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Symmetry breaking and restoration using the equation-of-motion technique for nonequilibrium quantum impurity models

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Abstract

The dynamics of correlated electrons in quantum impurity models is typically described within the nonequilibrium Green function formalism combined with a suitable approximation. One common approach is based on the equation-of-motion technique often used to describe different regimes of the dynamic response. Here, we show that this approach may violate certain symmetry relations that must be fulfilled by the definition of the Green functions. These broken symmetries can lead to unphysical behaviour. To circumvent this pathological shortcoming of the equation-of-motion approach we provide a scheme to restore basic symmetry relations. Illustrations are given for the Anderson and double Anderson impurity models.

1. Introduction

Describing the transport of electrons through an interacting region is a challenging task and typically involves the calculation of the dynamics of correlated electrons driven away from equilibrium [1–3]. In general, this many-body out-of-equilibrium problem cannot be solved exactly but for a few simple cases [4–7]. Excluding recent developments based on brute-force approaches such as time-dependent numerical renormalization-group techniques [8–10], iterative [11–13] or stochastic [14–18] diagrammatic techniques to real-time path integral formulations, wave function based approaches [19], or reduced dynamic approaches [20, 21], all suitable to relatively simple model systems, most theoretical treatments of quantum transport rely on approximations of some sort. One well studied approach is based on the nonequilibrium Green function (NEGF) formalism otherwise known as the Keldysh NEGF or the Schwinger–Keldysh formalism [22, 23], which is widely used to describe transport phenomena [24–26].

Based on the NEGF, an exact expression for the stationary current through an interacting system coupled to large non-interacting metallic leads in terms of the system’s Green function can be derived [27]:

\[ I = \frac{ie}{2\pi \hbar} \int d\varepsilon (\text{Tr}[f_L(\varepsilon - \mu_L)\Gamma_L(\varepsilon)(G^r(\varepsilon) - G^a(\varepsilon))] + \text{Tr}[\Gamma_L G^< (\varepsilon)] \right) \]

or equivalently

\[ I = \frac{e}{\hbar} \int d\varepsilon \text{Tr}[\Sigma_{0,L}^<(\varepsilon)G^< (\varepsilon) - \Sigma_{0,L}^r(\varepsilon)G^> (\varepsilon)] \]

where \( G^r, G^a, G^< \) and \( G^> \) are the system’s retarded, advanced, lesser and greater Green functions (GFs), which will be defined later below. The lesser tunnelling self-energy is given by \( \Sigma_{0,L}^< = i f_L(\varepsilon - \mu_L)\Gamma_L \), where \( f_L(\varepsilon - \mu_L) \) is the Fermi–Dirac distribution in the left lead and \( \Gamma_L \) is the matrix coupling the interacting system to the left reservoir with elements \( (\Gamma_L)_{mn}^L = 2\pi \rho_L(\varepsilon) t_{km} \) (where \( t_{km} \) is the hopping matrix elements between the system and...
the left reservoir, and \( \rho_s(\epsilon) \) is the density of states in the left lead). The calculation of the system’s GF required to obtain the current (or other observables) is far from trivial, excluding simple non-interacting cases. Most applications are based on perturbative diagrammatic techniques to obtain \( G^\tau, G^a, G^c \) and \( G^\gamma \) [28]. Alternatively, one can use the equation-of-motion (EOM) approach, which allows to deduce the system’s GFs by deriving the corresponding equations of motion [29–32]. In light of its simplicity, it has been used extensively to describe transport phenomena such as the Coulomb blockade [33] and the Kondo effect [31, 34, 35], providing qualitative and in some cases quantitative results. When applied to interacting systems, the EOM for the GF gives rise to an infinite hierarchy of equations of higher order GFs. A well-known approximation procedure is to truncate this hierarchy, thus introducing a mean-field like description to some observables. These equations for the GFs then need to be solved self-consistently for the resulting closed set of equations. Although successful, the EOM technique has its drawbacks [36, 50].

In this paper we show that while a closure can always be obtained, it is not clear a priori whether it fulfills symmetry relations that single particle GFs must obey. This failure can lead to solutions which are not physical, such as complex occupation of levels [50] and even finite currents at zero bias. We also propose an approach to fix this deficiency by imposing a set of rules to reconstruct GFs that fulfill basic symmetry relations. Illustrations are given for the Anderson model [37] at the Kondo regime and for the double Anderson model [38]. Our paper is organized as follows: in section 2 we describe the EOM approach and the single site and double site Anderson models. In section 3 we discuss symmetry relation for GFs and illustrate symmetry breaking for the aforementioned models with specific closures suitable to describe the Kondo effect. In section 4 we provide a recipe to restore the basic symmetry relations within the EOM approach and discuss implications for level occupancy and coherences, current, and sum rules for the Anderson model in the Kondo regime and the double Anderson model. Finally, in section 5 we conclude.

2. EOM technique and models

2.1. Equations of motion

The fundamental object of nonequilibrium many-body theory, is the contour ordered Green function [22, 23, 39],

\[
G(r_2, t_2, r_1, t_1) = \frac{-i}{\hbar} \langle T_C \hat{\Psi}_{H}(r_2, t_2) \hat{\Psi}_{H}^\dagger(r_1, t_1) \rangle, \tag{3}
\]

where the time variables (\( t_1 \) and \( t_2 \)) are along the Schwinger–Keldysh contour as depicted in figure 1, \( T_C \) is the contour time ordering operator which moves operators with earlier time arguments to the right, \( \hat{\Psi}_{H}/\hat{\Psi}_{H}^\dagger \) are the system’s annihilation/creation field operators in the Heisenberg picture (in what follows we omit the \( H \) index), and the average \( \langle \cdots \rangle \) should be interpreted as the trace over the many particle Hilbert space with the equilibrium \( (t = -\infty) \) density matrix.

