Quantum transport through a quantum dot: Combining the scattering-states numerical renormalization group with nonequilibrium Green functions

To cite this article: Frithjof B Anders and Sebastian Schmitt 2010 J. Phys.: Conf. Ser. 220 012021

View the article online for updates and enhancements.
Quantum transport through a quantum dot: combining the scattering-states numerical renormalization group with nonequilibrium Green functions

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Abstract.
Scattering states fulfill the correct boundary conditions of a current carrying open quantum system. Discretizing the energy continuum of these states allows for employing Wilson’s numerical renormalization group approach without violating the boundary conditions by using a finite size system. We evolve the analytically known steady-state density operator for a non-interacting quantum-system at finite bias to the full interacting problem by the time-dependent numerical renormalization group after switching on the local charging energy. Using a newly developed algorithm for steady-state nonequilibrium Green functions, we can calculate the current $I$ as function of bias voltage $V$ for arbitrary temperature and magnetic field. A comparison with second-order and GW Kadanoff-Baym-Keldysh results shows excellent agreement for weak interaction strength $U$.

1. Introduction
Quantum dots have been considered as possible building blocks for nano-electronics and for quantum information [1, 2]. Their physical properties are dominated by many-body effects at temperatures below the charging energy due to the quantization of the charge. Furthermore, such devices are fully controllable by external gate electrodes. Therefore, their investigation is of fundamental importance for our understanding of open quantum systems out of equilibrium.

The quantization of the electric charge dominates the electrical response of such quantum dots at low temperature leading to Coulomb blockade physics: for voltages smaller than the charging energy $U = E_c = e^2/2C$, where $C$ is the classical capacitance, transport can only occur via tunneling of single-electrons coining the name single-electron transistor (SET) for such devices – see the review by Kastner [1]. This blockade of charge transport is lifted in certain parameter regimes due to the Kondo effect [3]. Even when real charge fluctuations are suppressed, the remaining spin degree of freedom in the Coulomb blockade valley can fluctuate due to virtual spin-flip transitions at odd fillings of a quantum dot mediating charge transfer between the leads. As a consequence, a pinned many-body resonance at the chemical potential opens a new transport channel below a characteristic temperature $T_K$ which is exponentially dependent on the charging energy.
By now the properties of such nano-devices are well understood at zero bias in the crossover regime from high to low temperatures using non-perturbative approaches such as Wilson’s numerical renormalization group (NRG) [4]. In contrast to equilibrium conditions, the understanding of the real-time evolution and the steady-state nonequilibrium of many-particle quantum systems is still at its infancy. Over the past 40 years, the Keldysh technique [5] has proven to be the most successful approach to nonequilibrium dynamics as it furnishes a perturbative expansion for correlation functions. It is applicable to problems having a well defined ground state in equilibrium such as in semi-conductor quantum optics [6] where the band gaps act as a cutoff for any divergence in perturbation theory.

Quantum impurity models are used in the theory of quantum transport on the molecular level. Since most quantum impurity models exhibit infrared divergencies in the perturbation theory – for instance a local spin coupled anti-ferromagnetically to the spin of a metallic host [7] – the Keldysh diagrammatic approaches are only applicable in certain parameter regimes usually at high temperature, large bias or weak interactions. In these regimes, the infrared divergencies are cut off by temperature or voltage, both causing decoherence and a finite memory time. This is true, in particular, for the single impurity Anderson model [7]: the minimal model to describe Coulomb blockade physics and its lifting via a many-body resonance. Simple equation of motion techniques also fail for these type of problems [7] since they are not able to capture the correct infrared physics which develops through correlations in all orders.

Summing cumulants used in Hubbard decoupling schemes [8, 9, 10] to infinite order yields conserving approximations such as the Non-Crossing-Approximation (NCA). The NCA [11, 12, 13] and their extensions [14] based on skeleton expansion become unreliable at low temperatures and large magnetic fields [15] since the logarithmically divergence terms are only partially included. However, the combination of NCA and Keldysh techniques pioneered by Meir and Wingreen [16] has been a standard approach for calculating quantum transport in strongly correlated systems with ballistic leads in the 90ths [17]: for large values of $U$ it is better suitable than recent GW approaches [18] since it contains (i) exactly the atomic/molecular limit with arbitrary Coulomb repulsions and (ii) also predicts the correct low-energy scale [19].

For a certain topology of the couplings, the current is fully determined by the nonequilibrium (NEQ) spectral functions of the impurity [20, 21, 16]. For large voltage $V$ ($V/T_K \gg 1$) scaling functions in $V/T_K$ have been derived for the Kondo model [22, 23]. Such generalizations of the NCA or the “poor-man’s scaling” [7] to nonequilibrium can be backed in certain limits with field theoretical techniques [24]. In the Toulouse limit [25] the Kondo model has been solved exactly for finite bias [26] as well as in an AC field [27]. Using bosonisation and refermionisation, this model is mapped exactly onto a resonant level model. The Keldysh NCA solution for pulsed bias [28] agrees well with the exact solution at the Toulouse point [29].

Recently, a large number of different methods have been developed to tackle this difficult problem for arbitrary regimes. Using scattering states, perturbative methods [30], Quantum Monte Carlo methods [31] and the Bethe Ansatz approach [32] were extended to finite bias along the line of Hershfield’s expression of a steady-state density operator [33]. Schmitteckert applied the time-dependent density matrix renormalization group (DMRG) [34] to different interacting 1D wires [35] which agrees well with a field theoretical solution [36]. Iterative propagation of the density matrix [37] along the Keldysh contour allows the calculation of the current in the weakly correlate regime governed by short memory times. Wegner’s flow equation approach [38, 39] as well as the real-time renormalization group approach [40, 41] has been extended to a spin coupled anti-ferromagnetically to two leads.

