A mathematical account of the NEGF formalism

Horia Decebal Cornean, Valeriu Moldoveanu, Claude-Alain Pillet

A mathematical account of the NEGF formalism

H.D. CORNEAN[1], V. MOLDOVEANU[2], C.-A. PILLET[3]

[1]Department of Mathematical Sciences
Aalborg University
Fredrik Bajers Vej 7G, 9220 Aalborg, Denmark

[2]National Institute of Materials Physics
P.O. Box MG-7 Bucharest-Magurele, Romania

[3] Aix Marseille Univ, Université de Toulon, CNRS, CPT, Marseille, France

Abstract. The main goal of this paper is to put on solid mathematical grounds the so-called Non-Equilibrium Green's Function (NEGF) transport formalism for open systems. In particular, we derive the Jauho-Meir-Wingreen formula for the time-dependent current through an interacting sample coupled to non-interacting leads. Our proof is non-perturbative and uses neither complex-time Keldysh contours, nor Langreth rules of 'analytic continuation'. We also discuss other technical identities (Langreth, Keldysh) involving various many body Green's functions. Finally, we study the Dyson equation for the advanced/retarded interacting Green's function and we rigorously construct its (irreducible) self-energy, using the theory of Volterra operators.

1 Introduction

The computation of Green's functions (GFs) associated to interacting many-body quantum systems is one of the most fruitful and challenging problems in theoretical condensed matter physics. Among many applications of Green's functions techniques let us mention the linear response to an adiabatically switched perturbation (e.g. an external electric field or electron–electron interactions) which is embodied in a single or two-particle GF. Also, the equilibrium properties of an interacting system can be studied in the framework of the finite-temperature (Matsubara) formalism. The great advantage of GFs is that they can be obtained from perturbative approximations which satisfactorily capture plenty of physical phenomena. In some sense they are much simpler objects than N-particle wavefunctions which are difficult to compute even with the currently available hardware. It was already clear in the early '60s that non-equilibrium regimes cannot be described within ground-state perturbation theory based on the Gell-Mann and Low Theorem [GML] as the system does not return to the same initial state after the external driving is turned off.

In spite of this difficulty considerable efforts were spent to adapt the very appealing and successful diagrammatic expansion of the ground-state GF (see, e.g., [FW]) to the non-equilibrium setting and in particular to transport calculations for open quantum systems. The resulting theory of non-equilibrium Green's functions (NEGFs) nowadays surpasses in predictive power quantum kinetic (Boltzmann) equations[1], Kubo-Greenwood

[1]The Kadanoff-Baym equations lead to the Boltzmann equation under appropriate assumptions, see the review [Da].

formulas [Ku] and the Landauer-Büttiker approach to coherent transport (see, e.g., [Im]). Although the NEGF formalism was proposed and developed in the '60s by several authors [Sc, KB, Ke, Fu, Cr] to the best of our knowledge a review has not been available until '84 [Da]. Also, the first application of the Keldysh formalism to a transport problem has been presented in a series of papers by Caroli et al. [Ca1, Ca2, Co, Ca3]. It is interesting to note that in their first paper the authors introduced the partitioning transport setting which is nowadays standard textbook material (the setting will be described in the next section). The real breakthrough of the non-equilibrium GFs method to transport problems is due to Meir and Wingreen [MW]. They proposed a closed formula for the steady-state current across an interacting region which was then extended to the transient regime [JWM].

Given the fact that in the non-interacting case the single-particle GF reduces to the resolvent of the full Hamiltonian which can either be computed in perturbation theory or related to scattering theory, it is not surprising that some aspects of Green's functions methods have been also addressed from the mathematical point of view. Two such examples are the Green-Kubo formulation of linear response theory and the Landauer-Büttiker approach to coherent transport in mesoscopic systems. Both methods were rigorously established for independent electron (i.e., quasi-free) models with discrete and continuous geometries [AH, AP, AJPP2, BP, CJM, CDNP, N].

In the interacting case, and more generally for non quasi-free dynamics, mathematical constructions of current carrying steady states have been obtained within the perturbative approach [FMU, JP1, AJPP1, MMS]. The linear response theory of these nonequilibrium steady states (NESS) is also well understood at the mathematical level [JOP1, JOP2, JOP3]. Using the scattering theoretical approach developed in these works, we have recently obtained steady-states limits of the two-point GFs of an open mesoscopic sample [CMP1, CMP2, CM] for various, partitioning and non-partitioning protocols. We have also presented an alternative perturbative formula for the steady-state current and established the independence of the steady-state quantities on the initial state of the sample.

As a natural continuation of these results the present work aims at providing the first rigorous account of the Keldysh-Green's functions machinery which is rather inaccessible to the mathematical community in its original formulation. Indeed, for a beginner or a mathematically oriented reader the first unfamiliar technical object of the NEGF formalism is quite its starting point: the famous Keldysh contour introduced along with its associated countour-ordering operator which replaces the time-ordering operator of the equilibrium theory. In the simplest version of the theory (i.e., if the initial correlations are neglected) the contour runs from some initial time t_0 where the system is still in an *equilibrium* state to some later time t and then back to t_0. This unusual choice becomes even stranger when one adds a misleading picture in which the contour is slightly extended to the complex plane. If the initial state is correlated the Keldysh contour has an additional complex (Matsubara) 'hook' ($t \in [t_0 - \mathrm{i}\beta, t_0]$). Let us emphasize that this construction plays a crucial role in transport calculations where one uses formal identities for GFs whose time variables are seen on different 'branches' of the Keldysh contour.

If one carefully follows the development of the many-body perturbative approaches, *the only* 'raison d'être' of the Keldysh contour is quickly unraveled: it provides a systematic and convenient way to order time arguments of complicated products of interaction picture operators on the chronological (from t_0 to t) and anti-chronological (from t to t_0) time branches. These products appear naturally in the statistical average of a given observable in the non-equilibrium regime. A nice discussion on this point can be found in the review by Danielewicz [Da]. Moreover, a compact form amenable to a diagrammatic analysis via the Wick theorem is achieved by introducing contour-ordered GFs, the latter being nothing but Keldysh GFs. To sum up, the Keldysh contour helps one to reveal the formal analogy between the equilibrium many-body perturbation theory and the non-equilibrium one. Nevertheless, it is rather unfortunate that in order to study the non-equilibrium, one has to be familiar to the ground-state perturbation theory, Matsubara Green's functions, real-time GFs and so on [MSSL, Ne, ND, NDG, FVA]. According to a recent point of view [SvL], the non-equilibrium many-body perturbation formalism is the first one to be learned, the other ones being derived from it as simplified versions.