**Figure 1.** The Schwinger–Keldysh contour \( C \) consists of two oriented branches, \( C = C_+ \cup C_- \). The forward branch \( C_+ \) extending from \( t = -\infty \) to \( t \) and the backward branch \( C_- \) extending from \( t = \infty \) to \( -\infty \). By definition, any time on the backward branch (e.g. \( t_2 \)) comes after a time on the forward branch (\( t_1 \)). The thin line represents the real-time axis with the time variable \( \tau \).

The EOM for the contour ordered GF is obtained from the Heisenberg EOM for a Heisenberg operator \( \frac{\partial}{\partial t} \hat{A}(t) = \frac{i}{\hbar} [\hat{H}(t), \hat{A}(t)] + \frac{g}{\hbar^2} \hat{V}(t) \), where in our case \( \hat{H}(t) = \hat{H}_0 + \hat{V}(t) \). Here \( \hat{H}_0 \) stands for the one-body non-interacting part of \( \hat{H}(t) \), \( \hat{V}(t) = \hat{H}(t) - \hat{H}_0 \), and \([\hat{A}, \hat{B}]\) is the commutator. Let us consider a generic example. The EOM [40] for \( G(r_2, t_2, r_1, t_1) \) can be written as (omitting the \( r \) dependence for brevity)

\[
G(t_2, t_1) = g_2(t_2, t_1)(\langle \hat{\Psi}, \hat{\Psi}^\dagger \rangle) - \frac{i}{\hbar} \int_{t_{C}}^t d\tau g_2(t_2, \tau) \times \langle T_C [\hat{\Psi}(\tau), \hat{\Psi}(\tau)] \rangle, \tag{4}
\]

where \((ih \frac{\partial}{\partial \tau} - \epsilon) \hat{g}_2(t_2, t_1) = \delta(t_1 - t_2), [\hat{A}, \hat{B}] \) is the anti-commutator, and \( \epsilon \) is defined from the equation, \( \hat{g}_2(\tau, \tau) = \hat{g}_1(\tau, \tau) = [\hat{\Psi}(\tau), \hat{H}_0] \). For example, if \( \hat{H}_0 = \sum_{n}(\varepsilon_{n} - \mu)\hat{d}_{n}^{\dagger}\hat{d}_{n} \) and \( \hat{g}_i = \hat{d}_{i} \) then \( \epsilon = \varepsilon_i - \mu \). Following Langreth theorem [41], we can change the contour integration in equation (4) to integration along the real-time axis. This yields (see section 3 for the definitions of the different real-time GFs)

\[
G^\tau(t_2, t_1) = g_2^\tau(t_2, t_1)(\langle \hat{\Psi}, \hat{\Psi}^\dagger \rangle) + \int_{t_1}^{t_2} dt g_2^\tau(t_2, t_1)\hat{G}^\tau(t, t_1), \tag{5}
\]

\[
G^c(t_2, t_1) = g_2^c(t_2, t_1)(\langle \hat{\Psi}, \hat{\Psi}^\dagger \rangle) + \int_{t_0}^{t_2} dt g_2^c(t_2, t_1)\hat{G}^c(t, t_1) + \int_{t_0}^{t_1} dt g_2^c(t_2, t_1)\hat{G}^c(t, t_1), \tag{6}
\]

where the time variables (\( t_1 \) and \( t_2 \)) are along the real-time axis, \( G^\tau(t_2, t_1) \) is the retarded GF usually used to calculate the response of the system at time \( t_2 \) to an earlier perturbation of the system at time \( t_1 \). \( G^c(t_2, t_1) \) is the lesser GF which plays the role of the single particle density matrix, and \( \hat{G}(t_2, t_1) = -\frac{i}{\hbar} \langle T_C [\hat{\Psi}(t_2), \hat{\Psi}(t_1)] \rangle \) is a new GF generated by the EOM procedure. Depending on the Hamiltonian it can be a single particle GF or a many particle GF and can involve lead operators as well as system operators. In steady state, the GFs depend only on the difference in time, \( t = t_2 - t_1 \), which is simpler to express in Fourier space

\[
G^\tau(\omega) = g_2^\tau(\omega)(\langle \hat{\Psi}, \hat{\Psi}^\dagger \rangle) + \hat{g}_2^\tau(\omega)\hat{G}^\tau(\omega), \tag{7}
\]

\[
G^c(\omega) = g_2^c(\omega)(\langle \hat{\Psi}, \hat{\Psi}^\dagger \rangle) + \hat{g}_2^c(\omega)\hat{G}^c(\omega) + \hat{g}_2^c(\omega)\hat{G}^\tau(\omega). \tag{8}
\]
To simplify the notation we denote the Fourier transform of $G(t_2 - t_1) = G(t)$ as $G(\omega)$, i.e., functions with an argument ‘$\omega$’ are Fourier transforms of their time-domain counterparts. At this stage one has to evaluate $G(t_2, t_1)$ (\textit{G}(t) in steady state). Except for very simple cases, where an exact closure can be obtained, writing the EOM for $G(t_2, t_1)$ will produce new and/or ‘higher order’ GFs that need to be evaluated. This leads (in principle) to an infinite set of equations. The idea of the EOM method is therefore, to truncate this hierarchy of equations making a mean-field like approximation for the ‘higher order’ GFs through lower order functions. This is the Achilles heel of this method as there is no systematic way to fulfill. We will use two impurity models to demonstrate at what level of approximation the symmetry relations are violated and propose a scheme to restore symmetrization.

2.2. The impurity models

To illustrate the shortcomings of the EOM approach, we refer to the Anderson model [34, 37, 44] and the double Anderson model [38] to represent two different degrees of complexity to the Anderson model [34, 37, 44] and the double Anderson model.

Achilles heel of this method as there is no systematic way to 'higher order' GFs through lower order functions. This is the parameter $i_{lm}^m$ represents the coupling strength between the system and the contacts, and the index $m$ runs over the site index $\{\alpha, \beta\}$ in the double Anderson model.