In this paper, we report on the application of a scattering-states approach to quantum-transport though a single-electron transistor [1]. Oguri has pointed out [42] that discretizing the Lippmann-Schwinger states of a noninteracting quantum dot can serve as a single-particle basis which is current carrying. The scattering-state NRG (SNRG) approach consists of the following
steps to calculate the current through a SET for arbitrary temperature, bias, magnetic field and interaction strength $U$:

(i) construct the single-particle scattering states of the noninteracting Hamiltonian which contain the correct boundary conditions of the current-carrying open quantum system,

(ii) use the analytically known steady-state density operator [33] of a noninteracting quantum-dot for an initial NRG run at finite bias at a given temperature and coupling to the leads,

(iii) employ the time-dependent numerical renormalization group [43, 44] to propagate the steady-state density operator to the analytically unknown density operator at finite bias and charging energy, i.e. $\hat{\rho}_0(V,U=0,t=0) \rightarrow \hat{\rho}(V,U,t \rightarrow \infty)$,

(iv) use $\hat{\rho}(V,U)$ to calculate the steady-state nonequilibrium spectral functions [45] which enters the Meir-Wingreen formula [20, 21, 16] for the current.

The paper is organized as follows. In Sec. 2 we introduce the model and discuss briefly the two approaches used: the scattering-states numerical renormalization group in Sec. 2.2 and the Keldysh Green function technique in Sec. 2.7. The comparison between the SNRG and the Keldysh Green functions for small values of $U$ are discussed in Sec. 3.1. The IV characteristics of a quantum dot in the Kondo regime is presented in Sec. 3.2. While the zero-bias conductance remains independent of $U$ for a symmetric junction for $T \rightarrow 0$, the IV curves are strongly $U$ dependent for finite bias.

2. Theory

Quantum impurity models (QIM) are used to describe quantum transport on the molecular level. Their Hamiltonian $\mathcal{H}$

$$\mathcal{H} = \mathcal{H}_{\text{imp}} + \mathcal{H}_{\text{bath}} + \mathcal{H}_I$$

consists of three parts: an impurity part $\mathcal{H}_{\text{imp}}$ modelling the interacting device with a finite number of degrees of freedom, one or more Bosonic or Fermionic baths assigned to $\mathcal{H}_{\text{bath}}$ and the coupling of these subsystems by $\mathcal{H}_I$. Examples of such quantum impurities are a simple two-level system, a localized spin, a superconducting qubit, a molecule or a quantum dot. The leads provide two such fermionic baths at different chemical potentials, while dephasing of isolated spins or qubits is usually driven by bosonic fluctuations such as fluctuating electromagnetic fields or molecular vibrations [46].

2.1. Model

In this work, we restrict ourselves to a junction with a single spinful orbital coupled to a left (L) and a right (R) lead

$$\mathcal{H} = \sum_{\sigma=\pm1} \int d\epsilon (\epsilon - \mu_\sigma) c_{\epsilon,\sigma}^\dagger c_{\epsilon,\sigma} + \sum_{\sigma=\pm1} \left[ E_d + \frac{U}{2} - \frac{\sigma}{2} H \right] \hat{n}_{\sigma}^d + \frac{U}{2} \left( \sum_{\sigma} \hat{n}_{\sigma}^d - 1 \right)^2 + \sum_{\alpha\sigma} V_{\alpha\sigma} \int d\epsilon \sqrt{\rho_\alpha(\epsilon)} \left( d_{\sigma}^\dagger c_{\epsilon,\sigma} + c_{\epsilon,\sigma}^\dagger d_{\sigma} \right).$$

Here $\hat{n}_{\sigma}^d = d_{\sigma}^\dagger d_{\sigma}$ measures the orbital occupancy, $H$ denotes the external magnetic field and $U$ the local charging energy if the quantum dot level is doubly occupied. The Hartree term has been partially absorbed into the single-particle energy $E_d \rightarrow E_d + U/2$. The different chemical potentials $\mu_\alpha$ in both leads appear as a shift of the band centers and are functions of the external voltage $V = \mu_R - \mu_L$. For simplicity, we assume that both leads have the same density of states $\rho(\epsilon)$ characterized by the same band width $D$ but different band centers. This Hamiltonian is commonly used to model a single Coulomb-blockade resonance in ultra-small quantum dots [3, 16].
2.2. Definition of the scattering states

In the absence of the local Coulomb repulsion $H_U$

$$H_U = \frac{U}{2} \left( \sum_\sigma \hat{n}_\sigma^d - 1 \right)^2,$$  \hspace{1cm} (3)

the Hamiltonian (2) is diagonalized exactly [30, 33, 47, 31, 42, 48, 49] in the continuum limit by scattering states. These scattering-states are created by the operator $\gamma^\dagger_{\sigma\alpha}$

$$\gamma^\dagger_{\sigma\alpha} = \hat{c}^\dagger_{\sigma\alpha} + V_\alpha \sqrt{\rho_\alpha(\epsilon)} G^r_{0\sigma}(\epsilon) \left[ d^R_\alpha + \sum_{\alpha'} \int d\epsilon' \frac{V_{\alpha'}^r \rho_{\alpha'}(\epsilon')}{\epsilon - \epsilon'} \right].$$  \hspace{1cm} (4)