In our paper we establish a 'contour-free' viewpoint of the NEGF formalism. A certain advantage of this approach is that a mathematically oriented reader can get to the JMW formula without an a priori knowledge of many-body theory or Feynman diagrams. On the other hand, it should not come as a surprise that the non-equilibrium transport can be formulated without contour-ordered quantities given the fact that the seminal work of Kadanoff and Baym [KB] is written down only in terms of retarded/advanced and correlation GFs.

The paper is organized as follows:

- After this Introduction we continue with a description of the setting in Section 2. We are only dealing with discrete, partitioned systems; the partition-free case [SA] will be treated elsewhere. Note that we work right from the beginning at the thermodynamic limit, the only important properties of the reference state being the KMS property and gauge-invariance (i.e. it 'commutes' with the number operator).
- In Section 3 we introduce the NEGFs and we formulate our main results. Sections 4 and 5 contain all the proofs. Section 6 concludes the paper and lists some open problems. In the Appendix we prove a positivity lemma related to the dissipative properties of the retarded interacting GF.
- While in this work we shall use standard quantities (lesser, retarded/advanced GFs) and tools (Wick theorem, Dyson equation) from many-body perturbation theory, our proofs *do not* require two essential ingredients of the Keldysh formalism: the contour-ordering operator and the so called 'analytic continuation' Langreth rules [La, HJ]. Although a significant number of papers in the physical literature confirm the usefulness of these methods in specific calculations based on diagrammatic expansion, our approach shows that they are not mandatory for the study of non-equilibrium transport. In fact we are able to provide in Theorem 3.1 the first rigorous proof of the probably most famous by-product of the NEGF formalism, namely the Jauho-Meir-Wingreen (JMW) [JWM] formula for the time-dependent current through an interacting quantum dot without using contour-ordered GFs and Langreth rules; the only technical ingredients we need are the well known KMS condition (2.3) and the Duhamel identity (4.1). Along the way we also present 'contourless' derivations of the Langreth rules and of the Keldysh equation for the lesser Green's function.
- The JMW formula only involves lesser and retarded interacting GFs restricted to the small sample. When the restriction to the small sample of the initial state is the vacuum, we show in Proposition 3.6 how to express lesser GFs in terms of non-interacting advanced/retarded GFs and a lesser self-energy, which in principle can be computed in all orders of the interaction.
- Our final result, Proposition 3.7, is a rigorous formulation of a Dyson equation for the interacting advanced/retarded GFs, using the theory of Volterra operators. In the proof of Lemma 5.1 we also describe how one can compute the self-energy in any order of the interaction and we explicitly identify its leading terms.

Acknowledgments. The idea of a rigorous mathematical approach to the NEGF formalism appeared more than ten years ago, catalyzed by lively discussions with, among others, N. Angelescu, J. Dereziński, P. Duclos, P. Gartner, V. Jakšić, G. Nenciu, G. Stefanucci, and V. Zagrebnov. Financial support by Grant 4181-00042 of the Danish Council for Independent Research | Natural Sciences is gratefully acknowledged. The work of CAP was partly funded by Excellence Initiative of Aix-Marseille University-A*MIDEX, a French "Investissements d'Avenir" program. VM acknowledges financial support by the CNCS-UEFISCDI grant PN-III-P4-ID-PCE-2016-0221.

2 The model

In order to avoid technicalities which would only obscure the exposition we restrict ourselves to a simple model of a discrete sample $\mathscr{S}$ coupled to a finite collection of reservoirs $\mathscr{R}$ of spinless electrons within the partitioning

scenario used in our previous work [CMP2]. In this section, we briefly recall this setup and refer the reader to [CMP2] for a detailed discussion and results pertaining to the existence of steady states in this model.

2.1 The one-particle setup

Our main object of interest is a Fermi gas on a discrete structure $\mathscr{S}+\mathscr{R}$ (e.g., an electronic system in the tight-binding approximation). There, $\mathscr{S}$ is a finite set describing a confined sample and $\mathscr{R}=\mathscr{R}_1+\cdots+\mathscr{R}_m$ is a collection of infinitely extended reservoirs (or leads) which feed the sample $\mathscr{S}$.

The one-particle Hilbert space of the compound system is

$$\mathfrak{h}=\mathfrak{h}_{\mathscr{S}}\oplus\mathfrak{h}_{\mathscr{R}},\qquad \mathfrak{h}_{\mathscr{R}}=\oplus_{j=1}^{m}\mathfrak{h}_j,$$

where $\mathfrak{h}_{\mathscr{S}}=\ell^2(\mathscr{S})$ and $\mathfrak{h}_j$ is the Hilbert space of the j^{th} reservoir. Let $h_{\mathscr{S}}$, a self-adjoint operator on $\mathfrak{h}_{\mathscr{S}}$, be the one-particle Hamiltonian of the isolated sample. Denote by h_j the Hamiltonian of the j^{th} reservoir. The one-particle Hamiltonian of the decoupled system is

$$h_{\mathrm{D}}=h_{\mathscr{S}}\oplus h_{\mathscr{R}},\qquad h_{\mathscr{R}}=\oplus_{j=1}^{m}h_j.$$

The coupling of the sample to the reservoirs is achieved by the tunneling Hamiltonian

$$h_{\mathrm{T}}=\sum_{j=1}^{m}d_j\left(|\psi_j\rangle\langle\phi_j|+|\phi_j\rangle\langle\psi_j|\right),$$

where $\psi_j\in\mathfrak{h}_j$ and $\phi_j\in\mathfrak{h}_{\mathscr{S}}$ are unit vectors and $d_j\in\mathbb{R}$ a coupling constant. The one-particle Hamiltonian of the fully coupled system is

$$h=h_{\mathrm{D}}+h_{\mathrm{T}}.$$

In the following, we will denote by $1_{j/\mathscr{S}/\mathscr{R}}$ the orthogonal projection acting on the one-particle Hilbert space $\mathfrak{h}$ with range $\mathfrak{h}_{j/\mathscr{S}/\mathscr{R}}$.