3. Symmetry breaking in impurity models

3.1. Definitions and symmetry relations

In the Keldysh formalism the two time NEGF is defined on a contour (figure 1) [22]. In accordance with where on the contour the two times are placed one can define four real-time GFs [49]: the time ordered $G'$, anti-time ordered $G''$, lesser $G^<$, and greater $G^>$ GF:

$$G_{\alpha\beta}(t_2, t_1) = \begin{cases} \frac{i}{\hbar} \langle T \Psi_{\alpha}(t_2) \Psi_{\beta}(t_1) \rangle, & \text{for } t_2 > t_1, \\ \frac{i}{\hbar} \langle \Psi_{\beta}(t_1) \Psi_{\alpha}(t_2) \rangle, & \text{for } t_2 < t_1 \end{cases}$$

The first two terms on the RHS are similar to the Anderson impurity model Hamiltonian (extended to 2 sites), $V_{\sigma\sigma'}$ is the repulsion energy between two electrons on different sites (inter-site repulsion), and $i_{m}^m$ is the coupling strength for electron hopping between the two sites. The interaction between the system and the contacts is simply given by the tunnelling Hamiltonian [48]

$$\hat{H}_{\text{int}} = \sum_{m, \sigma, \bar{\kappa} \in \{L,R\}} i_{lm}^{m} c_{\bar{\kappa} \sigma}^\dagger d_{m\sigma} + \text{h.c.} \quad (13)$$

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The parameter $i_{lm}^m$ represents the coupling strength between the system and the contacts, and the index $m$ runs over the site index $\{\alpha, \beta\}$ in the double Anderson model.
following relations must hold:
\[ G_{\sigma\sigma}(t_2, t_1) = (G_{\sigma\sigma}^a(t_1, t_2))^*, \]
\[ G_{\sigma\sigma}^{<,>}(t_2, t_1) = -(G_{\sigma\sigma}^{<,>}(t_1, t_2))^*. \] (17)

In steady state these relations can be rewritten in Fourier space as:
\[ G_{\sigma\sigma}^{<,>}(\omega) = -(G_{\sigma\sigma}^{\alpha,\beta}(\omega))^*, \]
\[ G_{\sigma\sigma}^{\alpha,\beta}(\omega) = G_{\sigma\sigma}^{<,>}(\omega) - G_{\sigma\sigma}^{\alpha,\beta}(\omega). \] (18)

In what follows we show that the relations in equation (18) do not always hold when the GFs are obtained by the EOM technique with an arbitrary closure, thus leading to unphysical behaviour [50].

3.2. The Anderson model

Following the derivation in [28, 34, 48] we define the following contour ordered GF:
\[ G_{\sigma\sigma}(t, t') = -i \langle T \delta_d(\sigma)d^\dagger(\sigma)d(\sigma)d^\dagger(\sigma) \rangle, \]
\[ G_{2}(t, t') = -i \langle T \delta_{\bar{n}}(\sigma)d(\sigma)d^\dagger(\sigma) \rangle, \] (19) (20)

where \( \bar{\sigma} \) is the opposite spin of \( \sigma \). Various approximate decoupling procedures can be applied to the many particle GF [51]. Here we follow the approximation scheme used in [28, 34] where all electronic correlations containing at most one lead operator, are not decoupled and their EOM are calculated. Higher order GFs involving (opposite) spin correlations in the leads are set to zero, and the remaining higher order GFs involving lead and system degrees of freedom are decoupled such that
\[ F_{2}(t, t') = -\frac{i}{\hbar} \langle T \delta_{\bar{n}}(\sigma)d(\sigma)d^\dagger(\sigma) \rangle - \delta_{\bar{k}g} \langle \epsilon_{\bar{k}} - \mu_{L,R} \rangle G_{\sigma\sigma}(t, t'). \]

In what follows, we show that the symmetry relation for the lesser GF, \( G_{\sigma\sigma}^{<,>}(\omega) = -(G_{\sigma\sigma}^{\alpha,\beta}(\omega))^* \), is not satisfied. In turn, this implies that \( \langle n_{\sigma} \rangle = -\frac{i}{\hbar} \int_{-\infty}^{\infty} G_{\sigma\sigma}(\omega) d\omega \) (the occupation number) is a complex number, which of course is not physical. Following the same derivation given below one can show that the greater GF is not an imaginary function either. All other symmetry requirements are fulfilled for the Anderson impurity model.

Within the approximation scheme of [34], the lesser GF is given by:
\[ G_{\sigma\sigma}^{<,>}(\omega) = g^{<,>}(\omega) - g^{<,>}(\omega)UP^{a}(\omega)g^{\alpha}(\sigma) \Sigma^{\alpha}(\omega)g^{\alpha}(\omega) \times UP^{a}(\omega)g^{\alpha}(\sigma) \Sigma^{\alpha}(\omega)g^{\alpha}(\omega) - g^{<,>}(\omega)UP^{a}(\omega)g^{\alpha}(\sigma) \Sigma^{\alpha}(\omega)g^{\alpha}(\omega) \times UP^{a}(\omega)g^{\alpha}(\sigma) \Sigma^{\alpha}(\omega)g^{\alpha}(\omega), \] (21)

The self-energies are given by:
\[ \Sigma^{<,>}_{\sigma}(\omega) = \sum_{k \in \{L,R\}} |t_{\sigma k}|^2(\hbar \omega - \epsilon_{\sigma k} \pm i0^+)^{-1}, \]
\[ \Sigma^{\alpha,\beta}_{\sigma}(\omega) = \sum_{k \in \{L,R\}} A_{k}^{(j)} |t_{\sigma k}|^2(\hbar \omega + \epsilon_{\sigma k} - \epsilon_{\sigma} - i\epsilon)^{-1}, \]
\[ - U \pm i0^+)^{-1} + (\hbar \omega - \epsilon_{\sigma k} - \epsilon_{\sigma} \pm i0^+)^{-1}, \]
\[ j = 1, 3 \]
\[ \Sigma^{<,>}_{\sigma}(\omega) = \Sigma^{<,>}_{\sigma}(\omega) + \Sigma^{\alpha,\beta}_{\sigma}(\omega). \] (22) (23) (24) (25) (26)

Here \( \Sigma^{<,>}_{\sigma}(\omega) \) is the exact self-energy for the non-interacting case, while \( \Sigma^{\alpha,\beta}_{\sigma}(\omega) \) are the self-energies due to the tunnelling of the \( \bar{\sigma} \) electron, with \( A_{k}^{(1)} = f_{\bar{\sigma}}(\epsilon_{\sigma k} - \mu_{k}) \) and \( A_{k}^{(3)} = 1 \).

