\omega} E_{d\sigma} \hat{\sigma}_3 \hat{\Phi}_{\sigma\omega}. \end{aligned} \tag{5}$$

Here, we have defined $\Delta = \Delta_L + \Delta_R$, and

$$i\Delta_\lambda = -\sum_{k,\lambda} \frac{|V_{k\lambda}|^2}{\omega - \epsilon_{k\lambda} + i\eta^+}. \tag{6}$$

In analogy to the equilibrium version of the renormalized theory (RPT) of Hewson [25, 37, 26], we can express the action Eq.(5) in terms of a set of "renormalized" parameters $\tilde{U}$, $\tilde{\epsilon}_{d\sigma}$ and $\tilde{\Delta}$. The fields are rescaled accordingly via the wave-function renormalization factor z given by $z^{-1} = 1 - \partial\Sigma^R_{\sigma\omega}/\partial\omega\Big|_{\omega=0}$.

Here, we seek to construct a renormalized perturbation theory to treat deviations from particle-hole symmetry, represented by the paramater $\tilde{\epsilon}_{d\sigma} = zE_{d\sigma}$ which is assumed to be small compared to the energy scale determined by the renormalized quasi-particle spectral width $\tilde{\Delta} = z\Delta$. Thus,

$$S[\hat{\Phi}^\dagger, \hat{\Phi}; U, E_{d\sigma}, \Delta] \;=\; S[\tilde{\Phi}^\dagger, \tilde{\Phi}; \tilde{U}, \tilde{\epsilon}_{d\sigma}, \tilde{\Delta}] + \delta S[\tilde{\Phi}^\dagger, \tilde{\Phi}; \lambda_1, \lambda_2, \lambda_3]. \tag{7}$$

In order to preserve the original action and thus avoid over counting, one must include counterterms proportional to the parameters λ_1, λ_2 and λ_3. These counterterms are defined as $\lambda_1 = -z\Sigma^R_\sigma(0,0)$, $\lambda_2 = z - 1$ and $\lambda_3 = z^2\left(U - \Gamma_{\uparrow\downarrow}(0,0)\right)$, respectively. Their values are determined in order to satisfy the RG conditions imposed on the retarded Green's function

$$\begin{aligned}
\tilde{\Sigma}^R_{\sigma\omega}\Big|_{\omega=0,T=0,V=0} &= 0, \\
\frac{\partial}{\partial\omega}\tilde{\Sigma}^R_{\sigma\omega}\Big|_{\omega=0,T=0,V=0} &= 0, \\
\tilde{\Gamma}_{\uparrow\downarrow}(0,0) = z^2\Gamma_{\uparrow\downarrow}(0,0) &= \tilde{U},
\end{aligned} \tag{8}$$

at every order in $\tilde{U}$. For the particle-hole symmetric case, the retarded self-energy in equilibrium has been obtained up to second order in $\tilde{u} = \tilde{U}/(\pi\tilde{\Delta})$ [25, 37, 26]. This equilibrium expression can be extended to non-thermal steady states, *e.g.* the one that ensues when the system is experiencing a voltage drop across the interaction region that is constant in time. This extension is based on Ward identities [36, 27, 1, 32]. As a result, one obtains an expression for the selfenergy of the local propagator near the strong-coupling fixed point and at particle-hole symmetry and zero magnetic field

$$\tilde{\Sigma}^R_{\sigma\omega} \;=\; -i\frac{\tilde{\Delta}\tilde{u}^2}{2}\left[\left(\frac{\omega}{\tilde{\Delta}}\right)^2 + \left(\frac{\pi T}{\tilde{\Delta}}\right)^2 + \zeta\left(\frac{V}{\tilde{\Delta}}\right)^2 - \frac{\zeta}{3}\left(\frac{\pi TV}{\tilde{\Delta}}\right)^2\right] + O(T^4, V^4, \tilde{u}^3). \tag{9}$$

At zero magnetic field, it has been shown by Hewson [25, 26] that the counterterm λ_1 cancels the Hartree contribution up to order $\tilde{u}^2$. To the same order, there are no contributions from the counterterms λ_2 and λ_3 [25, 26]. This renormalized action, exact up to terms of order $\tilde{u}^2$ constitutes the reference system around which our perturbative scheme of dual fermions is defined. In the next section, the bare dual fermion Green's function is introduced.