2.2 The many-body setup

We shall now describe the Fermi gas associated with the one-particle model introduced previously and extend this model by adding many-body interactions between the particles in the sample $\mathscr{S}$. In order to fix our notation and make contact with the one used in the physics literature let us recall some basic facts. We refer to [BR2] for details on the algebraic framework of quantum statistical mechanics that we use here.

$\Gamma_-(\mathfrak{h})$ denotes the fermionic Fock space over $\mathfrak{h}$ and $\Gamma_-^{(n)}(\mathfrak{h})=\mathfrak{h}^{\wedge n}$, the n-fold completely antisymmetric tensor power of $\mathfrak{h}$, is the n-particle sector of $\Gamma_-(\mathfrak{h})$. For $f\in\mathfrak{h}$, let $a(f)/a^*(f)$ be the annihilation/creation operator on $\Gamma_-(\mathfrak{h})$. In the following $a^\#$ stands for either a or a^*. The map $f\mapsto a^*(f)$ is linear while $f\mapsto a(f)$ is anti-linear, both maps being continuous, $\|a^\#(f)\|=\|f\|$. The underlying algebraic structure is characterized by the canonical anti-commutation relations (CAR for short)

$$\{a(f),a^*(g)\}=\langle f|g\rangle\mathbb{1},\qquad \{a(f),a(g)\}=0, \tag{2.1}$$

and we denote by $\mathrm{CAR}(\mathfrak{h})$ the C^*-algebra generated by $\{a^\#(f)\,|\,f\in\mathfrak{h}\}$, i.e., the norm closure of the set of polynomials in the operators $a^\#(f)$. Note that if $\mathfrak{g}\subset\mathfrak{h}$ is a subspace, then we can identify $\mathrm{CAR}(\mathfrak{g})$ with a subalgebra of $\mathrm{CAR}(\mathfrak{h})$.

The second quantization of a unitary operator u on $\mathfrak{h}$ is the unitary $\Gamma(u)$ on $\Gamma_-(\mathfrak{h})$ acting as $u\otimes u\otimes\cdots\otimes u$ on $\Gamma_-^{(n)}(\mathfrak{h})$. The second quantization of a self-adjoint operator q on $\mathfrak{h}$ is the self-adjoint generator $\mathrm{d}\Gamma(q)$ of the

strongly continuous unitary group $\Gamma(\mathrm{e}^{\mathrm{i}tq})$, i.e., $\Gamma(\mathrm{e}^{\mathrm{i}tq}) = \mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma(q)}$. If $\{f_\iota\}_{\iota\in I}$ is an orthonormal basis of $\mathfrak{h}$ and q a bounded self-adjoint operator, then

$$\mathrm{d}\Gamma(q) = \sum_{\iota,\iota'\in I} \langle f_\iota | q | f_{\iota'}\rangle\, a^*(f_\iota) a(f_{\iota'}),$$

holds on $\Gamma_-(\mathfrak{h})$. If q is trace class (in particular, if q is finite rank), then $\mathrm{d}\Gamma(q)$ is bounded and belongs to $\mathrm{CAR}(\mathfrak{h})$.

A unitary operator u on $\mathfrak{h}$ induces a Bogoliubov automorphism of $\mathrm{CAR}(\mathfrak{h})$

$$A \mapsto \gamma_u(A) = \Gamma(u) A \Gamma(u)^*,$$

such that $\gamma_u(a^\#(f)) = a^\#(uf)$. If $t \mapsto u_t$ is a strongly continuous family of unitary operators on $\mathfrak{h}$, then $t \mapsto \gamma_{u_t}$ is a strongly continuous family of Bogoliubov automorphisms of $\mathrm{CAR}(\mathfrak{h})$. In particular, if $u_t = \mathrm{e}^{\mathrm{i}tp}$ for some self-adjoint operator p on $\mathfrak{h}$, we call γ_{u_t} the quasi-free dynamics generated by p.

The quasi-free dynamics generated by the identity I is the gauge group of $\mathrm{CAR}(\mathfrak{h})$ and $N = \mathrm{d}\Gamma(I)$ is the number operator on $\Gamma_-(\mathfrak{h})$,

$$\vartheta^t(a^\#(f)) = \mathrm{e}^{\mathrm{i}tN} a^\#(f) \mathrm{e}^{-\mathrm{i}tN} = a^\#(\mathrm{e}^{\mathrm{i}t} f) = \begin{cases} \mathrm{e}^{-\mathrm{i}t} a(f) & \text{for } a^\# = a; \\ \mathrm{e}^{\mathrm{i}t} a^*(f) & \text{for } a^\# = a^*. \end{cases}$$

The algebra of observables of the Fermi gas is the gauge-invariant subalgebra of $\mathrm{CAR}(\mathfrak{h})$,

$$\mathrm{CAR}_\vartheta(\mathfrak{h}) = \{A \in \mathrm{CAR}(\mathfrak{h}) \,|\, \vartheta^t(A) = A \text{ for all } t \in \mathbb{R}\}.$$

It is the C^*-algebra generated by the set of all monomials in the $a^\#$ containing an equal number of a and a^* factors. In particular, it is contained in the so-called even part of $\mathrm{CAR}(\mathfrak{h})$ which consists of all elements invariant under the involutive morphism Θ which maps $a^\#(f)$ to $-a^\#(f)$.