The local retarded resonant level Green function

$$G^r_{0\sigma}(\omega) = \left[ \omega + i\delta - (E_d + \frac{U}{2} - \sigma \frac{H}{2}) - \sum_\alpha V^r_\alpha \int d\epsilon \frac{\rho_\alpha(\epsilon)}{\omega + i\delta - \epsilon} \right]^{-1}$$  \hspace{1cm} (5)

enters as expansion coefficient. Defining $\tilde{V} = \sqrt{V^2_L + V^2_R}$, we will use $r_{R(L)} = V_{R(L)}/\tilde{V}$ and

$$\Delta(\omega) = \tilde{V}^2 \sum_\alpha r^2_\alpha \int d\epsilon \frac{\rho_\alpha(\epsilon)}{\omega + i\delta - \epsilon} = \Re[\Delta(\omega)] - i\Gamma(\omega)$$  \hspace{1cm} (6)

in the rest of the paper, where $\Gamma(0) = \Gamma = \sum_\alpha \pi V^2_\alpha \rho(0)$.

For infinitely large leads, these scattering states diagonalize the Hamiltonian (2) for $U = 0$:

$$\mathcal{H}_0 = \mathcal{H}(U = 0) = \sum_{\alpha=L,R;\sigma} \int d\epsilon \epsilon \gamma^\dagger_{\epsilon\sigma\alpha} \gamma_{\epsilon\sigma\alpha}.$$  \hspace{1cm} (7)

Note that these scattering states are complex and current carrying. This is embedded in the complex expansion coefficients $G^r_{0\sigma}(\epsilon)$ reflecting the continuum limit. Time-reversal symmetry manifests itself in the symmetric spectrum for left and right movers. To avoid any contribution from bound states, we will implicitly assume a wide band limit: $D \gg \max\{|E_d|, \Gamma, |V|, |H|\}$, where $\Gamma_\alpha = \pi V^2_\alpha \rho(0)$ and $\Gamma = \Gamma_L + \Gamma_R$.

Hershfield has shown that the density operator for such a noninteracting current-carrying quantum system retains its Boltzmannian form [33]

$$\hat{\rho}_0 = \frac{e^{-\beta(\mathcal{H}_0 - \hat{Y}_0)}}{\text{Tr}[e^{-\beta(\mathcal{H}_0 - \hat{Y}_0)}]}, \quad \hat{Y}_0 = \sum_{\alpha\sigma} \mu_\alpha \int d\epsilon \gamma^\dagger_{\epsilon\sigma\alpha} \gamma_{\epsilon\sigma\alpha}$$  \hspace{1cm} (8)

even for finite bias. The $\hat{Y}_0$ operator accounts for the occupation of the left- and right-moving scattering states, and $\mu_\alpha$ for the different chemical potentials of the leads. Therefore, all steady-state expectation values of operators can be calculated using $\hat{\rho}_0$ which includes the finite bias. In the absence of a Coulomb repulsion $U$, the problem is well understood. The current expectation value [42] calculated with this density-operator $\hat{\rho}_0$ reproduces the standard result [20, 21, 16] for noninteracting devices. The knowledge of the analytical form of $\hat{\rho}_0$, however, makes this steady-state model accessible to a NRG approach [4, 49].

The expansion coefficients in the definition of $\gamma^\dagger_{\epsilon\sigma\alpha}$ in Eq. (4) contain the complex single-particle Green function $G^r_{0\sigma}(\epsilon)$ which we separate in modulus and phase

$$G^r_{0\sigma}(\epsilon) = |G^r_{0\sigma}(\epsilon)| e^{-i\Phi_\sigma(\epsilon)}.$$  \hspace{1cm} (9)
This phase $\Phi_\sigma(\epsilon)$ is absorbed into the new scattering states $\gamma^\dagger_{\sigma\alpha} \rightarrow \tilde{\gamma}^\dagger_{\sigma\alpha} = \gamma^\dagger_{\sigma\alpha} e^{i\Phi_\sigma(\epsilon)}$ by a gauge transformation. The impurity operator $d^\dagger_{\sigma}$ is expanded into left and right mover contributions

$$d^\dagger_{\sigma} = r_R d^\dagger_{\sigma R} + r_L d^\dagger_{\sigma L}$$

using the inversion of Eq. (4). These two new operators are defined as

$$d^\dagger_{\sigma\alpha} = \bar{V} \int d\epsilon \sqrt{\rho(\epsilon)} |G^\sigma_{0\sigma}(\epsilon)| \tilde{\gamma}^\dagger_{\sigma\alpha} ,$$

and obey the anti-commutator relation \( \{d_{\sigma\alpha}, d^\dagger_{\sigma'\alpha'}\} = \delta_{\sigma\sigma'}\delta_{\alpha\alpha'} \).

2.3. Discretization of the scattering states

The scattering-states numerical renormalization group (SNRG) approach \[49\] starts from a logarithmic discretization of the scattering-states continuum $\tilde{\gamma}_{\sigma\alpha}$ controlled by the parameter $[50, 4] \Lambda > 1$. The discretized version of the noninteracting Hamiltonian (7) is mapped \[50, 4\] onto a semi-infinite Wilson chain Hamiltonian $H_0(\Lambda)$

$$H_0(\Lambda) = \lim_{m \rightarrow \infty} H^0_m$$

$$H^0_m = \sum_{\sigma\alpha} \sum_{n=0}^{m} w_{n\sigma\alpha} f^\dagger_{n\sigma\alpha} f_{n\sigma\alpha} + \sum_{\sigma\alpha} \sum_{n=0}^{m-1} (t_{n\sigma\alpha} f^\dagger_{n\sigma\alpha} f_{n+1\sigma\alpha} + t^*_{n\sigma\alpha} f^\dagger_{n+1\sigma\alpha} f_{n\sigma\alpha}) (12)$$

whose tight-binding matrix elements $t_{n\sigma\alpha}$ decay exponentially $t_{n\sigma\alpha} \propto \Lambda^{-n/2}$. We use $d_{\sigma\alpha}$ defined in Eq. (11) as starting vector $f^\dagger_{0\sigma\alpha} = d_{\sigma\alpha}$ for the Householder transformation \[4\] and obtain the tight-binding coefficients \[4\] of the Wilson chain (12). It is straightforward to show that the energy of the first link corresponds to the energy of the original quantum-dot orbital: $w_{0\sigma\alpha} = E_d + U/2 - \sigma H/2$.