3. The dual Fermion Green's function

The bare dual fermion bare Green's function is given by the expression [1, 32]

$$\mathbf{G}^{f(0)}_{\sigma\omega} \;=\; -\mathbf{g}_{\sigma\omega}\left[\mathbf{g}_{\sigma\omega} - \mathbf{D}^{-1}_{\sigma\omega}\right]^{-1}\mathbf{g}_{\sigma\omega} = \sum_{n=1}^{\infty}\mathbf{g}_{\sigma\omega}\left[\mathbf{D}_{\sigma\omega}\mathbf{g}_{\sigma\omega}\right]^n. \tag{10}$$

Here, we have defined $\mathbf{D}_{\sigma\omega} = \tilde{\epsilon}_{d\sigma}\hat{\sigma}_3$. For convenience we switch from the dynamical index representation $+-$ to the trigonal representation [38] in what follows. Both representations are linked by a similarity transformation

$$\hat{\mathbf{G}}^f_{\sigma\omega} = \hat{L}\hat{\sigma}_3\mathbf{G}^f_{\sigma\omega}\hat{L}^\dagger = \begin{pmatrix} G^{f,R}_{\sigma\omega} & G^{f,K}_{\sigma\omega} \\ 0 & G^{f,A}_{\sigma\omega} \end{pmatrix}, \tag{11}$$

where we defined $\hat{L} = (1 - i\hat{\sigma}_2)/\sqrt{2}$ and $\hat{\sigma}_2$ is the 2nd Pauli matrix. Under this transformation the matrix $\mathbf{D}_{\sigma\omega} \rightarrow \hat{L}\hat{\sigma}_3\mathbf{D}_{\sigma\omega}\hat{L}^\dagger = \tilde{\epsilon}_{d\sigma}\mathbf{1}$ becomes proportional to the identity. Moreover, the retarded component of the dual fermion Green's function becomes

$$G^{f(0),R}_{\sigma\omega} = \sum_{n=1}^{\infty} \left(\tilde{\epsilon}_{d\sigma}\right)^n \left(g^R_{\sigma\omega}\right)^{n+1} = \frac{\tilde{\epsilon}_{d\sigma}\left(g^R_{\sigma\omega}\right)^2}{1 - \tilde{\epsilon}_{d\sigma}g^R_{\sigma\omega}}. \tag{12}$$

The advanced Green's function then follows from the usual relation $G^{f(0),A}_{\sigma\omega} = \left(G^{f(0),R}_{\sigma\omega}\right)^*$. In the steady-state and up to $O(\tilde{u}^4)$, the Keldysh component of the dual fermion Green's function is given by [1, 32]

$$G^{f(0),K}_{\sigma\omega} = \left(1 - 2\tilde{f}(\omega, T, V)\right)\left(G^{f(0),A}_{\sigma\omega} - G^{f(0),R}_{\sigma\omega}\right). \tag{13}$$

Here, up to $O(\tilde{u}^4)$, the non-equilibrium distribution function is given by the expression [1, 32]

$$\tilde{f}(\omega, T, V) = \frac{\tilde{\Delta}_L f_0(\omega + \alpha_L V, T) + \tilde{\Delta}_R f_0(\omega - \alpha_R V, T)}{\tilde{\Delta}_L + \tilde{\Delta}_R}, \tag{14}$$

where $f_0(\omega, T)$ denotes the Fermi distribution and $\alpha_L + \alpha_R = 1$.

Note, that by substituting the definition of the retarded renormalized Green's function of the reference system

$$g^R_{\sigma\omega} = \left(\omega + i\tilde{\Delta} - \tilde{\Sigma}^R_{\sigma\omega}\right)^{-1} \tag{15}$$

into Eq.(12), one concludes that as $\tilde{\epsilon}_{d\sigma} \rightarrow 0$ then $G^{f(0),R}_{\sigma\omega} \rightarrow 0$, and hence the dual fermion contribution to the perturbed self-energy vanishes in the p-h symmetric limit, as expected.

On the other hand, in the limit $\tilde{\epsilon}_{d\sigma} \rightarrow \infty$, we have the non-trivial result [30, 1]

$$\lim_{\tilde{\epsilon}_{d\sigma}\rightarrow\infty} G^{f(0),R}_{\sigma\omega} = -g^R_{\sigma\omega}. \tag{16}$$

The relation between the dual fermion Green's function and the local Green's function associated with the $d^\dagger_\sigma, d_\sigma$ operators of Eq. (1) in Keldysh space is

$$\mathbf{G}_{\sigma\omega} = -\tilde{\epsilon}^{-1}_{d\sigma}\hat{\sigma}_3 + \left(\mathbf{g}_{\sigma\omega}\hat{\sigma}_3\tilde{\epsilon}_{d\sigma}\right)^{-1}\mathbf{G}^f_{\sigma\omega}\left(\hat{\sigma}_3\mathbf{g}_{\sigma\omega}\tilde{\epsilon}_{d\sigma}\right)^{-1}. \tag{17}$$

Here, the dressed dual fermion Green's function $\mathbf{G}^f_{\sigma\omega}$ is a solution of the Dyson equation

$$\mathbf{G}^f_{\sigma\omega} = \mathbf{G}^{f(0)}_{\sigma\omega} + \mathbf{G}^{f(0)}_{\sigma\omega}\mathbf{\Sigma}^f_{\sigma\omega}\mathbf{G}^f_{\sigma\omega}, \tag{18}$$

where $\mathbf{\Sigma}^f_{\sigma\omega}$ is the dual fermion self-energy which will be discussed in the next section.

