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Non-equilibrium steady-states for interacting open systems: exact results

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Under certain conditions we prove the existence of a steady-state transport regime for interacting mesoscopic systems coupled to reservoirs (leads). The partitioning and partition-free scenarios are treated on an equal footing. Our time-dependent scattering approach is *exact* and proves, among other things, the independence of the steady-state quantities from the initial state of the sample, and that the stationary current vanishes at zero bias. Closed formulas for the steady-state current amenable for perturbative calculations w.r.t. the interaction strength are also derived. In the partitioning case we calculate the first order correction and recover the mean-field (Hartree-Fock) results.

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I. INTRODUCTION

The theoretical modeling of time-dependent transport has been an active area of research in the last few years[1–3]. Transient currents are calculated using the Keldysh formalism[4], and the electron-electron interaction (EEI) effects are accounted for via time-dependent density functional theory (TDDFT) or many-body perturbative (MBP) methods. But no matter which metod one uses and how simple the system is, one recovers an old and often avoided question in non-equilibrium transport: does there exist a non-equilibrium steady-state (NESS), and if yes, is it unique?

Recently, Kurth *et al.*[5] presented TDDFT simulations for a single-level quantum dot (QD) in the Coulomb blockade regime. By selecting a suitable exchange-correlation potential they noticed that the system does not evolve to a steady state but rather follows charging/discharging cycles. Moreover, Myöhänen *et al.*[3] and Puig *et al.*[6] emphasized that different approximation schemes for the interaction self-energy lead to different steady-states, i.e, in the long-time limit the numerical simulations lead to different values of the current. These recent findings cleary show that the crossover to a steady-state (if any) is a non-trivial aspect which is revealed only by a fully time-dependent formalism for open and interacting systems. We remind here that following Ref.[4] the Keldysh formalism was extensively used to compute the stationary currents by assuming i) that such a steady state is achieved and ii) that the interaction strength is rather small such that a perturbative approach makes sense. The first assumption implies that it is sufficient to work directly with the Fourier transforms of the Green functions. The second assumption allows one to exploit diagrammatic techniques and conserving approximations for the interaction self-energy[7]. Given the results mentioned above one faces three questions: 1) How legitimate is it to take for granted the steady-state quantities of the Keldysh formalism especially in the presence of electron-electron interaction ? 2) Is the result of Kurth *et al.*[5] universal? 3) Is it possible to establish the existence of a stationary current in the long-time limit *before* selecting a given approximation scheme for the explicit calculations of the interaction effects?

In this note we prove that an interacting sample evolves to a NESS provided: i) all single-particle eigenstates of the isolated sample become resonances (with positive width) when the leads are coupled and ii) the interaction strength is small enough to ensure convergence of a certain perturbation expansion. These conditions are met for large quantum dots coupled to broad leads. Condition i) is also fulfilled if the bias applied on the leads covers the entire spectrum of the sample (wide-band limit). We follow the scattering approach to the NESS of open quantum systems advocated by Ruelle[17] and implemented, in the fermionic case, by Fröhlich et al.[18] and Jakšić et al.[20–22]. The existence of a steady-state is rigorously proved by deriving explicit expressions for both the lesser Green's function and the current in the infinite time limit. Our method is exact in the interaction and needs neither Langreth rules, nor Dyson equations for Keldysh-Green's functions. It provides convergent expansions in terms of the interaction strength, i.e., it shows that the NESS is an analytic function of the interaction.

Moreover, the proof of the steady-limit covers the two complementary but different transport scenarios: the partitioning approach of Caroli *et al.*[11] and the partition-free setting coined by Cini[12]. Let us briefly remind them here. In the partitioning approach the central region (sample) is coupled to *biased* leads at some initial instant. In contrast, the partition-free setup starts from a coupled and unbiased system, a bias being switched at $t = t_0$. Both settings have also received interest from the mathematical point of view[13–16,21].

The content of the paper is as follows: Section II sets the model and some notations needed for the partitioning and partition-free settings. We formulate our main result, the steady state limit of the lesser Green's function, in Section III. The expression for the steady currents is derived in Section IV, along with the Landauer-Büttiker

formula which holds if the Coulomb effects are considered up to the 1st order term in the interaction strength. We outline the proof of our results in Section V and conclude in Section VI with some general comments.

II. MODEL AND NOTATIONS

Our system consists of a finite sample S coupled to M semi-infinite leads labeled by γ. It is described by a discrete model: sites from the lead γ are denoted by $\{i_\gamma\}_{i\geq 0}$ and $\{m\}_{m\in S}$ are the sites of the sample. We denote by $\mathcal{H}_S$ and $\mathcal{H}_L$ the one particle Hilbert spaces of the sample and leads. The one particle Hilbert space of the compound system is $\mathcal{H} = \mathcal{H}_L \oplus \mathcal{H}_S$ and $\mathcal{F}$ denotes the fermionic Fock space over $\mathcal{H}$. The one particle Hamiltonian of the noninteracting sample is h_S, an arbitrary self-adjoint operator on $\mathcal{H}_S$. In terms of the on-site creation/annihilation operators on $\mathcal{F}$, the Hamiltonian and number operator of the sample are

$$H_S = \sum_{m,n\in S} \langle m|h_S|n\rangle\, a_m^\dagger a_n, \qquad N_S = \sum_{m\in S} a_m^\dagger a_m.$$