The lesser self-energies are defined as [35]:
\[ \Sigma^{<,>}_{\sigma}(\omega) = \Sigma^{<,>}_{\sigma}(\omega) = i(\epsilon_{\sigma} - \mu_{L,R}) \]
\[ + f_{\bar{\sigma}}(\epsilon - \mu_{L,R}) \Gamma_{\sigma}(\omega), \] (27) (28) (29)

where \( \Gamma_{\sigma}(\omega) = -2i\text{Im}(\Sigma^{<,>}_{\sigma}(\omega)), j = 0, 1, 3, \) and \( K = L, R, \) applying the principle of reducio ad absurdum, we assume \( G_{\sigma\sigma}^{<,>}(\omega) \) to be imaginary. Since it must hold for any real value of \( \langle n_{\sigma} \rangle \) between 0 and 1, we argue that the terms multiplying \( U\langle n_{\sigma} \rangle \) in equation (21) must be imaginary. That is (omitting \( \omega \) for brevity)
\[ A_{1} = g^{<,>}P^{\alpha}g_{\sigma}^{\alpha} + g^{<,>}P^{\alpha}g_{\sigma}^{\alpha} - U(g^{<,>}P^{\alpha}g_{\sigma}^{\alpha}g^{\alpha}(\omega) + g^{<,>}P^{\alpha}g_{\sigma}^{\alpha}g^{\alpha}(\omega) + g^{<,>}P^{\alpha}g_{\sigma}^{\alpha}g^{\alpha}(\omega) + g^{<,>}P^{\alpha}g_{\sigma}^{\alpha}g^{\alpha}(\omega) + g^{<,>}P^{\alpha}g_{\sigma}^{\alpha}g^{\alpha}(\omega) + g^{<,>}P^{\alpha}g_{\sigma}^{\alpha}g^{\alpha}(\omega), \] (30)

must be imaginary. Moreover, Since \( A_{1} \) must be imaginary for any value of \( \bar{U} \), the terms not multiplying it, should be imaginary as well, i.e.,
\[ A_{2} = g^{<,>}P^{\alpha}g_{\sigma}^{\alpha} + g^{<,>}P^{\alpha}g_{\sigma}^{\alpha}, \] (31)

should be imaginary. Up to here we only used the fact that \( \langle n_{\sigma} \rangle \) is a real quantity and we assumed \( U \) to be real as well.
By definition $g_1^2$ and $g_2^2$ are imaginary, thus, for $A_2$ to be imaginary, the following identity must hold:

$$\text{Im}(g'P')g_2^2 + \text{Im}(P'g_2^2)g_1^2 = 0.$$  \hfill (33)

In other words we demand $\text{Re}(A_2) = 0$. Substituting equations (24) and (25) into (33), we get:

$$\text{Im}(g'P')g_2^2 \Sigma_2^\alpha g_2^\alpha = -\text{Im}(P'g_2^2)g_1^2 g_1^\alpha.$$  \hfill (34)

Thus, if the equality in equation (34) is true, our assumption that $G_{2,\alpha}^\infty$ is imaginary is correct. Using the definitions for $g_1^\alpha$ and $g_2^\alpha$, the last equality can be rewritten as:

$$\text{Im}(g'P') \frac{-i\omega}{(\omega - \varepsilon_4 - U)^2 + \text{Im}(\Sigma'_4)}^2 = \text{Im}(P'g_2^2) \frac{i\omega}{(\omega - \varepsilon_4)^2 + \text{Im}(\Sigma_4')}^2,$$  \hfill (35)

where $\varepsilon_4 = \varepsilon_4 + \text{Re}(\Sigma'_4)$ and $\varepsilon_4 = \varepsilon_4 + \text{Re}(\Sigma_4')$. Starting with the LHS of equation (35), we look at $g'P'$:

$$g'P' = \frac{(\omega - \varepsilon_4 - U - i\text{Im}(\Sigma'_4))(\omega - \varepsilon_4 - i\text{Im}(\Sigma_4'))}{(\omega - \varepsilon_4)^2 + \text{Im}(\Sigma_4')} \times \frac{\text{Re}(\Sigma'_4) + U\text{Re}(\Sigma_4')}{\text{Im}(\Sigma_4')^{-1}} + i\text{Im}(\Sigma'_4)^{-1}.$$  \hfill (36)

To simplify the notation we denote: $a_0 = \omega_0 - \varepsilon_0$, $a_1 = \text{Re}(\Sigma'_4)$, $a_4 = \omega_4 - \varepsilon_4 - U$ and $b_j = \text{Im}(\Sigma'_4)$ with $j = 0, 1, 4$. Rewriting the equation for $g'P'$:

$$g'P' = \frac{a_4 - ib_4}{a_0a_4 - b_0b_4 + Ua_1 - (a_0b_4 + a_4b_0 - Ub_1).}$$  \hfill (37)

Denote $D = a_0a_4 - b_0b_4 + Ua_1$ and $E = a_0b_4 + a_4b_0 - Ub_1$, so we can rewrite equation (37) as:

$$g'P' = \frac{a_4D + b_4E - i(b_4D - a_4E)}{D^2 + E^2}.$$  \hfill (38)

Finally:

$$\text{Im}(g'P') = -\frac{b_4D - a_4E}{D^2 + E^2},$$  \hfill (39)

and the LHS of equation (35) is given by:

$$\text{LHS} = \frac{i\omega b_4}{(a_0)^2 + (b_0)^2} \frac{b_4D - a_4E}{D^2 + E^2}.$$  \hfill (40)