It is convenient to express Eqs. (17) in the trigonal representation, by applying the transformation defined in Eq.(11), which leads to

$$\hat{\mathbf{G}}_{\sigma\omega} = \hat{L}\hat{\sigma}_3\mathbf{G}_{\sigma\omega}\hat{L}^\dagger = -\tilde{\epsilon}_{d\sigma}^{-1}\mathbf{I} + \tilde{\epsilon}_{d\sigma}^{-2}\hat{\mathbf{g}}_{\sigma\omega}^{-1}\hat{\mathbf{G}}_{\sigma\omega}^{f}\hat{\mathbf{g}}_{\sigma\omega}^{-1}. \tag{19}$$

Similarly, the Dyson equation becomes in the trigonal representation

$$\hat{\mathbf{G}}_{\sigma\omega}^{f} = \hat{\mathbf{G}}_{\sigma\omega}^{f(0)} + \hat{\mathbf{G}}_{\sigma\omega}^{f(0)}\hat{\mathbf{\Sigma}}_{\sigma\omega}^{f}\hat{\mathbf{G}}_{\sigma\omega}^{f}, \tag{20}$$

where the dual-fermion self-energy adopts the matrix form

$$\hat{\mathbf{\Sigma}}_{\sigma\omega}^{f} = \begin{pmatrix} \Sigma_{\sigma\omega}^{f,R} & \Sigma_{\sigma\omega}^{f,K} \\ 0 & \Sigma_{\sigma\omega}^{f,A} \end{pmatrix}. \tag{21}$$

In particular, solving for the retarded component of the non-equilibrium local Green's function from Eq.(17), we have

$$G_{\sigma\omega}^{R} = -\tilde{\epsilon}_{d\sigma}^{-1} + \tilde{\epsilon}_{d\sigma}^{-2}\left(g_{\sigma\omega}^{R}\right)^{-1} G_{\sigma\omega}^{f,R}\left(g_{\sigma\omega}^{R}\right)^{-1}. \tag{22}$$

This exact expression can be combined with the solution of the Dyson equation for the retarded component of the dual-fermion Green's function obtained from Eq.(18),

$$G_{\sigma\omega}^{f,R} = \frac{G_{\sigma\omega}^{f(0),R}}{1 - G_{\sigma\omega}^{f(0)}\Sigma_{\sigma\omega}^{f,R}}, \tag{23}$$

to obtain an explicit expression for the retarded component of the local non-equilibrium Green's function

$$G_{\sigma\omega}^{R} = \left(\omega - \tilde{\epsilon}_{d\sigma} + i\tilde{\Delta} - \tilde{\Sigma}_{E_d,\sigma\omega}^{R}\right)^{-1}. \tag{24}$$

Here, we have defined the retarded component of the non-equilibrium self-energy by

$$\tilde{\Sigma}_{E_d,\sigma\omega}^{R} = \tilde{\Sigma}_{\sigma\omega}^{R} + \frac{\Sigma_{\sigma\omega}^{f,R}}{1 + g_{\sigma\omega}^{R}\Sigma_{\sigma\omega}^{f,R}}. \tag{25}$$

4. The dual fermion self-energy

In order to obtain an approximation for the dual fermion self-energy, we consider the sum of ladder diagrams, with the effective quasi-particle interaction defined by the renormalized vertex $\tilde{U}$ of Eq. (8). In the trigonal representation, the non-equilibrium dual-fermion self-energy matrix, expressed in terms of the dual fermion vertex $\hat{\mathbf{\Gamma}}^f$, is

$$\hat{\mathbf{\Sigma}}_{\sigma\omega}^{f} = \frac{1}{2}\int_{-\infty}^{+\infty}\frac{d\omega'}{2i\pi}\left\{\Gamma_{\sigma,-\sigma}^{f,K}\left(\hat{\gamma}^1\hat{\mathbf{G}}_{-\sigma\omega'}^{f(0)}\hat{\gamma}^1\right) + \Gamma_{\sigma,-\sigma}^{f,A}\left(\hat{\gamma}^1\hat{\mathbf{G}}_{-\sigma\omega'}^{f(0)}\hat{\gamma}^2\right) + \Gamma_{\sigma,-\sigma}^{f,R}\left(\hat{\gamma}^2\hat{\mathbf{G}}_{-\sigma\omega'}^{f(0)}\hat{\gamma}^1\right)\right\}, \tag{26}$$

where $\hat{\gamma}^1 = \mathbf{1}$ and $\hat{\gamma}^2 = \hat{\sigma}_1$.