The semi-infinite leads are described by the Hamiltonian $H_L = \sum_\gamma H_\gamma$ and number operator $N_L = \sum_\gamma N_\gamma$, where

$$H_\gamma = \tau_L \sum_{i\geq 0} \left(a_{i_\gamma}^\dagger a_{(i+1)_\gamma} + a_{(i+1)_\gamma}^\dagger a_{i_\gamma} \right), \quad N_\gamma = \sum_{i\geq 0} a_{i_\gamma}^\dagger a_{i_\gamma}.$$

We also need the tunneling Hamiltonian H_T, some constant potential H_B applied to the leads and the electron-electron interaction in the sample V,

$$H_T = \tau \sum_{\gamma=1}^{M} \left(a_{0_\gamma}^\dagger a_{m_\gamma} + a_{m_\gamma}^\dagger a_{0_\gamma} \right), \qquad H_B = \sum_{\gamma=1}^{M} v_\gamma N_\gamma,$$
$$V = \frac{\xi}{2} \sum_{m,n\in S} v(m,n)\, a_m^\dagger a_m a_n^\dagger a_n.$$

Here, τ is the coupling strength, $m_\gamma \in S$ the contact site of the sample with lead γ, v_γ a constant potential, ξ the interaction strength and $v(m,n)$ a pair potential. The differences $v_\alpha - v_\beta$ define the bias between the corresponding leads. By convention all the v_γ vanish in the partitioning case, so that $H_B = 0$. For both partitioning ('p')/partition-free ('pf') settings we assume that the switching (of the coupling to the leads H_T/of the bias H_B) happens suddenly at $t = 0$. A smooth switching can also be treated up to some technicalities[23], and does not influence the results.

The Hamiltonians H_S, H_L, H_T, H_B as well as

$$H_0 = H_S + H_L + H_B, \qquad H = H_0 + H_T,$$

act in the Fock space $\mathcal{F}$ as the second quantized versions of single particle tight-binding Hamiltonians $h_S, h_L, h_T, h_B, h_0, h$ acting on $\mathcal{H}$. Similar relations hold for the number operators N_S, N_γ, N_L and $N = N_S + N_L$. We denote by $\mathcal{F}_L$ and $\mathcal{F}_S$ the subspaces of $\mathcal{F}$ where $N_S = 0$ and $N_L = 0$ respectively. The full dynamics of the system is generated by the Hamiltonian

$$K = H + V.$$

We now introduce the initial state of the system as thermodynamic limit of states defined by density matrices on the sample coupled to finite leads of length Λ. Indicating this infrared cutoff by the superscript $^{(\Lambda)}$, we set

$$\rho_{L,\vec{\mu}}^{(\Lambda)} = \frac{\mathrm{e}^{-\beta(H_L^{(\Lambda)} - \sum_\gamma \mu_\gamma N_\gamma^{(\Lambda)})}}{\mathrm{Tr}_{\mathcal{F}_L^{(\Lambda)}}\{\mathrm{e}^{-\beta(H_L^{(\Lambda)} - \sum_\gamma \mu_\gamma N_\gamma^{(\Lambda)})}\}},$$

for $\vec{\mu} = [\mu_1, ..., \mu_M]$ and, for any leads observable $\mathcal{O}_L$,

$$\langle \mathcal{O}_L \rangle_{L,\vec{\mu}} = \lim_{\Lambda\to\infty} \mathrm{Tr}_{\mathcal{F}_L}\{\rho_{L,\vec{\mu}}^{(\Lambda)} \mathcal{O}_L\}.$$

We recall that this state is characterized by the two-point function

$$\langle a_{j_\alpha}^\dagger a_{i_\gamma} \rangle_{L,\vec{\mu}} = \delta_{\alpha\gamma} \langle i_\gamma | F_\gamma(h_\gamma) | j_\gamma \rangle,$$

and Wick's theorem. There, $F_\gamma(\varepsilon) = (1 + \mathrm{e}^{\beta(\varepsilon - \mu_\gamma)})^{-1}$ denotes the Fermi-Dirac function of lead γ.

In the 'p' setting, the initial state is the product state defined by

$$\langle \mathcal{O}_L \mathcal{O}_S \rangle_{\mathrm{p}} = \langle \mathcal{O}_L \rangle_{L,\mathrm{p}} \langle \mathcal{O}_S \rangle_{S,\mathrm{p}}$$

for any observables $\mathcal{O}_{L/S}$ of the leads/sample. There,

$$\langle \mathcal{O}_L \rangle_{L,\mathrm{p}} = \langle \mathcal{O}_L \rangle_{L,\vec{\mu}}, \qquad \langle \mathcal{O}_S \rangle_{S,\mathrm{p}} = \mathrm{Tr}_{\mathcal{F}_S}\{\rho_{S,\mathrm{p}} \mathcal{O}_S\},$$

where $\rho_{S,\mathrm{p}}$ is an arbitrary density matrix on $\mathcal{F}_S$. In the 'pf' case the leads and sample are coupled and have the same chemical potential μ_0, i.e.,

$$\langle \mathcal{O} \rangle_{\mathrm{pf}} = \lim_{\Lambda\to\infty} \mathrm{Tr}_{\mathcal{F}^{(\Lambda)}}\{\rho_{\mathrm{pf}}^{(\Lambda)} \mathcal{O}\},$$

where

$$\rho_{\mathrm{pf}}^{(\Lambda)} = \frac{\mathrm{e}^{-\beta(H_S + H_L^{(\Lambda)} + H_T + V - \mu_0 N^{(\Lambda)})}}{\mathrm{Tr}_{\mathcal{F}^{(\Lambda)}}\{\mathrm{e}^{-\beta(H_S + H_L^{(\Lambda)} + H_T + V - \mu_0 N^{(\Lambda)})}\}}.$$