In contrast to the standard NRG \[50, 4\], the impurity degree of freedom has been included into $H_0(\Lambda)$ since not the leads but the full scattering states have been discretized. Any complex phase of the tight-binding parameters $t_n$ can be absorbed into the creation (annihilation) operators $f^\dagger_{n\sigma\alpha}(f_{n\sigma\alpha})$ of an electron on the chain link $n$ with spin $\sigma$ and $\alpha (=\text{left/right})$ mover by a local gauge transformation.

The NRG solves $H_0(\Lambda)$ by iteratively diagonalizing the series of Hamiltonians $H^0_m$. Hereby, the discarding of the high-energy states at the end of each iteration circumvents the exponentially increasing dimension of the many-body Fock space: the Fock space of the next Hamiltonian $H_{m+1}$ is spanned only by the lowest $N_s$ eigenstates of $H_m$ plus the degrees of freedom of the additional chain link $m+1$. The difference $\Delta H_m = H_{m+1} - H_m$ combined with rescaling of the energy scale provides the renormalization group equation of the problem \[4\] which is the core of the NRG iteration procedure.

In the SNRG, however, the current operator acquires energy dependent phases $\Phi_\sigma(\epsilon)$ from the gauge transformation when expanded in the scattering states. Since it remains an open question how to set up a Wilson chain for which the current operator is local, we calculate \[21, 33, 42\] the IV curve using the bias-dependent spectrum of the retarded Green function $\rho_\sigma(\omega, V) = -3m|G^\sigma_{0\sigma}(\omega, V)|/\pi$

$$I(V) = \frac{G_0}{e} \sum_{\sigma} \int_{-\infty}^{\infty} d\omega \left[ f(\omega - \mu_L) - f(\omega - \mu_R) \right] \pi \Gamma \rho_\sigma(\omega, V)$$

where $f(\omega)$ denotes the Fermi function, and $G_0 = (e^2/h)4\Gamma_L\Gamma_R/\Gamma^2$. This expression remains valid even for finite $U$ \[20, 21, 16\].
2.4. Local Coulomb interaction

In order to include the local Coulomb interaction, the number operator $\hat{n}_\sigma^d = d^\dagger_\sigma d_\sigma$ must be expanded in the new orbitals $d^\dagger_\sigma \sigma$. It consists of two contributions: a density term and a backscattering term $\hat{n}_\sigma^d = \hat{n}_\sigma^0 + \hat{O}_\sigma^{\text{back}}$, where

$$\hat{n}_\sigma^0 = \sum_\alpha r_\alpha^2 d^\dagger_\sigma \sigma d_\sigma \sigma$$  \hspace{1cm} (14)

and the backscattering term is defined as

$$\hat{O}_\sigma^{\text{back}} = r_{LR} \left( d^\dagger_{\sigma R} d_{\sigma L} + d^\dagger_{\sigma L} d_{\sigma R} \right).$$  \hspace{1cm} (15)

The local Coulomb interaction term

$$U \hat{n}_\uparrow^d \hat{n}_\downarrow^d = U \left( \hat{n}_\uparrow^0 \hat{n}_\downarrow^0 + \sum_\sigma \hat{O}_\sigma^{\text{back}} \hat{n}_\sigma^0 + \hat{O}_\uparrow^{\text{back}} \hat{O}_\downarrow^{\text{back}} \right)$$  \hspace{1cm} (16)

leads to a mixing of left and right movers, since $\hat{O}_\sigma^{\text{back}}$ does not commute with $Y_0$. However, the term $H_0^U$,

$$H_0^U = \frac{U}{2} \left( \sum_\sigma \hat{n}_\sigma^0 - 1 \right)^2,$$  \hspace{1cm} (17)

commutes with $\hat{Y}_0$ and can be absorbed into the steady-state density operator $\hat{\rho}_0 \rightarrow \hat{\rho}_0 = \exp[-\beta (H_0 - \hat{Y}_0)]/Z$ with $H_0 = H_0^i + H_0^U$ using the arguments given in Ref. [24].