Here, the dual-fermion vertex components are defined by the matrix

$$\hat{\mathbf{\Gamma}}_{\sigma,-\sigma}^{f} = \left[\mathbf{1} - \tilde{U}\hat{\sigma}_1\hat{\mathbf{\Pi}}_{\sigma,-\sigma}^{f(0)}(\omega)\right]^{-1}\hat{\sigma}_1\tilde{U} = \begin{pmatrix} \Gamma_{\sigma,-\sigma}^{f,K} & \Gamma_{\sigma,-\sigma}^{f,R} \\ \Gamma_{\sigma,-\sigma}^{f,A} & 0 \end{pmatrix}, \tag{27}$$

where the polarisation matrix is defined by

$$\hat{\mathbf{\Pi}}^{f(0)}_{\sigma,-\sigma}(\omega) = \begin{pmatrix} 0 & \Pi^{A}_{\sigma,-\sigma}(\omega) \\ \Pi^{R}_{\sigma,-\sigma}(\omega) & \Pi^{K}_{\sigma,-\sigma}(\omega) \end{pmatrix}. \tag{28}$$

The different components of the polarization insertion in the trigonal representation are given by the expressions [38]

$$\Pi^{f,K}_{\sigma,-\sigma}(\omega) = -\frac{1}{2}\int_{-\infty}^{+\infty}\frac{d\omega'}{2i\pi}\left\{G^{f(0),K}_{\sigma,\omega+\omega'}G^{f(0),K}_{-\sigma\omega'} + G^{f(0),R}_{\sigma,\omega+\omega'}G^{f(0),A}_{-\sigma\omega'} + G^{f(0),A}_{\sigma,\omega+\omega'}G^{f(0),R}_{-\sigma\omega'}\right\}, \tag{29}$$

$$\Pi^{f,R}_{\sigma,-\sigma}(\omega) = -\frac{1}{2}\int_{-\infty}^{+\infty}\frac{d\omega'}{2i\pi}\left\{G^{f(0),R}_{\sigma,\omega+\omega'}G^{f(0),K}_{-\sigma\omega'} + G^{f(0),K}_{\sigma,\omega+\omega'}G^{f(0),A}_{-\sigma\omega'}\right\}, \tag{30}$$

$$\Pi^{f,A}_{\sigma,-\sigma}(\omega) = \left[\Pi^{f,R}_{\sigma,-\sigma}(\omega)\right]^{*}. \tag{31}$$

In particular, at $\omega = 0$, $T = 0$, $V = 0$, and to zero order in $\tilde{U}$, one has

$$\Pi^{f(0),R}_{\sigma,-\sigma}(0) = \Pi^{f(0),A}_{\sigma,-\sigma}(0) = \frac{1}{\pi\tilde{\Delta}} + \frac{1}{\pi\tilde{\Delta}}\frac{\tilde{\epsilon}^2_{d,-\sigma}\tan^{-1}(\tilde{\epsilon}_{d\sigma}) - \tilde{\epsilon}^2_{d\sigma}\tan^{-1}(\tilde{\epsilon}_{d,-\sigma})}{\tilde{\epsilon}_{d\sigma}\tilde{\epsilon}_{d,-\sigma}\left(\tilde{\epsilon}_{d\sigma} - \tilde{\epsilon}_{d,-\sigma}\right)}. \tag{32}$$

The dual fermion vertex components are thus obtained as

$$\begin{aligned}
\Gamma^{f,R}_{\sigma,-\sigma} &= \frac{\tilde{U}_s}{1 - \tilde{U}_s\Pi^{f,R}_{\sigma-\sigma}(\omega)}, \\
\Gamma^{f,A}_{\sigma,-\sigma} &= \frac{\tilde{U}_s}{1 - \tilde{U}_s\Pi^{f,A}_{\sigma,-\sigma}(\omega)}, \\
\Gamma^{f,K}_{\sigma,-\sigma} &= -\frac{\tilde{U}_s^2\Pi^{f,K}_{\sigma,-\sigma}(\omega)}{\left(1 - \tilde{U}_s\Pi^{f,R}_{\sigma,-\sigma}(\omega)\right)\left(1 - \tilde{U}_s\Pi^{f,A}_{\sigma,-\sigma}(\omega)\right)}.
\end{aligned} \tag{33}$$

Note that the Keldysh component of the dual fermion vertex is of higher order in the effective quasiparticle interaction $\tilde{U}_s$ than the retarded and advanced components.