Now we turn to analyse the RHS of equation (35). We start by evaluating $P'g_2^2$. Using the same notation as we did for $g'P'$, we get:

$$P'g_2^2 = \frac{g_2^2}{1 + g_2^2 \Sigma_2^\alpha g_2^\alpha U} = \frac{a_0D + b_0E + i(b_0D - a_0E)}{D^2 + E^2}.$$  \hfill (41)

Here we used $\text{Im}(\Sigma') = -\text{Im}(\Sigma^\alpha)$. Finally:

$$\text{Im}(P'g_2^2) = \frac{b_0D - a_0E}{D^2 + E^2}. \hfill (42)$$

The RHS of equation (35) is given by:

$$\text{RHS} = \frac{b_0D - a_0E}{D^2 + E^2} \frac{i\omega b_0}{(a_0)^2 + (b_0)^2}.$$  \hfill (43)

The equality (equation (35)) now reads:

$$\frac{b_4}{(a_0)^2 + (b_0)^2} \frac{b_4D - a_4E}{D^2 + E^2} = \frac{b_0D - a_0E}{D^2 + E^2} \frac{b_0}{(a_0)^2 + (b_0)^2},$$  \hfill (44)

or

$$\frac{b_4^2D - a_4b_4E}{(a_0)^2 + (b_0)^2} = \frac{b_0^2D - a_0b_0E}{(a_0)^2 + (b_0)^2}.$$  \hfill (45)

Substituting $D = a_0a_4 - b_0b_4 + Ua_1$ and $E = a_0b_4 + a_4b_0 - Ub_1$ one can easily show that the equality does not hold. Thus, our assumption is wrong and $G_{2,\alpha}^\infty$ is not an imaginary function as it should be by definition.

If one is only interested in the Coulomb blockade regime, it is not necessary to go to the level of approximation presented here (which is essential to obtain the Kondo effect). For the Coulomb blockade regime one can turn to the approximation presented in [33], where on top of the approximations described above we also neglect the simultaneous hopping of electron pairs to and from the system. This approximation does not violate the symmetry relations of the single particle GF (see appendix A for further discussion), but as pointed above, it does not reproduce the Kondo peaks at low temperatures.

3.3. The double Anderson model

For the double Anderson model we follow the derivation given in [52], and define the following contour ordered GF:

$$G_{ab}^\sigma (\tau, \tau') = -\frac{i}{\hbar} \langle T_{\sigma} d_{a\sigma} (\tau) d_{b\sigma}^\dagger (\tau') \rangle,$$  \hfill (46)

$$G_{ab\gamma}^\sigma (\tau, \tau') = -\frac{i}{\hbar} \langle T_{\gamma} d_{a\gamma} (\tau) d_{b\gamma}^\dagger (\tau') \rangle,$$  \hfill (47)

where $\sigma = s, \bar{s}$. The approximations used in [52] are: (a) neglect the simultaneous hopping of electron pairs to and from the system, (b) assume that $F_2(\tau, \tau') = -\frac{1}{\hbar} \langle T_{\sigma} C_{\bar{k}\sigma} (\tau) N_{\gamma} (\tau) d_{a\sigma}^\dagger (\tau') \rangle \approx -\frac{1}{\hbar} \sum_{\gamma = 0, \bar{0}} \langle T_{\gamma} C_{\bar{k}\gamma} (\tau) N_{\gamma} (\tau) \rangle d_{a\gamma}^\dagger (\tau')$, where $n(\tau)$ is the number operator of one of the electrons of the system, and $(i\hbar \frac{\partial}{\partial \omega_0} - \varepsilon_{\alpha\beta} )g_\alpha (\tau, \tau_1) = \delta (\tau - \tau_1)$, and (c) higher order GFs of the form $-\frac{1}{\hbar} \langle T_{\gamma} C_{\bar{k}\gamma} (\tau) N_{\gamma} (\tau) \rangle d_{a\gamma}^\dagger (\tau')$ are decoupled to $-\frac{1}{\hbar} \langle n_{\gamma} (\tau) \rangle \langle T_{\gamma} C_{\bar{k}\gamma} (\tau) \rangle d_{a\gamma}^\dagger (\tau') - \frac{1}{\hbar} \langle T_{\gamma} C_{\bar{k}\gamma} (\tau) \rangle d_{a\gamma} (\tau) d_{b\gamma} (\tau') \rangle$. These approximations lead to the following equations for the retarded and advanced GF (omitting $(\omega)$ for brevity):

$$G_{ab\gamma}^\sigma (\tau, \tau') = (\omega_0 - \varepsilon_{ab\gamma} - \Sigma_{0\gamma}^\sigma)^{-1} \times \delta_{\gamma\bar{\gamma}} + h_{\gamma\bar{\gamma}}^{\sigma} G_{ab\gamma}^\sigma (\tau, \tau'),$$  \hfill (48)

$$G_{ab\gamma}^\sigma (\tau, \tau') = (\omega_0 - \varepsilon_{ab\gamma} - \Sigma_{0\gamma}^\sigma)^{-1} \times \delta_{\gamma\bar{\gamma}} + h_{\gamma\bar{\gamma}}^{\sigma} G_{ab\gamma}^\sigma (\tau, \tau'),$$  \hfill (49)

The equations for the various $G_{ab\gamma}^\sigma (\omega)$, $\alpha$, are provided in appendix B. Given the expressions for the retarded and advanced GF (equations (48) and (49)), one can show (see
appendix B for a full proof) that \((G_{\alpha\beta}^{>\ell}(\omega))^\dagger \neq (G_{\beta\alpha}^{<\ell}(\omega))^\dagger\). Moreover, we find that none of the symmetry relations in equation (18) hold. In the following section we propose a symmetrization scheme that restores all the symmetries of the single particle GF.