For later reference, we also define the leads state

$$\langle \cdot \rangle_{L,\mathrm{pf}} = \langle \cdot \rangle_{L,\vec{\mu}=[\mu_0,...,\mu_0]}.$$

The *lesser Green's function* is defined as

$$G_{\boxdot\, xy}^{<}(t,s) = \mathrm{i}\, \langle a_y^\dagger(s) a_x(t) \rangle_{\boxdot},$$

where x, y are sites from either leads or sample, $a_x(t) = \mathrm{e}^{\mathrm{i}tK} a_x \mathrm{e}^{-\mathrm{i}tK}$ and $\boxdot$ stands for either 'p' or 'pf'. This object plays a central role in the Keldysh approach and allows to compute both the particle density and the currents. Our main concern being the existence of steady currents, we are primarily interested in its large time behaviour $t, s \to \infty$ for constant $t - s$.

III. THE EXISTENCE OF THE STEADY-STATE

For $|\phi\rangle \in \mathcal{H}$, we set

$$a(|\phi\rangle) = \sum_x \langle\phi|x\rangle\, a_x, \quad a^\dagger(|\phi\rangle) = \sum_x \langle x|\phi\rangle\, a_x^\dagger,$$

and let $a^\#(|\phi\rangle)$ denote either $a(|\phi\rangle)$ or $a^\dagger(|\phi\rangle)$. If q is a self-adjoint operator on $\mathcal{H}$ and Q denotes its second quantized version, then the well known identity

$$\mathrm{e}^{\mathrm{i}Q} a^\#(|\phi\rangle)\mathrm{e}^{-\mathrm{i}Q} = a^\#(\mathrm{e}^{\mathrm{i}q}|\phi\rangle), \tag{1}$$

holds. The interaction picture operators

$$\mathcal{A}_x^\#(t) = \mathrm{e}^{-\mathrm{i}tH} a_x^\#(t)\mathrm{e}^{\mathrm{i}tH}, \tag{2}$$

satisfies the equation of motion

$$\mathcal{A}_x^\#(t) = a_x^\# + \mathrm{i}\int_0^t [\mathrm{e}^{-\mathrm{i}uH} V \mathrm{e}^{\mathrm{i}uH}, \mathcal{A}_x^\#(u)]\mathrm{d}u. \tag{3}$$

By Eq.(1) we have

$$\begin{aligned} \mathrm{e}^{-\mathrm{i}uH} V \mathrm{e}^{\mathrm{i}uH} &= \frac{\xi}{2}\sum_{m,n\in S} v(m,n) \\ &\times a^\dagger(\mathrm{e}^{-\mathrm{i}uh}|m\rangle) a(\mathrm{e}^{-\mathrm{i}uh}|m\rangle) a^\dagger(\mathrm{e}^{-\mathrm{i}uh}|n\rangle) a(\mathrm{e}^{-\mathrm{i}uh}|n\rangle). \end{aligned} \tag{4}$$

Thus, the Dyson expansion of $\mathcal{A}_x^\#(t)$ obtained by iteration of Eq.(3) is a sum of iterated integrals involving monomials of the type

$$\mathcal{M}(|\phi_1\rangle, \ldots, |\phi_k\rangle) = a^{\#_1}(|\phi_1\rangle)\cdots a^{\#_k}(|\phi_k\rangle), \tag{5}$$

each $|\phi_j\rangle$ being either $|x\rangle$ or $\mathrm{e}^{-\mathrm{i}uh}|m\rangle$ for some $m \in S$ and $u \in [0,t]$ (so that, in particular $|\langle\Psi|\mathcal{M}|\Phi\rangle| \leq 1$ for any unit vector $|\Psi\rangle, |\Phi\rangle \in \mathcal{F}$). Moreover, one easily sees that this expansion converges for *any* t. In fact, a careful study of this expansion shows that, under suitable assumptions, it remains convergent even for $t = \infty$.

Theorem III.1. *Assume that the single particle Hamiltonian h has neither eigenvalue nor real resonance. If the interaction strength ξ is small enough, then the limits*

$$\mathcal{A}_x^\# = \lim_{t\to\infty} \mathcal{A}_x^\#(t),$$

exist. Moreover, a convergent expansion of $\mathcal{A}_x^\#$ in powers of the interaction strength ξ is obtained by setting $t = \infty$ in the Dyson expansion of $\mathcal{A}_x^\#(t)$.