In order to obtain analytical approximations to the transport coefficients, defined in Eq. (2), which are exact up to $O(\tilde{u}^3)$, we define an effective dual-fermion interaction from the expression for the dual-fermion vertex at $\omega = 0$, $V = 0$, and $T = 0$ by

$$\tilde{U}^{f}_{\sigma,-\sigma} = \Gamma^{f,A}_{\sigma,-\sigma}\Big|_{\omega=0,V=0,T=0} = \Gamma^{f,R}_{\sigma,-\sigma}\Big|_{\omega=0,V=0,T=0} = \frac{\tilde{U}_s}{1 - \tilde{U}_s\Pi^{f,R}_{\sigma,-\sigma}(0)}. \tag{34}$$

Up to order $O(\tilde{u}^3)$ we have that the self-energy of the non-symmetric system defined by Eq.(25) reduces to the expression

$$\tilde{\Sigma}^{R}_{E_d,\sigma\omega} = \tilde{\Sigma}^{R}_{\sigma\omega} + \Sigma^{f,R}_{\sigma\omega} + O(\tilde{u}^3). \tag{35}$$

5. Transport coefficients

With the results of the previous sections, we are in a position to calculate the experimentally accessible transport coefficients α and γ defined in Eq. (2). From the Meir-Wingreen expression [39] for the charge current through the quantum dot,

$$I = \frac{e}{2\hbar}\sum_{\sigma}\int d\omega\frac{4\Delta_L\Delta_R}{\Delta_L + \Delta_R}A_{\sigma}(\omega, T, V)\left[f_L(\omega) - f_R(\omega)\right] \tag{36}$$

where $f_{L,R} = f(\omega - \mu_{L,R})$ is the Fermi function for the left/right lead, respectively, and $A_\sigma(\omega, T, V) = -\pi^{-1}\Im G^R_{\sigma\omega}$ is the local spectral function. Expanding the differential conductance $dI/dV \equiv G(T, V, B)$ up to second order in V, T, and B, one obtains the expression [1]

$$\frac{G(T,0,B) - G(T,V,B)}{G(0,0,0)} = c_V \left(\frac{eV}{\tilde{\Delta}}\right)^2 - c_{TV} \left(\frac{eV}{\tilde{\Delta}}\right)^2 \left(\frac{k_B T}{\tilde{\Delta}}\right)^2 - c_{VE_d} \left(\frac{eV}{\tilde{\Delta}}\right) + c_{TVE_d} \left(\frac{eV}{\tilde{\Delta}}\right)^2 . \tag{37}$$

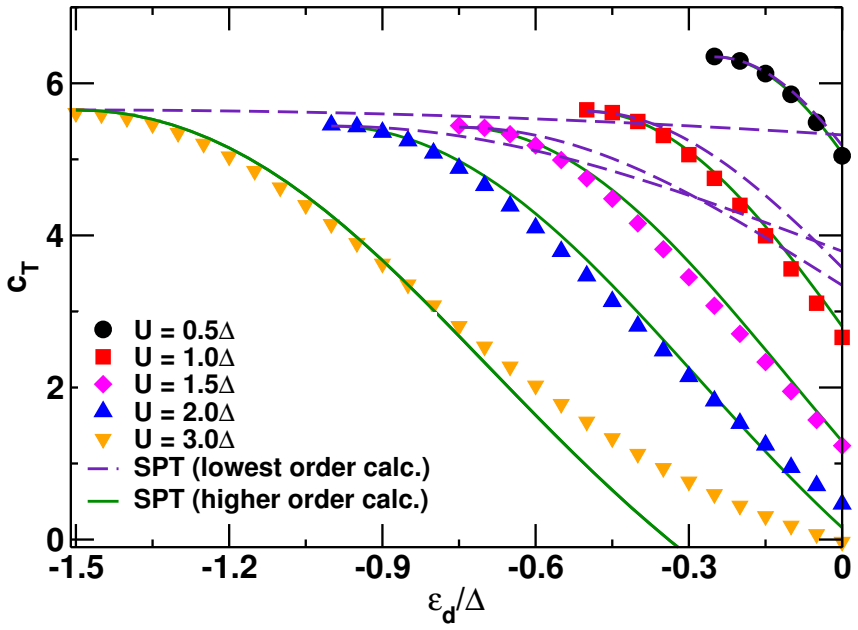

Figure 1. The transport coefficient c_T versus the asymmetry parameter ϵ_d/Δ: Continuous lines are the renormalized rSPT results including higher-order terms. Dashed lines are the renormalized rSPT results at the lowest order. Symbols are the NRG results for the same set of parameters. The particle-hole symmetric reference system is located at $\epsilon_d = -U/2$.

In particular, for the linear-response conductance ($V \to 0$), we have the relations

$$\begin{aligned} \frac{G(T, V=0, B=0)}{G(0,0,0)} &= 1 - c_T \left(\frac{k_B T}{\tilde{\Delta}}\right)^2 , \\ \frac{G(T=0, V=0, B)}{G(0,0,0)} &= 1 - c_B \left(\frac{g\mu_B B}{\tilde{\Delta}}\right)^2 . \end{aligned} \tag{38}$$

In Fig. 1, we show the renormalized rSPT result for c_T, defined in Eq.(38), obtained by including the higher-order dual-fermion contributions as described in section 4. The linear-response conductance can also be calculated via the NRG, which yields essentially exact results for this quantity [13, 34]. Clearly, the renormalized rSPT results for c_T are in excellent agreement with NRG calculations, even at relatively large values of the asymmetry parameter ϵ_d/Δ and Coulomb interaction U. We also display the results (dashed lines in Fig. 1) obtained from the rSPT calculation at the lowest order [34], where the improvement upon inclusion of higher order contributions is evident. A similar level of agreement with the NRG is obtained for the transport coefficient c_B, as shown in Fig. 2.