4. Symmetry restoration

4.1. Guidelines to restore symmetry

The customary route to calculate the NEGF is as follows: (a) calculate the retarded GF and use it to obtain the advanced GF (by demanding \(G_{\alpha\beta}^{\ell}(\omega) = (G_{\beta\alpha}^{\ell}(\omega))^\dagger\)), (b) Calculate the lesser/greater GF and symmetrize the lesser/greater to fulfil the quantum Onsager relations [53], hence obeying \(G_{\alpha\beta}^{<\ell}(\omega) = -(G_{\beta\alpha}^{<\ell}(\omega))^\dagger\). In most applications of NEGF the advanced GF is not directly calculated and thus, the symmetry breakage does not always stand out. In fact, this common procedure restores the relation between the advanced and retarded GF and between the lesser/greater and their complex conjugate, but does not necessarily restore the relation \(G_{\alpha\beta}^{\ell}(\omega) - G_{\beta\alpha}^{\ell}(\omega) = G_{\alpha\beta}^{<\ell}(\omega) - G_{\beta\alpha}^{<\ell}(\omega)\). It can be shown that violation of the latter leads to violation of the fluctuation dissipation relation, \(G^> = -\beta\varepsilon_0(\varepsilon - \mu_0)(G^> - G^0)\), at equilibrium. This oversimplified procedure can result in different values for the currents depending on how it is calculated, cf equation (1) or (2). It may also lead to finite currents at zero-bias voltage (see section 4.3 for more), which is physically incorrect.

In order to restore the symmetry relations that are imposed by the definitions of the GF (equation (18)), we suggest the following procedure:

(i) Calculate the retarded/advanced GF matrices \((G'/G^0)\) separately and use them to define ‘new’ retarded/advanced GF matrices \(\tilde{G}' = 0.5(\tilde{G}' + (\tilde{G}'^\dagger)^\dagger)\) and \(\tilde{G}^0 = 0.5(\tilde{G}^0 + (\tilde{G}^0)^\dagger)\).

(ii) Use the ‘new’ retarded/advanced GF matrices \((\tilde{G}' / \tilde{G}^0)\) to calculate the lesser/greater GF matrices \((\tilde{G}^< / \tilde{G}^>)\).

Again, use them to define ‘new’ lesser/greater GF matrices \(\tilde{G}^< = 0.5(\tilde{G}^< + (\tilde{G}^<)^\dagger)\).

(iii) Calculate the two anti-Hermitian matrices \(A = \tilde{G}^- - \tilde{G}^<\) and \(B = \tilde{G}^r - \tilde{G}^>\). Define the difference anti-Hermitian matrix \(C = A - B\), and redefine the retarded and advanced GFs \(\tilde{G}' = \tilde{G}' + C/2\), and \(\tilde{G}^0 = \tilde{G}^0 - C/2\).

The resulting GFs (\(\tilde{G}'\), \(\tilde{G}^a\), \(\tilde{G}^<\), and \(\tilde{G}^>\)) obey all the symmetry relations of equation (18) by construction. Note that if the original GFs obeyed the symmetry relations to begin with, our symmetrization procedure will not alter them in any way.

We now turn to perform detailed calculations for both the Anderson and double Anderson models. For the Anderson model, we use the closure described in section 3.2 while for the double Anderson model we use the closure described in section 3.3. The resulting EOMs were solved self-consistently in Fourier space with a frequency discretization of \(N_{\omega} = 2^{14} - 2^{16}\) depending on the model parameters. Typically, <15 self-consistent iterations were needed to converge the results.

Convergence was declared when the population values at subsequent iteration steps did not change within a predefined tolerance value chosen as \(10^{-6}\). For each set of calculations we have applied the above symmetrization scheme and compared the results to those obtained without restoring symmetry, as detailed for each model.

4.2. Anderson impurity model

First, we address the effects of symmetry breakage in the Anderson model. The closure used is sufficient to describe the appearance of the Kondo resonances at low temperatures, as seen in the upper panel of figure 2, where we plot the density of states as a function of energy for several temperatures, all calculated with symmetry restoration. The development
of Kondo peaks in the density of states as the temperature decreases is clearly evident, signifying a regime of strong correlations which is qualitatively captured by the simple EOM approach when symmetry is restored.

In the lower panel of figure 2 we show one of the main flaws of the EOM approach for the Anderson impurity model, where we plot the value of $\langle n_\uparrow \rangle$ as a function of the source–drain bias voltage with and without symmetry restoration. The most notable effect is the appearance of an imaginary portion to $\langle n_\uparrow \rangle$ as the source–drain bias voltage is increased. To obtain the results, without symmetry restoration, only the real part of $\langle n_\uparrow \rangle$ was used to converge the self-consistent equations for the GFs. By applying the symmetrization scheme proposed in section 4.1 to the lesser GF calculated in section 3.2, we restore the relation $\rho_{\alpha\beta}^{\sigma\sigma^*} (\omega) = -(\rho_{\beta\alpha}^{\sigma\sigma^*} (\omega))^*$. This is sufficient to obtain a real value for $\langle n_\uparrow \rangle$, as clearly shown in the lower panel of figure 2. All other symmetry relation are not violated here and thus, our symmetrization procedure does not affect them at all. Interestingly, taking only the real part of $\langle n_\uparrow \rangle$ provides identical results when compared to the results obtained after the full symmetrization procedure. However, this is only true for the simple case of the single site impurity model and does not hold for more complex systems.

4.3. The double Anderson model

We now turn to discuss the impact of symmetry breaking for the double Anderson model. This system is more involved compared to the single site Anderson model and thus, the level of closure used is somewhat simpler, as explained in section 3.3. While for the case of a single site Anderson model only the relation $\rho_{\alpha\beta}^{\sigma\sigma^*} (\omega) = -(\rho_{\beta\alpha}^{\sigma\sigma^*} (\omega))^*$ breaks down, in the double Anderson model we find that all 3 symmetries described by equation (18) are violated. This can be traced to the more complex form of the Hamiltonian for the double Anderson model, where each site is only coupled to one of the leads and transport in enabled by the direct hopping term between the two sites.