2.2.1 Locally interacting dynamics

The quasi-free dynamics generated by h describes the sample coupled to the leads and $H = \mathrm{d}\Gamma(h)$ is the corresponding many-body Hamiltonian

$$\tau_H^t(a^\#(f)) = \mathrm{e}^{\mathrm{i}tH} a^\#(f) \mathrm{e}^{-\mathrm{i}tH} = a^\#(\mathrm{e}^{\mathrm{i}th} f).$$

The group τ_H commutes with the gauge group ϑ so that it leaves $\mathrm{CAR}_\vartheta(\mathfrak{h})$ invariant. In the following, we shall consistently denote one-particle operators with lower-case letters and capitalize the corresponding second quantized operator, e.g., $H_\mathscr{S} = \mathrm{d}\Gamma(h_\mathscr{S})$, $H_\mathscr{R} = \mathrm{d}\Gamma(h_\mathscr{R})$, etc. We shall also denote the corresponding groups of automorphism by $\tau_{H_\mathscr{S}}$, $\tau_{H_\mathscr{R}}$, etc.

For $x \in \mathscr{S}$ we denote by $|x\rangle = \delta_x \in \mathfrak{h}_\mathscr{S}$ the Kronecker delta at x and by $a_x^\# = a^\#(\delta_x)$ the corresponding creation/annihilation operators. We allow for interactions between particles in the sample $\mathscr{S}$. However, particles in the leads remain free. The interaction energy within the sample is described by

$$W = \frac{1}{2} \sum_{x,y\in\mathscr{S}} w(x,y) N_x N_y.$$

where $N_x = a_x^* a_x$ and w is a two-body potential satisfying $w(x,y) = w(y,x) \in \mathbb{R}$ and $w(x,x) = 0$ for all $x, y \in \mathscr{S}$. For normalization purposes, we also assume that $\sup_{x,y\in\mathscr{S}} |w(x,y)| = 1$. For any self-adjoint $W \in \mathrm{CAR}_\vartheta(\mathfrak{h})$ and any value of the interaction strength $\xi \in \mathbb{R}$ the operator

$$K = H + \xi W,$$

is self-adjoint on the domain of H. Moreover $\tau_K^t(A) = \mathrm{e}^{\mathrm{i}tK} A \mathrm{e}^{-\mathrm{i}tK}$ defines a strongly continuous group of $*$-automorphisms of CAR($\mathfrak{h}$) leaving invariant the subalgebra CAR$_\vartheta(\mathfrak{h})$. This group describes the full dynamics of the Fermi gas, including interactions. Another important operator is

$$K_D = H_{\mathscr{S}} + \xi W + H_{\mathscr{R}},$$

which describes the dynamics of the interacting but uncoupled system. Note that $K = K_D + H_T$.

2.2.2 States of the Fermi gas

A state on CAR($\mathfrak{h}$) is a linear functional

$$\mathrm{CAR}(\mathfrak{h}) \ni A \mapsto \langle A \rangle \in \mathbb{C},$$

such that $\langle A^* A \rangle \geq 0$ for all A and $\langle \mathbb{1} \rangle = 1$. A state is gauge-invariant if $\langle \vartheta^t(A) \rangle = \langle A \rangle$ for all $t \in \mathbb{R}$. Note that if $\langle \cdot \rangle$ is a state on CAR($\mathfrak{h}$) then its restriction to CAR$_\vartheta(\mathfrak{h})$ defines a state on this subalgebra. We shall use the same notation for this restriction.

A state $\langle \cdot \rangle$ on CAR($\mathfrak{h}$) induces a GNS representation $(\mathscr{H}, \pi, \Omega)$ where $\mathscr{H}$ is a Hilbert space, π is a $*$-morphism from CAR($\mathfrak{h}$) to the bounded linear operators on $\mathscr{H}$ and $\Omega \in \mathscr{H}$ is a unit vector such that $\pi(\mathrm{CAR}(\mathfrak{h}))\Omega$ is dense in $\mathscr{H}$ and $\langle A \rangle = (\Omega | \pi(A) \Omega)$ for all $A \in \mathrm{CAR}(\mathfrak{h})$. Let ρ be a density matrix on $\mathscr{H}$ (a non-negative, trace class operator with $\mathrm{tr}(\rho) = 1$). The map $A \mapsto \mathrm{tr}(\rho \pi(A))$ defines a state on CAR($\mathfrak{h}$). Such a state is said to be normal w.r.t. $\langle \cdot \rangle$. From the thermodynamical point of view $\langle \cdot \rangle$-normal states are close to $\langle \cdot \rangle$ and describe local perturbations of this state.

Given a self-adjoint operator ϱ on $\mathfrak{h}$ satisfying $0 \leq \varrho \leq I$, the formula

$$\langle a^*(f_1) \cdots a^*(f_k) a(g_l) \cdots a(g_1) \rangle_\varrho = \delta_{kl} \det\{\langle g_j | \varrho | f_i \rangle\},$$

defines a unique gauge-invariant state on CAR($\mathfrak{h}$). This state is called the quasi-free state of density ϱ. It is uniquely determined by the two point function $\langle a^*(f) a(g) \rangle_\varrho = \langle g | \varrho | f \rangle$. An alternative characterization of quasi-free states on CAR($\mathfrak{h}$) is the usual fermionic Wick theorem

$$\langle \varphi(f_1) \cdots \varphi(f_k) \rangle_\varrho = \begin{cases} 0, & \text{if } k \text{ is odd;} \\ \displaystyle\sum_{\pi \in \mathscr{P}_k} \varepsilon(\pi) \prod_{j=1}^{k/2} \langle \varphi(f_{\pi(2j-1)}) \varphi(f_{\pi(2j)}) \rangle_\varrho, & \text{if } k \text{ is even;} \end{cases}$$

where $\varphi(f) = 2^{-1/2}(a^*(f) + a(f))$ is the field operator, $\mathscr{P}_k$ denotes the set of pairings of k objects, i.e., permutations satisfying $\pi(2j-1) < \min(\pi(2j), \pi(2j+1))$ for $j = 1, \ldots, k/2$, and $\epsilon(\pi)$ is the signature of the permutation π.