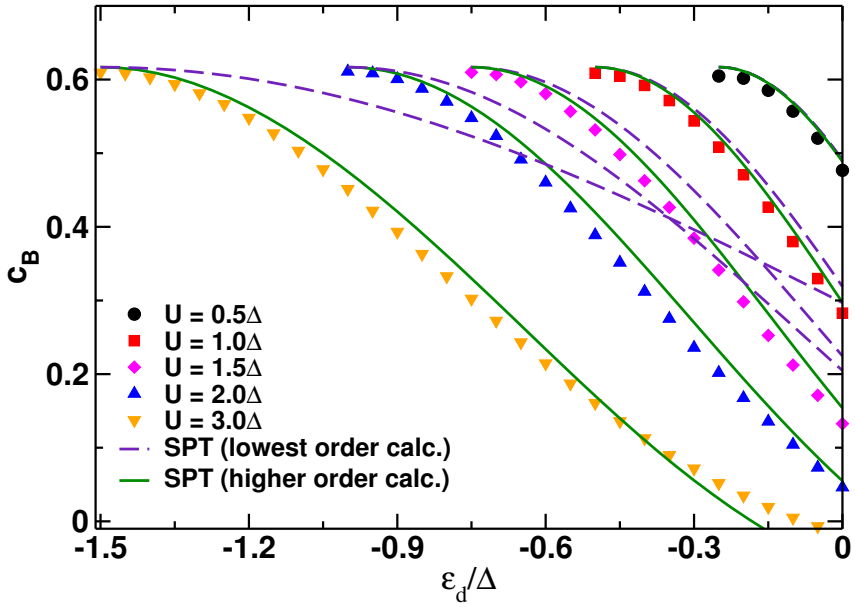

Figure 2. The transport coefficient c_B as a function of the asymmetry parameter ϵ_d/Δ: Continuous lines are the renormalized rSPT results including higher-order terms. Dashed lines are the renormalized rSPT results at the lowest order. Symbols are the NRG results for the same set of parameters.

6. Conclusion

In summary, we have reviewed the renormalized rSPT approach to non-thermal steady states in the Anderson model. By construction, this approach captures the strong-coupling nature of the fixed point. We present an extension to higher orders and compared these higher-order results to NRG calculations. As a result, the renormalized rSPT predictions are in excellent agreement with the (essentially) exact NRG results. The renormalized rSPT is a versatile approach for the out-of-equilibrium properties at sufficiently low energies and temperatures that can also be applied to more complicated models or more general steady states, that ensue by applying finite voltage and temperature differences across the system [40]. We also elucidated the role of Ward identities in calculating the out-of-equilibrium properties and clarified several controversial statements that appeared in the literature.

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Appendix A: Violation of Oguri's Ward identity in certain RPT schemes

In this appendix we briefly clarify a few controversial statements that appeared in the literature on the validity and the range of applicability of Oguri's Ward identity. Particle number conservation and the conservation of spin in a magnetic field lead to relations among derivatives of the proper local selfenergy $\Sigma(\omega)$ of the Anderson Hamiltonian, Eq. (1), with respect to $E_{d\sigma}$, magnetic field B, and ω through Ward identities. These identities were first obtained by Yamada

and Yosida [16]. The extensions to finite voltages is due to Oguri [36] who showed that

$$\frac{\partial}{\partial V}\tilde{\mathbf{\Sigma}}(\omega,T,V)\Big|_{V=0} = -\gamma\left(\frac{\partial}{\partial\omega}+\frac{\partial}{\partial\tilde{\epsilon}_d}\right)\tilde{\mathbf{\Sigma}}(\omega,T,V=0), \tag{39}$$

here given in terms of renormalized quantities and where $\tilde{\mathbf{\Sigma}}$ is the selfenergy matrix on the Keldysh contour as in Eq.(21). The parameter $\gamma = (\Delta_L\alpha_L - \Delta_R\alpha_R)/(\Delta_L+\Delta_R)$. To demonstrate that the relation (39) is valid at each order of perturbation theory, we here explicitly demonstrate that the sunset diagram, shown in Fig. 3, fulfills Oguri's Ward identity. A general proof can be obtained following similar arguments [27].

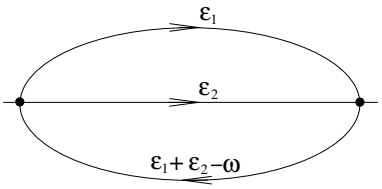

Figure 3. The sunset diagram appears in second order in the renormalized coupling constant and is part of the 'reference system' of the renormalized rSPT approach.