Remark. The first hypothesis of the previous theorem requires some comments. The spectrum of $h_L + h_B$ is continuous, filling the union of $[v_\gamma - 2\tau_L, v_\gamma + 2\tau_L]$. If all the eigenvalues of the isolated sample h_S are embedded in these bands and if the coupling to the leads τ is weak enough then all these eigenvalues will generically turn into resonances of positive width. In such circumstances, the spectrum of h is continuous and coincides with that of $h_L + h_B$. Moreover, one can show that for any x, y in either the leads or the sample,

$$\int_0^\infty |\langle x|\mathrm{e}^{-\mathrm{i}th}|y\rangle|\,\mathrm{d}t < \infty. \tag{6}$$

However, as the coupling τ increases, some resonances may become real, cross a band boundary and turn into an eigenvalue of h, invalidating (6). The first hypothesis in Theorem III.1 is meant to ensure the validity of Eq.(6).

Let w be an operator on $\mathcal{H}$ such that $|\langle\phi|w|\psi\rangle| \leq 1$ for all unit vectors $|\phi\rangle, |\psi\rangle \in \mathcal{H}$. Replacing each term (5) in the Dyson expansion of $\mathcal{A}_x^\#$ by $\mathcal{M}(w|\phi_1\rangle, \ldots, w|\phi_k\rangle)$ does not alter the convergence of this expansion. We denote by $\mathcal{A}_x^\#[w]$ the operator obtained from this modified Dyson expansion.

We are now in position to state our main result (recall that $h_B = 0$ in the 'p' case):

Theorem III.2. *Under the assumptions of Theorem III.1 one has, for any s,*

$$\begin{aligned} \mathcal{G}^<_{\boxdot xy}(s) &= \lim_{t\to\infty} G^<_{\boxdot xy}(t, t-s) \\ &= \mathrm{i}\langle \mathcal{A}_y^\dagger[\mathrm{e}^{-\mathrm{i}s(h_L+h_B)}\omega_+^\dagger]\mathcal{A}_x[\omega_+^\dagger]\rangle_{L,\boxdot}. \end{aligned} \tag{7}$$

There, ω_+ denotes the Møller operator[8]

$$\omega_+|\phi\rangle = \lim_{t\to-\infty} \mathrm{e}^{\mathrm{i}th}\mathrm{e}^{-\mathrm{i}th_0} p_L|\phi\rangle, \tag{8}$$

where p_L projects on the leads subspace $\mathcal{H}_L$.

In Section V, we shall outline the proofs of Theorems III.1, III.2. Complete mathematical details will be given elsewhere[23]. We conclude this section with several remarks.

1. Asymptotic completeness[8] implies that

$$\begin{aligned} \omega_+^\dagger|\psi\rangle &= \lim_{t\to-\infty} \mathrm{e}^{\mathrm{i}th_0}\mathrm{e}^{-\mathrm{i}th}|\psi\rangle \\ &= \lim_{t\to-\infty} p_L \mathrm{e}^{\mathrm{i}t(h_L+h_B)}\mathrm{e}^{-\mathrm{i}th}|\psi\rangle, \end{aligned} \tag{9}$$

is unitary from $\mathcal{H}$ to $\mathcal{H}_L$ so that the object under the expectation on the RHS of Eq.(7) has a convergent expansion as described above. Moreover, the expectation is w.r.t. the leads state $\langle\,\cdot\,\rangle_{L,\boxdot}$ which does not depend on the interaction V, i.e., satisfies Wick's theorem.

2. Eq.(7) implies right away that the expected particle number in the sample reaches a steady value in the long-time limit

$$\lim_{t\to\infty}\langle N_S(t)\rangle_{\boxdot} = -\mathrm{i}\sum_{m\in S} \mathcal{G}^<_{\boxdot,mm}(0).$$

In fact, one can show that, under the assumptions of Theorem III.1, the system reaches a NESS $\langle\,\cdot\,\rangle_{\boxdot+}$ described by

$$\begin{aligned} \langle a_{x_1}^{\#_1}\cdots a_{x_k}^{\#_k}\rangle_{\boxdot+} &= \lim_{t\to\infty}\langle a_{x_1}^{\#_1}(t)\cdots a_{x_k}^{\#_k}(t)\rangle_{\boxdot} \\ &= \langle \mathcal{A}_{x_1}^{\#_1}[\omega_+^\dagger]\cdots\mathcal{A}_{x_k}^{\#_k}[\omega_+^\dagger]\rangle_{L,\boxdot}. \end{aligned}$$

In the 'p' case, this NESS is *independent* on the initial state of the sample $\rho_{S,\mathrm{p}}$. Moreover, in the special case $\vec{\mu} = [\mu_0, \ldots, \mu_0]$, $\langle \cdot \rangle_{\mathrm{p}+}$ is the unique equilibrium state of the interacting system at inverse temperature β and chemical potential μ_0.

3. In the non-interacting case ($V = 0$), the NESS satisfies Wick's theorem with the two points function $\langle a_y^\dagger a_x \rangle_{\boxdot+} = \langle x|\rho_+|y\rangle$, where the one-particle density operator ρ_+ is given by[13,14]

$$\rho_+ = \omega_+ \left(\bigoplus_\gamma F_\gamma(h_\gamma) \right) \omega_+^\dagger. \tag{10}$$

IV. THE STEADY-STATE CURRENT

The current operator of lead α

$$J_\alpha = -\frac{\mathrm{d}}{\mathrm{d}t} N_\alpha(t)\Big|_{t=0} = -\mathrm{i}[K, N_\alpha] = -\mathrm{i}[H, N_\alpha],$$

is the second quantized version of the single-particle current $j_\alpha = -\mathrm{i}[h, p_\alpha]$, where p_α projects on lead α. Its statistical average is[4]

$$\langle J_\alpha(t) \rangle_{\boxdot} = \tau(G^<_{\boxdot m_\alpha 0_\alpha}(t,t) - G^<_{\boxdot 0_\alpha m_\alpha}(t,t)). \tag{11}$$