2.5. Time-dependent numerical renormalization group (TD-NRG) approach

Starting from an equilibrated system for times $t \leq 0$, the initial Hamiltonian $H_i$ is changed to $H_f$ by a sudden quench at $t = 0$. Then, the density matrix $\hat{\rho}(t)$ evolves as

$$\hat{\rho}(t) = e^{-iH_f t} \hat{\rho}_0 e^{iH_f t}$$  \hspace{1cm} (18)

starting from its initial value $\hat{\rho}_0$ at $t = 0$. If $H_{i}(t)$ describes a quantum impurity problem and $\hat{O}$ is an impurity operator, it was recently shown that the real-time dynamics of the expectation value of $O(t) = \langle \hat{O}(t) \rangle$ can be assessed [43, 44] by evaluating

$$O(t) = \sum_m \sum_{r,s} \rho_{r,s}^{\text{red}}(m) O_{s,r} e^{-i(E_m - E_s)t}$$  \hspace{1cm} (19)

where $O_{s,r}(m)$ denotes the matrix elements of the operator $\hat{O}$ at NRG iteration $m$, $E_m^r$ the NRG eigenenergy of state $|r\rangle$ and $\rho_{r,s}^{\text{red}}$ is the reduced density matrix

$$\rho_{r,s}^{\text{red}}(m) = \sum_e \langle r, e; m | \hat{\rho}_0 | s, e; m \rangle.$$  \hspace{1cm} (20)

The derivation of Eq. (19) requires a complete basis set of the Wilson chain. It was shown that the set of all discarded states of the NRG truncation procedure [43, 44] provides such a
complete basis set. The full Fock-space of the Wilson-chain of length \( N \) is spanned by this complete basis set \( \{ | l, e; m \rangle \} \)

\[
\hat{I} = \sum_{m} \sum_{l,e} | l, e; m \rangle \langle l, e; m | \quad (21)
\]

where \( l \) labels a discarded state at iteration \( m \), and \( e \) denotes the set of quantum numbers characterizing the chain links from \( m + 1 \) to \( N \). At each iteration \( m \), we can also partition the Fock-space into two parts

\[
\hat{I} = \sum_{m} \sum_{l,e} | l, e; m \rangle \langle l, e; m | = T_m^- + T_m^+
\]

where \( r \) accounts for all states which are present at iteration \( m \). The derivation of Eq. (19) makes heavy use of the different possibilities of partitioning of the complete Fock-space of the Wilson chain.

When applying the time-dependent NRG, we have to iteratively diagonalize not only the initial Hamiltonian \( K_i = H_i - Y_0 \) but also the final Hamiltonian \( H_f \) (here \( H_f = H_i + U \hat{n}_d^\dagger \hat{n}_d \)) using their corresponding Wilson chains (12) and the RG equation described above. The approximate eigenstates of the non-interacting \( H_i(N) \) obtained from the initial NRG run are used for a faithful representation of the steady-state density operator \( \hat{\rho}_0 \) at the inverse temperature \( 1/T = \beta_N \propto \Lambda^{N/2} \) and the finite bias \( V \). The iteratively obtained eigenstates of \( H_f(m) \) and their overlap matrix elements with the eigenstates of \( H_i(m) \) allows to construct a matrix representation of \( \hat{\rho}(t) \).

In contrast to the standard RG procedure which eliminates high energy degrees of freedom, the TD-NRG sums up the contributions from all discarded states via Eq. (19): the usage of a complete basis set ensures that the initial condition \( O(t \to 0^+) = \text{Tr} \left[ \hat{\rho}_0 \hat{O} \right] \) is always fulfilled up to machine precision of \( 10^{-15} \) accuracy.

2.6. Steady-state Green function

In Sec. 2.2 we have argued that the analytic form of the steady-state nonequilibrium density operator is only known explicitly \[33\] for \( U = 0 \). This allows for applying the NRG approach to construct a faithful representation of \( \hat{\rho}_0(V, U = 0) \). Since switching on the local Coulomb interaction is a \( 1/N \) effect in the coupled system of the two leads and quantum dot, we can assume that for infinitely large leads (i) a steady-state is reached after some characteristic but finite time which is (ii) unique and independent of the initial condition. Then, the time averaging of the density operator

\[
\hat{\rho}_\infty = \lim_{T \to \infty} \frac{1}{T} \int_0^T dt \hat{\rho}(t)
\]

projects out the steady-state contributions to the density operator \( \hat{\rho}(t) = \exp(-iH_ft) \hat{\rho}_0 \exp(iH_ft) \) even in a finite size system: only the energy diagonal terms contribute in accordance with the condition \( [H_f, \hat{\rho}_\infty] = 0 \). Even though \( \hat{\rho}_\infty \) remains unknown analytically, we can construct it systematically using the TD-NRG described above.

The steady-state retarded Green function (GF) is defined as

\[
G_{A,B}^{\rho}(t) = -i \text{Tr} \left[ \hat{\rho}_\infty [\hat{A}(t), \hat{B}]_s \right] \Theta(t),
\]

(24)
where \( [\hat{A}(t), \hat{B}]_s \) denotes the commutator for Bosonic, and the anti-commutator for Fermion correlation functions. The GF can be calculated \[45\] using the TD-NRG \[43, 44\] and extending ideas developed for equilibrium Green functions \[51\] which utilized the partitioning properties \[22\] of the complete basis set. In contrast to the equilibrium, however, two reduced-density matrices, \( \rho^{red}_{r,s}(m) \) and \( \tilde{\rho}^{red}_{r,s}(m) \) must be introduced \[45\]. One of the contributions to the (anti-)commutator can be written as

\[
\text{Tr} \left[ \rho_\infty (t) B \right] = \sum_{m=m_{\text{min}}}^{N} \sum_{r,s} \sum_{k} \delta_{E_m,E_{m'}} A_{r,k}^m e^{i(E_m - E_{m'})t} B_{k,s}^m \rho^{red}_{r,s}(m) + \sum_{m=m_{\text{min}}}^{N-1} \sum_{r,s} \sum_{k_1,k_2} A_{k_1}^m e^{i(E_{k_1} - E_m)t} B_{k_2}^m \tilde{\rho}^{red}_{k_2,k_1}(m),
\]

where the recursion relation for the second reduced density matrix \( \tilde{\rho}^{red}_{k_2,k_1}(m) \) reads