Specifically, the lesser component of $\tilde{\mathbf{\Sigma}}$ is considered which, on the Keldysh contour, is simply given by

$$\tilde{\Sigma}^{<}(\tau) = \tilde{U}^2\tilde{G}^{<}(\tau)\tilde{G}^{<}(\tau)\tilde{G}^{>}(-\tau) \tag{40}$$

or after Fourier transformation to frequency variables

$$\tilde{\Sigma}^{<}(\omega,T,V) \;=\; -2\pi i\tilde{U}^2\int d\epsilon_1\int d\epsilon_2\tilde{f}(\epsilon_1)\tilde{f}(\epsilon_2)\tilde{f}(\omega-\epsilon_1-\epsilon_2)\tilde{A}(\epsilon_1)\tilde{A}(\epsilon_2)\tilde{A}(\epsilon_1+\epsilon_2-\omega),$$

where

$$\tilde{A}(x) = \frac{1}{\pi}\frac{\tilde{\Delta}}{(x-\tilde{\epsilon}_d)^2+\tilde{\Delta}^2} \tag{41}$$

is the bare local renormalized spectral density which obeys the identity

$$\left(\frac{\partial}{\partial x}+\frac{\partial}{\partial\tilde{\epsilon}_d}\right)\tilde{A}(x) = 0. \tag{42}$$

Note that here, $\tilde{\epsilon}_d = zE_d$ is the renormalized, voltage and temperature independent local resonance level. The effective distribution function $\tilde{f}(\omega,V)$ is given by the expression

$$\tilde{f}(\omega,V) = \sum_{\lambda=L,R}\frac{\Delta_\lambda}{\Delta_L+\Delta_R}f_0(\omega-\alpha_\lambda V), \tag{43}$$

where the chemical potential at lead $\lambda = L,R$ is $\mu_L = \alpha_L V$, $\mu_R = -\alpha_R V$, with $\alpha_L+\alpha_R = 1$. Equation (40) implies

$$\begin{aligned}\lim_{V\to0}\tilde{f}(\omega,V) &= f_0(\omega),\\ \frac{\partial\tilde{f}(\epsilon,V)}{\partial V}\Big|_{V=0} &= \gamma\left(-\frac{\partial f_0(\epsilon)}{\partial\epsilon}\right),\end{aligned} \tag{44}$$

where f_0 is the usual Fermi function.

Consider the voltage derivative of the self-energy expression in Eq. (40), which can be written

$$\frac{\partial}{\partial V}\tilde{\Sigma}^{<}(\omega,T,V)\Big|_{V=0} = -2\pi i\tilde{U}^2\gamma\left(I_1+I_2+I_3\right), \tag{45}$$

with the help of Eq. (44) and where we have defined

$$\begin{aligned}
I_1 &= \int d\epsilon_1 \int d\epsilon_2 \tilde{A}(\epsilon_2)\tilde{A}(\epsilon_1+\epsilon_2-\omega)f_0(\epsilon_2)f_0(\omega-\epsilon_1-\epsilon_2)\left\{\tilde{A}(\epsilon_1)\left(-\frac{\partial f_0(\epsilon_1)}{\partial\epsilon_1}\right)\right\}\\
I_2 &= \int d\epsilon_1 \int d\epsilon_2 \tilde{A}(\epsilon_1)\tilde{A}(\epsilon_1+\epsilon_2-\omega)f_0(\epsilon_1)f_0(\omega-\epsilon_1-\epsilon_2)\left\{\tilde{A}(\epsilon_2)\left(-\frac{\partial f_0(\epsilon_2)}{\partial\epsilon_2}\right)\right\}\\
I_3 &= \int d\epsilon_1 \int d\epsilon_2 \tilde{A}(\epsilon_1)\tilde{A}(\epsilon_2)f_0(\epsilon_1)f_0(\epsilon_2)\left\{\tilde{A}(\epsilon_1+\epsilon_2-\omega)\left(-\frac{\partial}{\partial\epsilon_1}f_0(\omega-\epsilon_1-\epsilon_2)\right)\right\}.
\end{aligned} \tag{46}$$

We now focus on the term I_1 of Eq.(45) and apply the identity

$$\tilde{A}(\epsilon_1)\left(-\frac{\partial f_0(\epsilon_1)}{\partial\epsilon_1}\right) = -\tilde{A}(\epsilon_1)\left(\frac{\partial}{\partial\epsilon_1}+\frac{\partial}{\partial\tilde{\epsilon}_d}\right)f_0(\epsilon_1) = -\left(\frac{\partial}{\partial\epsilon_1}+\frac{\partial}{\partial\tilde{\epsilon}_d}\right)\left\{\tilde{A}(\epsilon_1)f_0(\epsilon_1)\right\}. \tag{47}$$