We introduce the interaction picture current operator

$$\mathcal{J}_\alpha(t) = \mathrm{e}^{-\mathrm{i}tH} \mathrm{e}^{\mathrm{i}tK} J_\alpha \mathrm{e}^{-\mathrm{i}tK} \mathrm{e}^{\mathrm{i}tH}, \tag{12}$$

which is similar to $\mathcal{A}_x(t)$, Eq.(3) being replaced by

$$\mathcal{J}_\alpha(t) = J_\alpha + \mathrm{i} \int_0^t [\mathrm{e}^{-\mathrm{i}uH} V \mathrm{e}^{\mathrm{i}uH}, \mathcal{J}_\alpha(u)] \mathrm{d}u. \tag{13}$$

Using Eq.(7) with $s = 0$ in Eq.(11) we get

$$I_{\alpha,\boxdot} = \lim_{t\to\infty} \langle J_\alpha(t) \rangle_{\boxdot} = \langle \mathcal{J}_\alpha[\omega_+^\dagger] \rangle_{L,\boxdot}, \tag{14}$$

where $\mathcal{J}_\alpha = \lim_{t\to\infty} \mathcal{J}_\alpha(t)$ is calculated by setting $t = \infty$ in the Dyson expansion generated by iteration of Eq.(13) and $\mathcal{J}_\alpha[\omega_+^\dagger]$ is obtained in the usual way from $\mathcal{J}_\alpha$. Comparing the final formulas for the two cases 'p' and 'pf', one realizes that $I_{\alpha,\mathrm{pf}}(\vec{v} = \vec{0}) = I_{\alpha,\mathrm{p}}(\vec{\mu} = [\mu_0,.., \mu_0])$. Since $J_\alpha = -\mathrm{i}[H + V, N_\alpha] = -\mathrm{i}[H^{(\Lambda)} + V, N_\alpha^{(\Lambda)}]$, one has

$$I_{\alpha,\mathrm{pf}}(\vec{v} = \vec{0}) = -\lim_{\Lambda\to\infty} \mathrm{Tr}_{\mathcal{F}^{(\Lambda)}} \{\rho_{\mathrm{pf}}^{(\Lambda)} \mathrm{i}[H^{(\Lambda)} + V, N_\alpha^{(\Lambda)}]\} = 0,$$

due to the cyclicity of the trace and the fact that $[\rho_{\mathrm{pf}}^{(\Lambda)}, H^{(\Lambda)} + V] = 0$. Thus both currents vanish in the absence of bias. This fact cannot be seen from the interacting Meir-Wingreen formula[4].

The interaction effects can be calculated perturbatively from Eq.(13). For the partitioning setting with identical leads having a hopping constant $\tau_L > 0$ one finds

$$I_{\alpha,\mathrm{p}} = I_{\alpha,\mathrm{LB}} + \mathcal{O}(\xi^2) + \mathcal{O}(\xi\tau^6), \tag{15}$$

where I_{LB} assumes a Landauer-like form

$$I_{\alpha,\mathrm{LB}} = \sum_\gamma \int_{-2\tau_L}^{2\tau_L} (F_\alpha(E) - F_\gamma(E)) |\mathcal{T}_{\alpha\gamma}^{\mathrm{MF}}(E,\xi)|^2 \mathrm{d}E \tag{16}$$

with the transmittance[25] $\mathcal{T}_{\alpha\gamma}^{\mathrm{MF}}(E,\xi)$ corresponding to a mean-field Hamiltonian $h_{S,\mathrm{MF}} = h_S + \xi v_{\mathrm{MF}}$ where

$$v_{\mathrm{MF}} = \sum_{m\in S} v_{H,m} |m\rangle\langle m| - \sum_{m,n\in S} v_{X,mn} |m\rangle\langle n| \tag{17}$$

and

$$v_{H,m} = \sum_{n\in S} v(m,n) \langle n|\rho_+|n\rangle, \quad v_{X,mn} = v(m,n) \langle n|\rho_+|m\rangle,$$

are Hartree and exchange terms, with the single-particle density operator ρ_+ given by Eq.(10).

V. PROOFS

We start by analysing the structure of $\mathcal{A}_x(t)$, following[21]. Iterating Eq.(3) and using Eq.(4), one obtains an infinite series involving iterated integrals of the multiple commutators

$$[\tilde{a}_{m_1}^\dagger(u_1) \cdots \tilde{a}_{n_1}(u_1), [\cdots, [\tilde{a}_{m_r}^\dagger(u_r) \cdots \tilde{a}_{n_r}(u_r), a_x] \cdots],$$

where $\tilde{a}_m(u) = a(\mathrm{e}^{-\mathrm{i}uh}|m\rangle)$. By repeated use of the algebraic identity

$$\begin{aligned} &[b_1 \cdots b_k, c_1 \cdots c_l] \\ &= \sum_{i=1}^k \sum_{j=1}^l (-1)^i \{b_i, c_j\} c_1 \cdots c_{j-1} b_1 \cdots \not{b}_i \cdots b_k c_{j+1} \cdots c_l, \end{aligned}$$