Given a strongly continuous group τ of $*$-automorphisms of CAR($\mathfrak{h}$) commuting with the gauge group ϑ, a state $\langle \cdot \rangle$ is a thermal equilibrium state at inverse temperature β and chemical potential μ if it satisfies the (β, μ)-KMS condition w.r.t. τ, i.e., if for any $A, B \in \mathrm{CAR}(\mathfrak{h})$ the function

$$F_{A,B}(s) = \langle A \tau^s \circ \vartheta^{-\mu s}(B) \rangle,$$

has an analytic continuation to the strip $\{0 < \mathrm{Im}\, s < \beta\}$ with a bounded continuous extension to the closure of this strip satisfying

$$F_{A,B}(s + \mathrm{i}\beta) = \langle \tau^s \circ \vartheta^{-\mu s}(B) A \rangle. \tag{2.2}$$

We shall say that such a state is a (β, μ)-KMS state for τ.

Remark 2.1. It is well known that for any $\beta > 0$ and $\mu \in \mathbb{R}$ the KMS states $\langle \cdot \rangle_H^{\beta,\mu}$ and $\langle \cdot \rangle_K^{\beta,\mu}$ are thermodynamic limits of the familiar grand canonical Gibbs states associated with the restrictions of the Hamiltonian H and K to finitely extended reservoirs with appropriate boundary conditions. See [BR2] for details.

2.2.3 The initial state

Let $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_m) \in \mathbb{R}_+^m$, $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_m) \in \mathbb{R}^m$ and denote by $\langle\cdot\rangle_{H_j}^{\beta_j,\mu_j}$ the unique (β_j, μ_j)-KMS state for τ_{H_j} on $\mathrm{CAR}(\mathfrak{h}_j)$. We say that a state $\langle\cdot\rangle$ on $\mathrm{CAR}(\mathfrak{h})$ is $(\boldsymbol{\beta}, \boldsymbol{\mu})$-KMS if it is a product state extension of the $\langle\cdot\rangle_{H_j}^{\beta_j,\mu_j}$ and some gauge-invariant state $\langle\cdot\rangle_{\mathscr{S}}$ on $\mathrm{CAR}(\mathfrak{h}_{\mathscr{S}})$, i.e., if

$$\langle A_1 A_2 \cdots A_m A_{\mathscr{S}}\rangle = \langle A_{\mathscr{S}}\rangle_{\mathscr{S}} \prod_{j=1}^{m} \langle A_j\rangle_{H_j}^{\beta_j,\mu_j}$$

holds for all $A_j \in \mathrm{CAR}(\mathfrak{h}_j)$ and $A_{\mathscr{S}} \in \mathrm{CAR}(\mathfrak{h}_{\mathscr{S}})$. We note that given a state $\langle\cdot\rangle_{\mathscr{S}}$ on $\mathrm{CAR}(\mathfrak{h}_{\mathscr{S}})$, such a product state extension exists and is unique (see [AM]). It describes a sample $\mathscr{S}$ whose state $\langle\cdot\rangle_{\mathscr{S}}$ is unentangled from the reservoirs which are all in thermal equilibrium. In particular, a $(\boldsymbol{\beta}, \boldsymbol{\mu})$-KMS state needs not be quasi-free. We shall need the following extension of the KMS condition (2.2) which follows from the CAR (2.1), the linearity, continuity and gauge invariance of states, the totality of monomials of the form $A_1 \cdots A_m A_{\mathscr{S}}$ with $A_j \in \mathrm{CAR}(\mathfrak{h}_j)$ and $A_{\mathscr{S}} \in \mathrm{CAR}(\mathfrak{h}_{\mathscr{S}})$ in $\mathrm{CAR}(\mathfrak{h})$, and the KMS condition (2.2): For any $A \in \mathrm{CAR}(\mathfrak{h})$ and $B \in \mathrm{CAR}(\mathfrak{h}_j)$ the function

$$F_{A,B}(s) = \langle A\tau_{H_j}^s \circ \vartheta^{-\mu_j s}(B)\rangle$$

has an analytic extension to the strip $\{0 < \mathrm{Im}\, s < \beta_j\}$ with a bounded continuous extension to the closure of this strip satisfying $F_{A,B}(s + \mathrm{i}\beta_j) = \langle \tau_{H_j}^s \circ \vartheta^{-\mu_j s}(B) A\rangle$ or

$$\langle A\tau_{H_j}^s \circ \vartheta^{-\mu_j s}(B)\rangle = \langle \tau_{H_j}^{s-\mathrm{i}\beta_j} \circ \vartheta^{-\mu_j (s-\mathrm{i}\beta_j)}(B) A\rangle$$

for all $s \in \mathbb{R}$. In particular, when $s = 0$, for any $A \in \mathrm{CAR}(\mathfrak{h})$ and $B = a^{\#}(f)$ with $f \in \mathfrak{h}_j$ we have the identity:

$$\langle A\, a^{\#}(f)\rangle = \langle a^{\#}(\mathrm{e}^{\beta_j(h_j - \mu_j)} f)\, A\rangle. \tag{2.3}$$

We also set

$$\varrho_{\mathscr{R}}^{\boldsymbol{\beta},\boldsymbol{\mu}} := \bigoplus_j \left(I + \mathrm{e}^{\beta_j(h_j - \mu_j)}\right)^{-1}, \tag{2.4}$$

which can also be seen as an operator on the whole $\mathfrak{h}$ by extending it by zero on $\mathfrak{h}_S$.

3 Main results

In this section we introduce the main objects of interest for the NEGFs machinery and we state our main results.

3.1 Retarded and advanced Green's Functions

For motivation purposes, let us first consider the non-interacting case, i.e., set $\xi = 0$. The one-body wave function then satisfies the Schrödinger equation

$$\mathrm{i}\partial_t \varphi(t) = h\varphi(t),$$

and the associated Cauchy problem with initial condition $\varphi(t_0) = \varphi_0 \in \mathfrak{h}$ is solved by the unitary propagator $\varphi(t) = \mathrm{e}^{-\mathrm{i}(t-t_0)h}\varphi_0$. In order to study the response of the system to time-dependent perturbations one investigates the corresponding inhomogeneous equation

$$(\mathrm{i}\partial_s - h)\varphi(s) = \psi(s).$$

To deal with perturbations that are localized in time, it makes sense to consider this equation in the Hilbert space $\mathscr{H} = L^2(\mathbb{R}, \mathrm{d}s; \mathfrak{h})$. The Fourier transform

$$\hat{\varphi}(\omega) = \int_{\mathbb{R}} \varphi(s) \mathrm{e}^{-\mathrm{i}\omega s} \mathrm{d}s,$$

maps the time-domain Hilbert space $\mathscr{H}$ unitarily onto the frequency-domain Hilbert space $L^2(\mathbb{R}, \frac{\mathrm{d}\omega}{2\pi}; \mathfrak{h})$ in such a way that

$$((\mathrm{i}\partial_s - h)\varphi)\hat{}(\omega) = (-\omega - h)\hat{\varphi}(\omega).$$