\[
\tilde{\rho}^{red}_{k_2,k_1}(m) = \sum_{r,s} \sum_{\alpha_{m+1}} \langle k_2, \alpha_{m+1}; m | s; m + 1 \rangle \rho^{red}_{r,s}(m + 1) \delta_{E_{m+1},E_{m+1}} \langle r; m + 1 | k_1, \alpha_{m+1}; m \rangle + \sum_{k',\alpha_{m+1}} \langle k_2, \alpha_{m+1}; m | k'; m + 1 \rangle \tilde{\rho}^{red}_{k',k}(m + 1) \langle k'; m + 1 | k_1, \alpha_{m+1}; m \rangle
\]

which is very similar to the recursion relation obeyed by reduced density matrix \( \rho^{red}_{r,s}(m) \). The matrix elements of the type \( \langle k'; m + 1 | k_1, \alpha_{m+1}; m \rangle \) are generated in the standard NRG algorithm. The Kronecker \( \delta_{E,E'} \) projects out the energy diagonal parts of the reduced density matrix since only those contribute to \( \rho_\infty \).

Details of its derivation are found in Ref. \[45\]. It was shown that the algorithm is identical to the equilibrium algorithm \[51\] if \( \mathcal{H}_i = \mathcal{H}_f \). Combining the Laplace transformation of both contributions \[25\] of the anti-commutator to \( G^r_{A,B}(z) \) yields the steady-state spectral function for the retarded GF which is used to calculate the current via Eq. \[13\].

2.7. The Kadanoff-Baym-Keldysh approach

In order to gauge the quality of the results for the SNRG for small values of \( U \) where perturbative approaches are applicable, we employ the nonequilibrium perturbation theory as formulated by Kadanoff, Baym \[52\] and Keldysh \[5\] on the usual Keldysh time contour, for example, see Refs. \[53, 54, 55\]. Since we are only interested in the steady-state properties, the information and correlations of the initial conditions are assumed to be lost. This is achieved by sending the initial time \( t_0 \to -\infty \) and dropping all correlation functions which involve the initial state. It is assumed, that the system reaches a steady state which is translational invariant in time. Therefore the single-particle Green function only depends on the difference between the two formerly independent times of particle creation and annihilation. The Fourier transform of the time difference leads to the formulation in frequency space for all Green functions of the steady state.

In the nonequilibrium steady-state formulation, two independent components of the contour ordered Green functions survive which are chosen to be the retarded and lesser Green functions, \( G^r(\omega) \) and \( G^<\omega) \) respectively. The advanced and greater functions are related via

\[
G^a(\omega) = G^r(\omega)^\dagger \\
G^>(\omega) = G^<\omega + G^r(\omega) - G^a(\omega)
\]

The solution of the retarded Green function at finite bias enters Eq. \[13\] to obtain the steady-state current.
The two relevant Green functions can be expressed as [56, 57]

\[
G^r_\sigma(\omega) = \frac{1}{\omega + i\delta - E_d - \Sigma^R_H - \Delta(\omega) - \Sigma^r_\sigma(\omega)}
\]

\[
G^\omega_\sigma(\omega) = G^r_\sigma(\omega) [2i f_L(\omega) \Gamma_L(\omega) + 2i f_R(\omega) \Gamma_R(\omega) + \Sigma^\omega_\sigma(\omega)] G^a_\sigma(\omega)
\]

where, again, \(\Delta(\omega) = \Delta_R(\omega) + \Delta_L(\omega)\) are the hybridization functions of the leads, \(\Gamma_\alpha(\omega)\) their imaginary parts (see Eq. (6)) and \(f_\alpha(\omega) = 1/\{\exp[\beta(\omega - \mu_\alpha)] + 1\}\) are the Fermi functions of the corresponding leads. The retarded and lesser self-energies, \(\Sigma^r_\sigma\) and \(\Sigma^\omega_\sigma\) respectively, include all correlation effects induced by the Coulomb interaction \(U\). \(\Sigma^H_\sigma\) accounts for the frequency independent Hartree energy shift.

We focus on three different approximations for the self-energy: (A) The direct expansion up to second order in \(U\), where noninteracting \(U = 0\) propagators are used as internal lines, labeled as \(2^{nd}U\), (B) full self-consistent evaluation of the second order skeleton diagram, and (C) the GW approximation (GWA). In the GW approximation (GWA) the bare Coulomb interaction \(U\) is screened by an infinite series of particle-hole excitations. The approximation (B) is called second Born approximation (2BA). In contrast to the usual 2BA no exchange contribution exists for our model with only one spinful orbital. Since the 2BA and the GWA are both evaluated self-consistently, the self-energies can be derived from a Luttinger-Ward functional [58] and are conserving approximations [59].