and of the canonical anti-commutation relations $\{a^\dagger(|\phi\rangle), a(|\psi\rangle)\} = \langle\psi|\phi\rangle$, $\{a(|\phi\rangle), a(|\psi\rangle)\} = 0$ we recast our expansion into the form

$$\begin{aligned} \mathcal{A}_x(t) = a_x + \sum_{r\geq 1} \xi^r \int_{0\leq u_r \leq \cdots \leq u_1 \leq t} \mathrm{d}u_1 \cdots \mathrm{d}u_r \\ \sum_{G\in\Gamma_r} C_r^G(u_1,.., u_r; x) \mathcal{M}_r^G(u_1,.., u_r; x), \end{aligned} \tag{18}$$

where each Γ_r is a finite set (of contraction diagrams). For each $G \in \Gamma_r$, $\mathcal{M}_r^G$ is a monomial of type (5) and C_r^G is a product of 'pairing factors' like $\langle y|\mathrm{e}^{-\mathrm{i}u_j h}|y'\rangle$ or $\langle y|\mathrm{e}^{-\mathrm{i}(u_j - u_k)h}|y'\rangle$, where $y, y' \in S \cup \{x\}$.

Our first assumption ensures that there exists a constant C_x such that

$$\int_0^\infty \max_{y,y'\in S\cup\{x\}} |\langle y|\mathrm{e}^{-\mathrm{i}uh}|y'\rangle| \, \mathrm{d}u \leq C_x.$$

A delicate combinatorial analysis then shows that (see Theorem 1.1 in[21])

$$\sum_{r\geq 1} |\xi|^r \int_{0\leq u_r \leq \cdots \leq u_1 \leq \infty} \mathrm{d}u_1 \cdots \mathrm{d}u_r \sum_{G\in\Gamma_r} |C_r^G(u_1,.., u_r; x)| < \infty,$$

provided $|\xi| \leq \Lambda_0 = 2/(27|S|^2 C_x v)$, where $|S|$ is the number of sites in the sample S and $v = \max_{n,m\in S} |v(n,m)|$. Thus, the expansion (18) converges uniformly w.r.t. $t \in [0,\infty]$. In particular, setting $t = \infty$ in Eq.(18) yields a convergent expansion of $\mathcal{A}_x$ (and taking adjoint gives an expansion for $\mathcal{A}_x^\dagger$). This proves Theorem III.1.

To prove Theorem III.2, we first notice that, according to Eq.(1), we get an expansion of

$$\begin{aligned}&\mathrm{e}^{-\mathrm{i}t(H_L+H_B)} a_x^\#(t-s) \mathrm{e}^{\mathrm{i}t(H_L+H_B)} \\ &= \mathrm{e}^{-\mathrm{i}t(H_L+H_B)} \mathrm{e}^{\mathrm{i}(t-s)H} \mathcal{A}_x^\#(t-s) \mathrm{e}^{-\mathrm{i}(t-s)H} \mathrm{e}^{\mathrm{i}t(H_L+H_B)},\end{aligned}$$

by replacing each factor $a^\#(|\psi\rangle)$ of any monomial $\mathcal{M}_r^G$ in Eq.(18) by $a^\#(\mathrm{e}^{-\mathrm{i}t(h_L+h_B)}\mathrm{e}^{\mathrm{i}(t-s)h}|\psi\rangle)$. Since Eq. (9) implies that

$$\lim_{t\to\infty} a^\#(\mathrm{e}^{-\mathrm{i}t(h_L+h_B)}\mathrm{e}^{\mathrm{i}(t-s)h}|\psi\rangle) = a^\#(\mathrm{e}^{-\mathrm{i}s(h_L+h_B)}\omega_+^\dagger|\psi\rangle),$$

one has

$$\begin{aligned}\lim_{t\to\infty} \mathrm{e}^{-\mathrm{i}t(H_L+H_B)} a_x^\#(t-s) \mathrm{e}^{\mathrm{i}t(H_L+H_B)} \\ = \mathcal{A}_x^\#[\mathrm{e}^{-\mathrm{i}s(h_L+h_B)}\omega_+^\dagger],\end{aligned}$$

and hence, $\mathcal{B}(t) = \mathrm{e}^{-\mathrm{i}t(H_L+H_B)} a_y^\dagger(t-s) a_x(t) \mathrm{e}^{\mathrm{i}t(H_L+H_B)}$ satisfies

$$\lim_{t\to\infty} \mathcal{B}(t) = \mathcal{A}_y^\dagger[\mathrm{e}^{-\mathrm{i}s(h_L+h_B)}\omega_+^\dagger]\mathcal{A}_x[\omega_+^\dagger]. \tag{19}$$

Notice that since the range of $\omega_+^\dagger$ is $\mathcal{H}_L$, the RHS of this identity is an observable of the leads. In the 'p' case, $H_B = 0$ and the state $\langle\cdot\rangle_\mathrm{p}$ is invariant under the dynamics of H_L. It follows that

$$\begin{aligned}\lim_{t\to\infty} \langle a_y^\dagger(t-s) a_x(t)\rangle_\mathrm{p} &= \lim_{t\to\infty} \langle \mathcal{B}(t)\rangle_\mathrm{p} \\ &= \langle \mathcal{A}_y^\dagger[\mathrm{e}^{-\mathrm{i}sh_L}\omega_+^\dagger]\mathcal{A}_x[\omega_+^\dagger]\rangle_\mathrm{p} \\ &= \langle \mathcal{A}_y^\dagger[\mathrm{e}^{-\mathrm{i}sh_L}\omega_+^\dagger]\mathcal{A}_x[\omega_+^\dagger]\rangle_{L,\mathrm{p}},\end{aligned}$$

which proves Theorem III.2 in the 'p' case.