Thus, the operator $\Omega = \mathrm{i}\partial_s - h$, with domain

$$\mathscr{H}^1 = H^1(\mathbb{R}, \mathrm{d}s; \mathfrak{h}) = \{\varphi \in \mathscr{H} \,|\, \|\varphi\|_1 = \|\sqrt{1+\omega^2}\hat{\varphi}\| < \infty\} \tag{3.1}$$

is self-adjoint on $\mathscr{H}$. Its spectrum fills the real axis and a simple calculation shows that the unitary group it generates is given by

$$(\mathrm{e}^{\mathrm{i}t\Omega}\varphi)(s) = \mathrm{e}^{-\mathrm{i}th}\varphi(s-t).$$

It follows that for $z \in \mathbb{C}_\pm = \{z \in \mathbb{C} \,|\, \pm \mathrm{Im}\, z > 0\}$ the resolvent

$$G_0^\pm(z) = (\Omega - z)^{-1} = \pm\mathrm{i}\int_{\mathbb{R}_\pm} \mathrm{e}^{-\mathrm{i}t(\Omega - z)} \mathrm{d}t,$$

has the time-domain expression

$$(G_0^\pm(z)\varphi)(s) = \pm\mathrm{i}\int_{\mathbb{R}} \theta(\pm(s'-s)) \mathrm{e}^{\mathrm{i}(s'-s)(h+z)}\varphi(s')\mathrm{d}s', \tag{3.2}$$

where θ denotes Heaviside step function.

We set $\mathbb{R}_\pm = \{s \in \mathbb{R} \,|\, \pm s > 0\}$ and observe that the boundary values $G_0^\pm(E) = G_0(E \pm \mathrm{i}0)$ are well defined as operators on the Fréchet space $\mathscr{H}_{\mathrm{loc}\mp} = L^2_{\mathrm{loc}}(\mathbb{R}_\mp, \mathrm{d}s; \mathfrak{h})$, with the semi-norm estimate

$$\|G_0^\pm(E)\varphi\|_T \leq T\|\varphi\|_T,$$

where $\|\varphi\|_T^2 = \int_0^T \|\varphi(\mp s)\|^2 \mathrm{d}s$. The 'integral kernel' of the operator $G_0^\mp(E) : \mathscr{H}_{\mathrm{loc}\pm} \to \mathscr{H}_{\mathrm{loc}\pm}$ is called retarded/advanced Green's function. In the physics literature it is usually denoted by $G_0^R(E|s,s')/G_0^A(E|s,s')$ or simply $G_0^R(s,s')/G_0^A(s,s')$ in the special case $E = 0$. Observing that for $f, g \in \mathfrak{h}$

$$\begin{aligned}
\langle f|G_0^R(E|s,s')|g\rangle &= -\mathrm{i}\theta(s-s')\mathrm{e}^{\mathrm{i}(s'-s)E}\left\langle\left\{\tau_H^{s'}(a^*(g)), \tau_H^s(a(f))\right\}\right\rangle,\\
\langle f|G_0^A(E|s,s')|g\rangle &= +\mathrm{i}\theta(s'-s)\mathrm{e}^{\mathrm{i}(s'-s)E}\left\langle\left\{\tau_H^{s'}(a^*(g)), \tau_H^s(a(f))\right\}\right\rangle,
\end{aligned}$$

leads to the definition of the retarded/advanced interacting Green's function

$$\begin{aligned}
\langle f|G^R(E|s,s')|g\rangle &:= -\mathrm{i}\theta(s-s')\mathrm{e}^{\mathrm{i}(s'-s)E}\left\langle\left\{\tau_K^{s'}(a^*(g)), \tau_K^s(a(f))\right\}\right\rangle,\\
\langle f|G^A(E|s,s')|g\rangle &:= +\mathrm{i}\theta(s'-s)\mathrm{e}^{\mathrm{i}(s'-s)E}\left\langle\left\{\tau_K^{s'}(a^*(g)), \tau_K^s(a(f))\right\}\right\rangle.
\end{aligned} \tag{3.3}$$

The decoupled retarded/advanced Green's function $G_D^{A/R}$ are defined similarly by replacing τ_K by τ_{K_D} in (3.3). We observe that for $f, g \in \mathfrak{h}_{\mathscr{R}}$, the CAR and the fact that there is no interaction in the reservoirs imply that

$$\begin{aligned}
\langle f|G_D^R(s,s')|g\rangle &= -\mathrm{i}\theta(s-s')\langle f|\mathrm{e}^{\mathrm{i}(s'-s)h_{\mathscr{R}}}|g\rangle,\\
\langle f|G_D^A(s,s')|g\rangle &= +\mathrm{i}\theta(s'-s)\langle f|\mathrm{e}^{\mathrm{i}(s'-s)h_{\mathscr{R}}}|g\rangle.
\end{aligned}$$