The analytic expressions for the self-energies read

\[
\Sigma^H_\sigma = U \int \frac{d\omega}{2\pi i} G^\omega_\sigma(\omega)
\]

\[
\Sigma^r_\sigma(\omega) = i \int \frac{dx}{2\pi} G^\omega_\sigma(x) W^r_\sigma(\omega - x) + i \int \frac{dx}{2\pi} G^r_\sigma(x) W^\omega_\sigma(\omega - x)
\]

\[
\Sigma^\omega_\sigma(\omega) = i \int \frac{dx}{2\pi} G^\omega_\sigma(x) W^\omega_\sigma(\omega - x)
\]

where the effective interactions are given by

\[
W^r_\sigma(\omega) = U^2 P^r_\sigma(\omega)
\]

\[
W^\omega_\sigma(\omega) = \frac{U^2 P^r_\sigma(\omega)}{1 - U^2 P^r_\sigma(\omega) P^\omega_\sigma(\omega)}
\]

\[
W^\omega_\sigma(\omega) = W^r_\sigma(\omega) P^\omega_\sigma(\omega) W^a_\sigma(\omega)
\]

\[
W^a_\sigma(\omega) = W^a_\sigma(\omega) P^\omega_\sigma(\omega) W^a_\sigma(\omega)
\]

and the particle-hole bubbles are

\[
P^r_\sigma(\omega) = -i \int \frac{dx}{2\pi} G^r_\sigma(x) G^\omega_\sigma(x - \omega) - i \int \frac{dx}{2\pi} G^\omega_\sigma(x) G^r_\sigma(x - \omega)
\]

\[
P^a_\sigma(\omega) = -i \int \frac{dx}{2\pi} G^a_\sigma(x) G^\omega_\sigma(x - \omega) - i \int \frac{dx}{2\pi} G^\omega_\sigma(x) G^a_\sigma(x - \omega)
\]

\[
P^\omega_\sigma(\omega) = -i \int \frac{dx}{2\pi} G^\omega_\sigma(x) G^\omega_\sigma(x - \omega)
\]

In the above expressions, the advanced and greater Green functions are determined via equations (27) and (28) and \(\bar{\sigma} = -\sigma\) denotes the opposite spin of \(\sigma\).

Equations (29)-(40) form a closed set solved self-consistently for the 2BA and GWA. For the \(2^{nd}U\)-approximation all particle-hole propagators (38)-(40) are evaluated only once with the
bare Green functions

\[ g_{\sigma}(\omega) = \frac{1}{\omega + i\delta - E_d - \Sigma_{H\sigma} - \Delta(\omega)} \]  

\[ g_{\sigma}^\leq(\omega) = g_{\sigma}(\omega) \left[ 2i f_L(\omega) \Gamma_L(\omega) + 2i f_R(\omega) \Gamma_R(\omega) \right] g_{\sigma}^\geq(\omega) \]  

Only the Hartree shift is included in order to determine the desired filling, and equation (34) is used as the effective interaction.

The GW approximation [61, 62] has been successfully applied to overcome some shortcomings of local-density calculations and estimate the screening of the Coulomb interactions in solid state physics. Recently, the method has been employed to calculate quantum transport through nanoscale devices. It furnished a conserving approximation and captures some essential many-body effects [63, 64, 57, 18]. It was shown to describe accurately the equilibrium properties in the weakly interacting regime and in asymmetric situations with a nearly empty or nearly full impurity orbital [65, 66]. In the strongly interacting Kondo regime \( \Gamma - U < E_d < -\Gamma \), the GW approximation produces an exponentially narrow peak in the spectral function at the Fermi level, which could be interpreted as remnants of the expected many-body resonance [66]. However, the line shape of this low energy resonance as well as the high-energy Hubbard peaks at \( \omega \approx E_d \) and \( \omega \approx E_d + U \) are not reproduced by this approximation [65, 66]. Additionally, for very large interaction strength \( U/\Gamma > 8 \), all those perturbative approaches favor unphysical magnetic solutions: these sets of equations are close to bifurcation points which might yield unphysical hysteretic response. This indicates restricted applicability of such approach to small values of \( U/\Gamma \).

**Figure 1.** Taken from Ref. [60]: Comparison of the SNRG and the Keldysh spectral functions obtained in second Born approximation (2BA) for \( U/\Gamma = 1, E_d = -U/2 \) for two values of the bias voltage at \( T = 0.006 \) and symmetric coupling \( R = 1 \). We add \( \rho(\omega) \) obtained in Hartree-Fock (HF) approximation as comparison (dashed line).
3. Results

3.1. Spectral functions for small charging energies $U$

All energies as well as the bias voltage are measured here in units of the single-particle charge fluctuation scale $\Gamma$. We used symmetric structureless leads characterized by a constant DOS $\rho_0 = 1/(2D)$ on the interval $[-D:D]$ where $D/\Gamma = 20$ is chosen.

For $U/\Gamma < 1$, the nonequilibrium spectral functions obtained with the SNRG and all three Keldysh approximations are identical [60]. In all cases, the major contribution stems from the Hartree-term $\Sigma^H$, which causes a level shift from $E_d \rightarrow E_d + \Sigma^H$. The line shape remains nearly identical to the $U = 0$ solution as can be seen in comparison with the $U = 0$ spectrum: the additional scattering introduced by the finite value of $U$ is much smaller than the resonant level width $\Gamma$. Furthermore, the spectrum – not shown here – remains almost bias independent.

A comparison between different spectral functions is depicted in Fig. 1 for moderate values of $U/\Gamma = 1$ and particle-hole symmetry. While for zero bias all curves agree, slight deviations between the SNRG solution and the Keldysh approach can be seen at small frequencies and large voltages. The perturbative approaches predict a slightly larger dephasing than the SNRG, leading to a stronger decrease of the spectral function around $\omega = 0$. Nevertheless, the overall agreement of all approaches is remarkable. Again, the line shape is dominated by the Hartree-shift and resonant level with $\Gamma$.

3.2. Transport in the Kondo regime

We have established the quality of the SNRG by comparing the SNRG spectral functions with the Keldysh spectral functions for small charging energy. These perturbative and conserving diagrammatic approximations only yield reliable results for small values of $U$ since higher order diagrams have been omitted.