To deal with the 'pf' case, we invoke standard perturbation theory (see e.g.[10]) to write

$$\langle \mathcal{O}\rangle_\mathrm{pf} = \frac{\langle \mathcal{D}\mathcal{O}\rangle_\mathrm{d}}{\langle \mathcal{D}\rangle_\mathrm{d}}. \tag{20}$$

There, $\langle\cdot\rangle_\mathrm{d}$ denotes the grand canonical ensemble for the decoupled dynamics H_0+V at inverse temperature β and chemical potential μ_0, *i.e.*, the product state

$$\langle \mathcal{O}_L\mathcal{O}_S\rangle_\mathrm{d} = \langle \mathcal{O}_L\rangle_{L,\mathrm{pf}} \frac{\mathrm{Tr}_{\mathcal{F}_S}\{\mathrm{e}^{-\beta(H_S+V-\mu_0 N_S)}\mathcal{O}_S\}}{\mathrm{Tr}_{\mathcal{F}_S}\{\mathrm{e}^{-\beta(H_S+V-\mu_0 N_S)}\}},$$

and

$$\begin{aligned}\mathcal{D} &= \mathrm{e}^{\beta(H_0+V-\mu_0 N)}\mathrm{e}^{-\beta(H+V-\mu_0 N)} \\ &= I + \sum_{k\geq 1}(-1)^k \int_0^\beta \mathrm{d}\tau_1 \cdots \int_0^{\tau_{k-1}} \mathrm{d}\tau_k \hat{H}_T(\tau_1)..\hat{H}_T(\tau_k),\end{aligned}$$

where $\hat{H}_T(u) = \mathrm{e}^{u(H_0+V)} H_T \mathrm{e}^{-u(H_0+V)}$. The state $\langle\cdot\rangle_\mathrm{d}$ being invariant under the dynamics of H_L+H_B, one has

$$\langle \mathcal{D} a_y^\dagger(t-s) a_x(t)\rangle_\mathrm{d} = \langle \mathcal{D}_t \mathcal{B}(t)\rangle_\mathrm{d},$$

where $\mathcal{D}_t = \mathrm{e}^{-\mathrm{i}t(H_L+H_B)}\mathcal{D}\mathrm{e}^{\mathrm{i}t(H_L+H_B)}$. It follows from Eq.(19) that

$$\begin{aligned}&\lim_{t\to\infty} \langle \mathcal{D} a_y^\dagger(t-s) a_x(t)\rangle_\mathrm{d} \\ &\quad = \lim_{t\to\infty} \langle \mathcal{D}_t \mathcal{A}_y^\dagger[\mathrm{e}^{-\mathrm{i}s(h_L+h_B)}\omega_+^\dagger]\mathcal{A}_x[\omega_+^\dagger]\rangle_\mathrm{d}.\end{aligned} \tag{21}$$

Introducing the partial trace

$$\mathcal{D}_L = \frac{\mathrm{Tr}_{\mathcal{F}_S}\{\mathrm{e}^{-\beta(H_S+V-\mu_0 N_S)}\mathcal{D}\}}{\mathrm{Tr}_{\mathcal{F}_S}\{\mathrm{e}^{-\beta(H_S+V-\mu_0 N_S)}\}},$$

we observe that, for any observable $\mathcal{O}_L$ of the leads,

$$\langle \mathcal{D}_t \mathcal{O}_L\rangle_\mathrm{d} = \langle \mathrm{e}^{-\mathrm{i}t(H_L+H_B)}\mathcal{D}_L \mathrm{e}^{\mathrm{i}t(H_L+H_B)}\mathcal{O}_L\rangle_{L,\mathrm{pf}}.$$

Since h_L+h_B has continuous spectrum, the dynamics of H_L+H_B is mixing w.r.t. the state $\langle\cdot\rangle_{L,\mathrm{pf}}$ (see e.g.[19]) so that

$$\begin{aligned}\lim_{t\to\infty} \langle \mathcal{D}_t \mathcal{O}_L\rangle_\mathrm{d} &= \lim_{t\to\infty} \langle \mathrm{e}^{-\mathrm{i}t(H_L+H_B)}\mathcal{D}_L \mathrm{e}^{\mathrm{i}t(H_L+H_B)}\mathcal{O}_L\rangle_{L,\mathrm{pf}} \\ &= \langle \mathcal{D}_L\rangle_{L,\mathrm{pf}} \langle \mathcal{O}_L\rangle_{L,\mathrm{pf}} = \langle \mathcal{D}\rangle_\mathrm{d} \langle \mathcal{O}_L\rangle_{L,\mathrm{pf}}.\end{aligned}$$

Applying this identity to the RHS of Eq.(21) and inserting the result into Eq.(20) proves Theorem III.2 in the 'pf' case.