Similar to the case of the Anderson model, as a result of symmetry breaking the occupation of the levels $\langle n_{\sigma\alpha} \rangle$ is a complex number. In addition, the relation $\rho_{\alpha\beta}^{\sigma\sigma} = -\frac{i\hbar}{2\pi} \int_{-\infty}^{\infty} \langle G_{\alpha\beta}^{\sigma\sigma} (\omega) \rangle^* d\omega$, should also fulfill certain symmetry relations, such as $\rho_{\alpha\beta}^{\sigma\sigma} = (\rho_{\beta\alpha}^{\sigma\sigma})^*$. In figure 3 we plot the real and imaginary parts of $\rho_{\alpha\beta}^{\sigma\sigma}$ and $\rho_{\beta\alpha}^{\sigma\sigma}$ for the case where the symmetry procedure has been applied (left panels) and for the bare case (right panels). The upper panels show the imaginary part of $\rho_{\alpha\beta}^{\sigma\sigma}$ and $\rho_{\beta\alpha}^{\sigma\sigma}$, which should show a mirror reflection about the zero axis (shown as thin solid line). This is, indeed, the case when symmetry is restored, however, it is destroyed when symmetry breaks down, in particular as the source–drain bias increases. A more dramatic effect is shown for the real part of $\rho_{\alpha\beta}^{\sigma\sigma}$ and $\rho_{\beta\alpha}^{\sigma\sigma}$ (lower panels). The two curves representing $\text{Re} (\rho_{\alpha\beta}^{\sigma\sigma})$ and $\text{Re} (\rho_{\beta\alpha}^{\sigma\sigma})$ should be identical (left panel when symmetry is restored) but are quite distinct when symmetry is not obeyed (right panel).

In figure 4 we plot the current as a function of the source–drain bias voltage for the double Anderson model.
coincide. However, when approximations are introduced or when the hierarchy is truncated, the calculation of the current based on the two different formulae will coincide only if the symmetry relation \(G_{\alpha\beta}^{rf}(\omega) - (G_{\alpha\beta}^{rf}(\omega))^{*} = (G_{\alpha\beta}^{rf}(\omega))^{*} - (G_{\alpha\beta}^{rf}(\omega))^{*}\) is preserved. Indeed, in the case of a single site Anderson model, even if symmetry is not restored, this relation holds and the two calculations yield identical values for the current. However, in the present case, all 3 symmetry relations are broken and thus, equations (1) and (2) give different results for the current, as clearly evident in figure 4. More significantly is the fact that equation (1) produces a finite value for the current even when the bias is zero, indicating the break down of the fluctuation dissipation relation. When symmetry is restored (solid curve) the two calculations are identical, as they should be, and the violation of the fluctuation dissipation relation is also resolved.

The symmetrization scheme proposed here is not a ‘magic cure’ and, in fact, does not resolve all issues of matter. It is well known that the lesser and greater GFs should obey a simple sum rule where the integral over the difference of their diagonal elements should always sum to 1:

\[
S_{\sigma\sigma} = \frac{-i\hbar}{2\pi} \int d\epsilon ((G_{\alpha\alpha}^{\sigma\sigma}(\epsilon))^{*} - (G_{\alpha\alpha}^{\sigma\sigma}(\epsilon))^{*}) = 1. \quad (50)
\]

In figure 5 we plot the sum rule as given by equation (50) for the double Anderson model where symmetry has been restored. A similar plot for the single site Anderson model yields a value of 1 regardless of whether symmetry has been restored or not within the closure discussed above. However, in the case of the more evolved double Anderson model, even when symmetry is restored and the GFs obey all 3 relations described in equation (18), the sum rule is violated. Nonetheless, the sum \(\sum_{\sigma\sigma} S_{\sigma\sigma} = N_e\), where \(N_e\) is the total number of electrons in the system at maximal occupancy, is indeed preserved when symmetrization is restored.

5. Summary

In this paper we have addressed the problem of symmetry breaking and restoring in the EOM approach to NEGF formalism. This formalism is based on deriving a hierarchy of equations of motion for the system’s Green functions and truncating this hierarchy at a desired (or tractable) order. Despite the uncontrolled approximation introduced by an arbitrary truncation, the closed set of equations is often used to describe the complex dynamics of correlated systems, including the Coulomb blockade and Kondo effect.

One shortcoming of the EOM approach, which has been the focus of the present study, is the fact that, a priori, for most situations it is impossible to determine whether the solution of the closed set of equations satisfies symmetry relation between the retarded, advanced, lesser and greater Green functions imposed by definition. For example, we have shown that for the Anderson model the relation \(G_{\alpha\beta}^{\sigma\sigma}(\omega) = -(G_{\beta\alpha}^{\sigma\sigma}(\omega))^{*}\) breaks down for a closure that is often used to describe the dynamics near the Kondo regime. We have also demonstrated that for the double Anderson model all 3 symmetry relations given by equation (18) break down for a lower level of closure. This faulty of the EOM approach leads to unphysical behaviour such as complex level occupations and finite current at zero source–drain bias (depending on how the current is evaluated).

We have also proposed a procedure to circumvent this deficiency by imposing symmetrization to the Green functions in such a way that all 3 symmetry relations are restored. The strength of the proposed approach is that it does not alter the GFs if symmetry is not broken. While this procedure eliminates some problems of physical importance and leads to real level occupations and vanishing current at zero source–drain bias (irrespective of how the current is evaluated), certain sum rules are still violated, indicating other problems with the EOM approach. Nonetheless, the symmetrized version of the EOM technique still describes the appearance of the Kondo peak and, as will be shown in future publication provides a quantitative description of the resonant transport for the double Anderson model even in the strong inter-dot coupling limit.