The spectral functions look quite different for larger values of $U$. A temperature dependent many-body resonance at $\omega = 0$ emerges when lowering $T$ below the characteristic low-energy scale $T_K$ as depicted in Fig. 2. The single lead calculation reduced the necessary number of NRG states $N_s$ keeps after each iteration significantly. $T_K$ depends exponentially on the charging energy.
Figure 3. Taken from Ref. [49]: nonequilibrium spectral functions for (a) a symmetric junction $R = 1$ and different value of the bias $V$, and (b) for a strongly asymmetric junction $R = 1000$. The charging energy is set to $U/\Gamma = 8$ and the single-particle level at $E_d = -U/2$ and $T \rightarrow 0$. The insets show the evolution of the Kondo-resonance. NRG Parameter: $\Lambda = 4$, $N_s = 2200$.

energy $U$ [67], i.e. $T_K \propto \exp(-\pi U/8\Gamma)$, and cannot be accessed by the diagrammatic methods described in Sec. 2.7 [60]. In addition, the single-particle resonance of the noninteracting problem splits into an upper and lower part with fractal weights which are the broaden atomic peaks at $E_d$ and $E_d + U$. The inset of Fig. 2 shows the evolution of the central many-body peak – $\rho(\omega = 0)$ – as a function of temperature. The logarithmic increase of $\rho(0)$ around $T \approx T_K$ as well as the saturation to the unitary limit $1/(\Gamma \pi)$ for $T \rightarrow 0$ is characteristic for the Kondo effect.

We have investigated [49] the bias dependence of the spectral functions for $U/\Gamma = 8$ in the quantum-point contact regime ($R = 1$) and in the tunneling regime ($R = 1000 \gg 1$).
The spectral function changes significantly with $V$ in the point-contact junction as depicted in Fig. 3(a): the many-body resonance at $\omega = 0$ decreases with increasing voltage on the scale of $T_K$. The onset of a splitting of the resonance is also observed for $|V| > \Gamma$.

As expected for the tunneling regime, the spectrum remains almost unaltered as shown in Fig. 3(b). A Kondo effect develops due to the interaction between the quantum dot and the lead which strongly coupled to the device; the weakly coupled lead only serves as probe.

The IV characteristic for a large charging energy $U/\Gamma = 8$ was calculated by inserting the spectra of Fig. 3 into Eq. (13). The results are shown for $R = 1$ and $R = 1000$ in Fig. 4. For better comparison, the current $I(V)$ has been normalized by $G_0$ which contains the prefactor $4R/(1 + R)^2$. For $R = 1000$, $G_0 = (e^2/h)4 \times 10^{-4}$: the current is strongly suppressed in the tunneling regime. In the quantum-point contact regime, the many-body resonance is destroyed with increasing voltage, and spectral weight is transferred to higher frequencies. As a consequence, the normalized current is initially lower than in the tunneling regime. This spectral weight loss accumulates at intermediate frequencies in the vicinity of the original atomic charge peaks. Hence, the current is enhanced once the voltage approaches the charging energy $U$.

The normalized current will saturate at $2\pi$ for very large voltages independent of $U$ due to the normalization of the Green function. At zero bias and odd integer fillings of the quantum-dot, the differential conductance is always given by values close to $G_0$ for $T \rightarrow 0$. For larger Coulomb interaction $U$, however, the current increases with bias significantly slower than predicted by the Hartree-Fock solution. Therefore, effective single-particle theories such as Hartree-Fock are unsuitable to describe interacting nano-devices and molecular junctions in the coherent regime at low temperature since they predict incorrect IV curves.

4. Conclusion
We have presented a novel non-perturbative approach to quantum-transport which extends the Wilson’s numerical renormalization group to open quantum systems. It includes the crossover from the Coulomb-blockade regime at high temperature to coherent transport at temperatures smaller than $T_K$. Since $T_K$ is exponentially dependent on the charging energy $U$, diagrammatic techniques fail to predict the correct energy scale and are only valid for small values of the
charging energy $U$.

Our approach uses a scattering-state description for the single-particle states and allows for simulation of a current-carrying open quantum system on a finite size system by including the correct boundary condition. Knowing the analytical form of the steady-state density operator for a noninteracting device at arbitrary bias [33], makes it possible to employ Wilson’s numerical renormalization to steady-state problems. By letting the system evolve from the Hartree-Fock solution to a full many-body problem at a finite value $U$, the time-dependent TD-NRG provides all information on the steady-state density matrix of the interacting system needed to calculate the steady-state spectral function at finite bias for arbitrary temperatures.

The scattering-states numerical renormalization group nonequilibrium spectra agree excellently with the diagrammatic Keldysh spectra for small values of $U$, establishing the reliability of the approach. The SNRG is suitable to access small and large interaction strength at arbitrary temperature in contrast to the Keldysh approaches such as second order Born or GW approximation which are limited to small values of $U$.

The scattering-states numerical renormalization group descriptions includes (i) Hubbard decoupling schemes [8, 9, 10] which are only applicable at high temperature as well as (ii) diagrammatic expansions in $U$ suitable for small values of the interaction strength. In addition, the SNRG does not suffer from artificial bifurcation points or unphysical magnetic solutions for large values of $U$ as seen in Hartree-Fock, second-order or GW approximation. Therefore, the method is suitable to investigate the IV characteristics of single-electron transistors in a finite magnetic field. A detailed study on the magneto-transport and the spin-currents relevant for spintronics is under way.

5. Acknowledgments
We would like to acknowledge financial support by the Deutsche Forschungsgemeinschaft under AN 275/6-1 and supercomputer support of the NIC, Forschungszentrum Jülich under project no. HHB000.

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