3.2 Other Green's Functions

For $s, s' \geq 0$ and $f, g \in \mathfrak{h}$, the interacting 'lesser' and 'greater' Green's functions are defined by

$$\begin{aligned} \langle f|G^<(s,s')|g\rangle &:= +\mathrm{i}\left\langle \tau_K^{s'}(a^*(g))\tau_K^{s}(a(f))\right\rangle, \\ \langle f|G^>(s,s')|g\rangle &:= -\mathrm{i}\left\langle \tau_K^{s}(a(f))\tau_K^{s'}(a^*(g))\right\rangle, \end{aligned} \tag{3.4}$$

and play an important role in the NEGF formalism. The decoupled 'lesser' and 'greater' Green's functions are obtained upon replacement of K by K_D in the above expressions. For $f, g \in \mathscr{H}_{\mathscr{R}}$, the fact that the restriction of the state $\langle\cdot\rangle$ to $\mathrm{CAR}(\mathfrak{h}_{\mathscr{R}})$ is the gauge-invariant quasi-free state with density $\varrho_{\mathscr{R}}^{\boldsymbol{\beta},\boldsymbol{\mu}}$ leads to the formulas

$$\begin{aligned} \langle f|G_D^<(s,s')|g\rangle &= +\mathrm{i}\langle f|\varrho_{\mathscr{R}}^{\boldsymbol{\beta},\boldsymbol{\mu}}\mathrm{e}^{\mathrm{i}(s'-s)h_{\mathscr{R}}}|g\rangle, \\ \langle f|G_D^>(s,s')|g\rangle &= -\mathrm{i}\langle f|(I-\varrho_{\mathscr{R}}^{\boldsymbol{\beta},\boldsymbol{\mu}})\mathrm{e}^{\mathrm{i}(s'-s)h_{\mathscr{R}}}|g\rangle. \end{aligned}$$

For completeness, let us mention two combinations of the 'lesser' and 'greater' Green's functions which also appear in the physics literature. We should not, however, use them in the following. The 'spectral function' is

$$\langle f|A(s,s')|g\rangle := \mathrm{i}\langle f|G^R(s,s') - G^A(s,s')|g\rangle = \mathrm{i}\langle f|G^>(s,s') - G^<(s,s')|g\rangle = \left\langle \left\{\tau_K^{s'}(a^*(g)), \tau_K^{s}(a(f))\right\}\right\rangle,$$

with the property that $A(t,t) = I$, while the 'Keldysh' Green's function is

$$\langle f|G^K(s,s')|g\rangle := \langle f|G^<(s,s') + G^>(s,s')|g\rangle = \left\langle \mathrm{i}\left[\tau_K^{s'}(a^*(g)), \tau_K^{s}(a(f))\right]\right\rangle.$$

3.3 The Jauho-Meir-Wingreen current formula

From Eq. (3.4) we see that the interacting lesser Green's function $G^<$ encodes all one-particle properties of the system. For example, the sample's particle density at time $t \geq 0$ is given by

$$\varrho(x,t) = \langle \tau_K^t(a_x^* a_x)\rangle = \mathrm{Im}\,\langle x|G^<(t,t)|x\rangle.$$

Computing the time derivative of the sample's particle number $N_{\mathscr{S}} = \mathrm{d}\Gamma(1_{\mathscr{S}})$ we obtain

$$\begin{aligned} \partial_t \tau_K^t(N_{\mathscr{S}}) = \tau_K^t(\mathrm{i}[K, N_{\mathscr{S}}]) = \tau_K^t(\mathrm{i}[H_T, N_{\mathscr{S}}]) \\ &= \sum_j d_j \tau_K^t(\mathrm{i}[\mathrm{d}\Gamma(|\phi_j\rangle\langle\psi_j| + |\psi_j\rangle\langle\phi_j|), \mathrm{d}\Gamma(1_{\mathscr{S}})]) \\ &= \sum_j d_j \tau_K^t(\mathrm{d}\Gamma(\mathrm{i}[|\phi_j\rangle\langle\psi_j| + |\psi_j\rangle\langle\phi_j|, 1_{\mathscr{S}}])) = \sum_j J_j(t) \end{aligned}$$

which allows us to identify the j^{th} term in the above sum

$$J_j(t) = \mathrm{i}d_j \tau_K^t\left(a^*(\psi_j)a(\phi_j) - a^*(\phi_j)a(\psi_j)\right),$$

with the particle current out of the j^{th} reservoir. Its expectation value in the initial state is

$$I_j(t) := \langle J_j(t)\rangle = d_j\left(\langle\phi_j|G^<(t,t)|\psi_j\rangle - \langle\psi_j|G^<(t,t)|\phi_j\rangle\right) = 2d_j\,\mathrm{Re}\,\langle\phi_j|G^<(t,t)|\psi_j\rangle, \tag{3.5}$$

where, in the last equality, we used the fact that $G^<(t,t)^* = -G^<(t,t)$. The main result of this paper is a rigorous proof of the JMW formula:

Theorem 3.1 (The Jauho-Meir-Wingreen formula)**.** *If the initial state $\langle\cdot\rangle$ is $(\boldsymbol{\beta},\boldsymbol{\mu})$-KMS, then the particle current out of the j^{th} reservoir at time $t>0$ is given by*

$$I_j(t) = -2d_j^2 \int_0^t \mathrm{d}s \int \mathrm{d}\nu_j(E)\, \mathrm{Im}\left\{ \mathrm{e}^{\mathrm{i}(t-s)E} \langle \phi_j | G^<(t,s) + G^R(t,s)[1+\mathrm{e}^{\beta_j(E-\mu_j)}]^{-1} | \phi_j \rangle \right\},$$

where ν_j denotes the spectral measure of h_j for the vector ψ_j.

Remark 3.2. The main feature of the JMW formula is that it only involves interacting Green functions restricted to the sample $\mathscr{S}$ (in spite of the fact that in (3.5) $\phi_j \in \mathfrak{h}_{\mathscr{S}}$ and $\psi_j \in \mathfrak{h}_j$). If one is interested in transient regimes, it seems that this formula is easier to deal with from a numerical point of view. But if one is interested in proving the convergence to a steady state value when $t\to\infty$, it is not very useful. Moreover, the JMW formula must be backed-up by systematic methods of calculating interacting GFs, which rely on Dyson equations and interaction self-energies.