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Appendix A

In what follows, we show that under the simpler closure (as used for example, in [33]), \(G_{\alpha\alpha}^{\sigma\sigma}(\omega) = -(G_{\sigma\alpha}^{\sigma\sigma}(\omega))^{*}\)
By definition $g^\omega(\omega)$ is imaginary. Since $G^\text{RHS}$, hence $G^\omega(\omega)$ to be imaginary one requires that (omitting $\omega$ for brevity):

$$G^\omega(\omega) = g^\omega U(n_\sigma)g^\omega + g^\omega U(n_\sigma)g^\omega,$$

is imaginary. Since $g^\omega(\omega)$ is an imaginary quantity as well, for $G^\omega(\omega)$ to be imaginary, the real part of $A_1$ needs to cancel, i.e.,

$$\text{Im}(g^\omega)g^\omega = \text{Im}(g^\omega)g^\omega.$$

Define

$$\epsilon_0 = \epsilon_\sigma + \text{Re}(\Sigma_0^\text{R}),$$

$$\Gamma = -\text{Im}(\Sigma)^0 = \text{Im}(\Sigma)^0,$$

and use it to rewrite the equation (A.7) as:

$$\Gamma \Sigma^\omega = -\frac{\Gamma \Sigma^\omega}{(\omega - \epsilon_0)^2 + \Gamma^2}.$$

Obviously the real part of $A_1$ cancels (the LHS equals the RHS), hence $G^\omega(\omega)$ is imaginary and fulfills the symmetry $G^\omega(\omega) = -(G^\omega(\omega))^\ast$.

Appendix B

Now we refer to section 3.3. In what follows we show that $(G^\omega_{\text{RHS}}(\omega))^\ast \neq (G^\omega(\omega))^\ast$. We start by presenting the retarded and advanced GFs in Fourier space (omitting $\omega$ for brevity):

$$(G^\omega_{\text{RHS}})^\ast = (\hbar \omega - \epsilon_0 - \Sigma_0^\text{R})^{-1} \times (\delta_{\alpha \beta} + h^\omega_{\alpha \beta}(G^\omega_{\text{RHS}})^\ast) + U(\Sigma^\omega_{\text{RHS}})^\ast + V(\Sigma^\omega_{\text{RHS}})^\ast + V(\Sigma^\omega_{\text{RHS}})^\ast.$$  

(11)

$$(G^\omega_{\text{RHS}})^\ast = (\hbar \omega - \epsilon_0 - \Sigma_0^\text{R})^{-1} \times (\delta_{\alpha \beta} + h^\omega_{\alpha \beta}(G^\omega_{\text{RHS}})^\ast) + U(\Sigma^\omega_{\text{RHS}})^\ast + V(\Sigma^\omega_{\text{RHS}})^\ast + V(\Sigma^\omega_{\text{RHS}})^\ast.$$  

(12)

For clarity we examine the simpler case where $V_\nu^\tau = 0$. Define the following GFs:

$$(g_{\nu}^\tau)^\ast = \frac{1}{\hbar \omega - \epsilon_0 - \Sigma_0^\text{R}},$$  

(13)

$$(g^\omega_{\text{RHS}})^\ast = \frac{1}{\hbar \omega - \epsilon_0 - U(\Sigma_0^\text{R})},$$  

(14)

$$(g^\omega_{\text{RHS}})^\ast = \frac{1}{\hbar \omega - \epsilon_0 - U(\Sigma_0^\text{R}) - \Sigma_0^\text{R}}.$$  

(15)

where $\Sigma_0$ is defined in equation (27). With these definitions we rewrite the equations for the retarded and advanced GFs:

$$(G^\omega_{\text{RHS}})^\ast = (\hbar \omega)^\ast G^\omega_{\text{RHS}}(G^\omega_{\text{RHS}})^\ast + (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast.$$  

(16)

$$(G^\omega_{\text{RHS}})^\ast = (\hbar \omega)^\ast + (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast.$$  

(17)

$$(G^\omega_{\text{RHS}})^\ast = (\hbar \omega)^\ast G^\omega_{\text{RHS}}(G^\omega_{\text{RHS}})^\ast,$$  

(18)

$$(G^\omega_{\text{RHS}})^\ast = (\hbar \omega)^\ast G^\omega_{\text{RHS}}(G^\omega_{\text{RHS}})^\ast.$$  

(19)

$$(G^\omega_{\text{RHS}})^\ast = (\hbar \omega)^\ast G^\omega_{\text{RHS}}(G^\omega_{\text{RHS}})^\ast.$$  

(20)

$$(G^\omega_{\text{RHS}})^\ast = (\hbar \omega)^\ast G^\omega_{\text{RHS}}(G^\omega_{\text{RHS}})^\ast.$$  

(21)

$$(G^\omega_{\text{RHS}})^\ast = (\hbar \omega)^\ast + (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast.$$  

(22)

$$(G^\omega_{\text{RHS}})^\ast = (\hbar \omega)^\ast + (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast.$$  

(23)

$$(G^\omega_{\text{RHS}})^\ast = (\hbar \omega)^\ast + (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast.$$  

(24)

$$(G^\omega_{\text{RHS}})^\ast = (\hbar \omega)^\ast + (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast.$$  

(25)

$$(G^\omega_{\text{RHS}})^\ast = (\hbar \omega)^\ast + (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast.$$  

(26)

$$(G^\omega_{\text{RHS}})^\ast = (\hbar \omega)^\ast + (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast.$$  

(27)

Simple substitutions now yield the following set of equations:

$$(G^\omega_{\text{RHS}})^\ast = (1 - (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast - (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast) - 1 \times (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast.$$  

(28)

$$(G^\omega_{\text{RHS}})^\ast = (1 - (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast - (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast) - 1 \times (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast.$$  

(29)

$$(G^\omega_{\text{RHS}})^\ast = (1 - (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast - (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast) - 1 \times (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast.$$  

(30)

and

$$(G^\omega_{\text{RHS}})^\ast = (1 - (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast - (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast) - 1 \times (\hbar \omega)^\ast U(\Sigma^\omega_{\text{RHS}})^\ast.$$  

(31)
should be equal. One can easily check that $X_1 \neq X_2$, thus $(G_{\alpha \beta}^\sigma(\omega))'$ is not equal to $(G_{\alpha \beta}^\sigma(\omega))^*$. The same can be done to show that $G_{\alpha \beta}^{\sigma \sigma}(\omega)^{<,>}$ is not equal to $-((G_{\alpha \beta}^\sigma(\omega))^*)^\dagger$ and $G_{\alpha \beta}^{\sigma \sigma'}(\omega)^{<,>}$ is not equal to $G_{\alpha \beta}^{\sigma \sigma'}(\omega)^{<,>}$.

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