Thus, inserting Eq. (47) into the integral I_1 we have

$$I_1 = -\int d\epsilon_1 \int d\epsilon_2 \tilde{A}(\epsilon_2)\tilde{A}(\epsilon_1+\epsilon_2-\omega)\tilde{f}(\epsilon_2)\tilde{f}(\omega-\epsilon_1-\epsilon_2)\left(\frac{\partial}{\partial\epsilon_1}+\frac{\partial}{\partial\tilde{\epsilon}_d}\right)\left\{\tilde{A}(\epsilon_1)f_0(\epsilon_1)\right\}. \tag{48}$$

Shifting the integration variable $\epsilon_1 \to \epsilon_1+\omega$, leads to

$$\begin{aligned}
I_1 &= -\int d\epsilon_1 \int d\epsilon_2 \tilde{A}(\epsilon_2)\tilde{A}(\epsilon_1+\epsilon_2)f_0(\epsilon_2)f_0(-\epsilon_1-\epsilon_2)\left(\frac{\partial}{\partial\omega}+\frac{\partial}{\partial\tilde{\epsilon}_d}\right)\left\{\tilde{A}(\epsilon_1+\omega)f_0(\epsilon_1+\omega)\right\}\\
&= -\left(\frac{\partial}{\partial\omega}+\frac{\partial}{\partial\tilde{\epsilon}_d}\right)\int d\epsilon_1 \int d\epsilon_2 \tilde{A}(\epsilon_2)\tilde{A}(\epsilon_1+\epsilon_2)f_0(\epsilon_2)f_0(-\epsilon_1-\epsilon_2)\tilde{A}(\epsilon_1+\omega)f_0(\epsilon_1+\omega)\\
&= -\left(\frac{\partial}{\partial\omega}+\frac{\partial}{\partial\tilde{\epsilon}_d}\right)\int d\epsilon_1 \int d\epsilon_2 \tilde{A}(\epsilon_2)\tilde{A}(\epsilon_1+\epsilon_2-\omega)f_0(\epsilon_2)f_0(\omega-\epsilon_1-\epsilon_2)\tilde{A}(\epsilon_1)f_0(\epsilon_1),
\end{aligned} \tag{49}$$

where, in the last line, we have shifted back the integration variable $\epsilon_1 \to \epsilon_1-\omega$.

The same type of manipulations can be applied to integrals I_2 and I_3. Adding the three terms together, we therefore obtain

$$\frac{\partial}{\partial V}\tilde{\Sigma}^{<}(\omega,T,V)\Big|_{V=0} = -\gamma\left(\frac{\partial}{\partial\omega}+\frac{\partial}{\partial\tilde{\epsilon}_d}\right)\tilde{\Sigma}^{<}(\omega,T,V=0), \tag{50}$$

which proves the validity of Oguri's Ward identity explicitly for the second order diagram of Fig. 3. A general perturbative proof can be constructed along similar lines [36]. Nonetheless, it has been argued that the identity is only valid at $V=0$ and that the limits $\omega\to 0$ and $V\to 0$ do not commute at $T=0$ but do so at non-zero temperature [41].

While there are no convincing indications that the strong-coupling fixed point at $T=0$, $\omega=0$, $V=0$ is singular, it should be clear that an important element in the explicit proof provided above, is the fact that the renormalized resonance level $\tilde{\epsilon}_d$ is independent of voltage and temperature. If this were not the case, there would be additional terms proportional to first-order-in-voltage derivatives of the type $\partial\tilde{\epsilon}_d/\partial V|_{V=0}$. As a result, it would no longer be possible to collect all terms in such a way as to satisfy the Ward identity. This is exactly what

happens in the non-equilibrium self-consistent perturbative scheme presented in [42]. There, the bare local renormalized spectral density of Eq. (41) is taken to be

$$\tilde{A}(x) = \frac{1}{\pi} \frac{\tilde{\Delta}}{(x - \tilde{\Delta}\cot(\pi\langle n_{d\sigma}\rangle))^2 + \tilde{\Delta}^2}, \tag{51}$$

where $\langle n_{d\sigma}\rangle$ is the average local occupation number of spin projection σ and is obtained from

$$\langle n_{d\sigma}\rangle = -i \int d\omega\, \tilde{G}^{<}_{\sigma}(\omega, T, V). \tag{52}$$

Notice that $\tilde{G}^{<}$ is related to $\tilde{\Sigma}^{<}$ via the identity $\tilde{G}^{<} = \tilde{G}^{A}\tilde{\Sigma}^{<}\tilde{G}^{R}$, where the hybridization term $i\tilde{\Delta}$ is included in the self-energy components [43]. Thus, in such a perturbative scheme, the Ward identity is violated as already pointed out in reference [43]. Moreover, this violation occurs even if only the Hartree value for $\langle n_{d\sigma}\rangle$ is used in Eq.(51).

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