VI. CONCLUSIONS

We give sufficient conditions for the existence of a steady-state regime for open interacting systems, using an approach based on time-dependent scattering theory. While the approach is perturbative w.r.t. the interaction strength, the existence of the stationary regime is general in the sense that it does not rely on a particular approximation scheme for the Coulomb effects. To our best knowledge, the steady-state regime is not proved within the Keldsyh formalism: the steady-state value of the current is derived by *assuming* that the two-time GFs depend only on time difference[4]. We perform the thermodynamic limit without making use of Langreth rules and Dyson equations. In the Keldysh approach it is not clear how to perform the thermodynamic limit on the *proper* interaction self-energy.

The smallness condition on ξ for the existence of the steady-state is also necessary. For example, if $v(m,n)$ is diagonal then V is a single-particle operator (Hartree-like potential) which can create bound states for large values of ξ, leading thus to oscillations similar to the ones observed in[2]. However, we conjecture that if one performs the ergodic limit $\lim_{T\to\infty}\frac{1}{T}\int_0^T J_\alpha(t)\mathrm{d}t$, a time-averaged steady-state could still be achieved even in the general interacting case. It would be interesting to investigate

the ergodic limit of the oscillating currents reported in Fig. 1 from[5], which seem to support our conjecture.

In the partitioning approach we have shown that the steady-state quantities *do not depend on the initial many-body configuration of the sample* $\rho_{S,\mathrm{p}}$. Moreover, one can allow other switching procedures of the bias or of the lead-sample coupling (not just the sudden one), and the steady state remains unchanged (the complete proof will be given in Ref. 23). Let us mention that very recently[27] we have shown that when ξ is allowed to be arbitrarily large and the system is in the off-resonant regime in which h has eigenvalues situated very far from the continuous spectrum, the *ergodic* cotunneling current *presents memory effects and depends on* $\rho_{S,\mathrm{p}}$ *if* $\xi \neq 0$. In the non-interacting case, we still have independence on $\rho_{S,\mathrm{p}}$.

Our results could be numerically implemented in both settings (partitioning and partition-free) and compared to the ones obtained from the Keldysh formalism. The second correction in Eq.(15) suggests significant differences for strong coupling to the leads.

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[1] S. Kurth *et al.*, Phys. Rev. B **72**, 035308 (2005).
[2] G. Stefanucci and C.-O. Almbladh, Phys. Rev. B **69**, 195318 (2004).
[3] P. Myöhänen *et al.* Phys. Rev. B **80**, 115107 (2009)
[4] A.-P. Jauho, N. S. Wingreen and Y. Meir., Phys. Rev. B **50**, 5528 (1994).
[5] S. Kurth *et al.* Phys. Rev. Lett. **104**, 236801 (2010).
[6] M. Puig von Friesen , C. Verdozzi and C.-O. Almbladh, Phys. Rev. B **82**, 155108 (2010).
[7] K. S. Thygesen and A. Rubio, Phys. Rev. B **77**, 115333 (2008).
[8] J. R. Taylor, *Scattering Theory: The Quantum Theory of Nonrelativistic Collisions.* Dover Publications (2006).
[9] M. L. Goldberger and K. M. Watson, *Collision theory.* Dover Publications (2004).
[10] R. Kubo, M. Toda and N. Hashitsume, *Statistical Physics II. Nonequilibrium Statistical Mechanics.* Springer, Berlin (1985).
[11] C. Caroli *et al.*, J. Phys. C **4**, 916 (1971).
[12] M. Cini, Phys. Rev. B. **22**, 5887 (1980).
[13] W. Aschbacher, V. Jakšić, Y. Pautrat and C.-A. Pillet, J. Math. Phys. **48**, 032101 (2007).
[14] G. Nenciu, J. Math. Phys. **48**, 033302 (2007).
[15] H. D. Cornean, H. Neidhardt and V. Zagrebnov, Ann. Henri Poincaré **10**, 61 (2009).
[16] H. D. Cornean, C. Gianesello and V. Zagrebnov, J. Phys. A: Math. Theor. **43**, 474011 (2010).
[17] D. Ruelle, J. Stat. Phys. **98**, 57 (2000).
[18] J. Fröhlich, M. Merkli and D. Ueltschi, Ann. Henri Poincaré **4**, 897 (2003).
[19] V. Jakšić and C.-A. Pillet, J. Stat. Phys. **108**, 787 (2002).
[20] W. Aschbacher, V. Jakšić, Y. Pautrat and C.-A. Pillet, in *Open Quantum Systems III*, Lecture Notes in Mathematics **1882**, Springer, New York, (2006).
[21] V. Jakšić, Y. Ogata and C.-A. Pillet, Ann. Henri Poincaré **8**, 1013 (2007).
[22] V. Jakšić, Y. Pautrat and C.-A. Pillet, Commun. Math. Phys. **285**, 175 (2009).
[23] H. D. Cornean, V. Moldoveanu and C.-A. Pillet, in preparation.
[24] A. L. Fetter, J. D. Walecka: *Quantum theory of many-particle systems* (Dover Publications, 2003).
[25] H. D. Cornean, A. Jensen, V. Moldoveanu, J. Math. Phys. **46**, 042106 (2005).
[26] G. Stefanucci, Phys. Rev. B **75**, 195115 (2007).
[27] H.D. Cornean, V. Moldoveanu, J. Phys. A: Math. Theor. **44**, 305002 (2011).