Remark 3.3. Let $\tilde{\mathfrak{h}}_j \subset \mathfrak{h}_j$ denote the cyclic subspace of h_j generated by ψ_j, i.e., the smallest h_j-invariant closed subspace of $\mathfrak{h}_j$ containing ψ_j. Set $\tilde{\mathfrak{h}} = \mathfrak{h}_{\mathscr{S}} \oplus (\oplus_j)\tilde{\mathfrak{h}}_j$ and denote by $\tilde{\mathfrak{h}}^\perp$ the orthogonal complement of $\tilde{\mathfrak{h}}$ in $\mathfrak{h}$. Let $\mathscr{O}$ be the $*$-subalgebra of CAR($\mathfrak{h}$) generated by $\{a(f)\,|\,f\in\tilde{\mathfrak{h}}\}$. One easily checks that $\mathscr{O}$ is invariant under the groups ϑ and τ_K. By the exponential law for fermions (see, e.g., Section 3.4.3 in [DeGe]) there exists a unitary map $U:\Gamma_-(\mathfrak{h})\to\Gamma_-(\tilde{\mathfrak{h}})\otimes\Gamma_-(\tilde{\mathfrak{h}}^\perp)$ such that $Ua(f)U^* = a(f)\otimes I$ for $f\in\tilde{\mathfrak{h}}$. Identifying in this way $\mathscr{O}$ with CAR($\tilde{\mathfrak{h}}$) and noticing that $W\in\mathscr{O}$, one easily shows that the restriction of the group τ_K to $\mathscr{O}$ is the Heisenberg dynamics generated by $\tilde{K} = \mathrm{d}\Gamma(\tilde{h}) + \xi W$ where $\tilde{h}$ is the restriction of h to $\tilde{\mathfrak{h}}$. Thus, as far as the dynamics on $\mathscr{O}$ is concerned, we may assume w.l.o.g. that ψ_j is a cyclic vector for h_j. Going to the induced spectral representation, this means that $\mathfrak{h}_j = L^2(\mathbb{R},\mathrm{d}\nu_j(E))$ where ν_j (the spectral measure of h_j for ψ_j) is a probability measure, h_j is multiplication by E and ψ_j is the constant function $\psi_j(E)=1$.

Theorem 3.1 is a direct consequence of Eq. (3.5) and the next result.

Proposition 3.4 (The Langreth identity)**.** *Assume that the initial state $\langle\cdot\rangle$ is $(\boldsymbol{\beta},\boldsymbol{\mu})$-KMS. Then, the following identity holds for all $j\in\{1,\dots,m\}$ and $t,t'\geq 0$,*

$$\langle\phi_j|G^<(t,t')|\psi_j\rangle = d_j\int_0^\infty \langle\phi_j|\big(G^R(t,s)|\phi_j\rangle\langle\psi_j|G_D^<(s,t') + G^<(t,s)|\phi_j\rangle\langle\psi_j|G_D^A(s,t')\big)|\psi_j\rangle \mathrm{d}s. \tag{3.6}$$

Remark 3.5. One should compare our results with formulas (12.11), (12.19), (12.21) and (13.3) in [HJ]. Our formula (3.6) corresponds to (12.19) and (13.3) in [HJ]. Haug and Jauho derive these two formulas in two steps: first using Keldysh contours (see (12.18) in [HJ]) and after that a Langreth-type 'analytic continuation' in order to come back to 'normal' integrals.

3.4 A decoupling Keldysh-like identity

As one can see from the JMW formula, one is left with computing correlation functions between points both situated in the sample $\mathscr{S}$. From a mathematical point of view, this is as complicated as the original problem. Nevertheless, in the physics literature one tries to rewrite the interacting lesser functions in terms of retarded/advanced GFs which afterward can be numerically computed by solving Dyson type equations. The next proposition shows how this is done:

Proposition 3.6 (A decoupling Keldysh identity)**.** *If the initial state $\langle\cdot\rangle$ is $(\boldsymbol{\beta},\boldsymbol{\mu})$-KMS and if its restriction to* CAR($\mathfrak{h}_{\mathscr{S}}$) *is the vacuum state, then there exists a continuous function*

$$\mathbb{R}_+\times\mathbb{R}_+ \ni (s,s') \mapsto S^<(s,s') = \sum_{x,x'\in\mathscr{S}} |x\rangle S^<_{xx'}(s,s')\langle x'| \in \mathscr{B}(\mathfrak{h}_{\mathscr{S}})$$

such that

$$\langle\phi|G^<(t,t')|\phi'\rangle = \int_0^\infty \mathrm{d}s \int_0^\infty \mathrm{d}s' \, \langle\phi|G_0^R(t,s)S^<(s,s')G_0^A(s',t')|\phi'\rangle, \tag{3.7}$$

for $\phi,\phi' \in \mathfrak{h}_{\mathscr{S}}$ *and* $t,t' \geq 0$. *Moreover,*

$$S^<_{xx'}(s,s') = \mathrm{i}\langle \mathscr{T}^*_{x'}(s')\mathscr{T}_x(s)\rangle$$

where

$$\mathscr{T}_x(s) = a(\mathrm{e}^{\mathrm{i}sh_D}h_T\delta_x) + \xi\tau_K^s(a_xV_x).$$

and

$$V_x = \sum_{y\in\mathscr{S}} w(x,y)N_y.$$

As a function of the interaction strength ξ, $S^<(s,s')$ *is entire analytic. The first two terms of its expansion*

$$S^<(s,s') = \sum_{n\geq 0}\xi^n S^{<(n)}(s,s')$$

are given by (recall (2.4) for the definition of $\varrho_{\mathscr{R}}^{\boldsymbol{\beta},\boldsymbol{\mu}}$*):*

$$S^{<(0)}_{xx'}(s,s') = \mathrm{i}\langle x|h_T\mathrm{e}^{-\mathrm{i}sh_{\mathscr{R}}}\varrho_{\mathscr{R}}^{\boldsymbol{\beta},\boldsymbol{\mu}}\mathrm{e}^{\mathrm{i}s'h_{\mathscr{R}}}h_T|x'\rangle = \mathrm{i}\sum_j d_j^2\left(\int \frac{\mathrm{e}^{\mathrm{i}(s'-s)E}}{1+\mathrm{e}^{\beta_j(E-\mu_j)}}\mathrm{d}\nu_j(E)\right)\langle x|\phi_j\rangle\langle\phi_j|x'\rangle,$$

and

$$\begin{aligned}
S^{<(1)}_{xx'}(s,s') = \mathrm{i}\sum_{y\in\mathscr{S}}\Big[\;& w(x,y)\Big(\langle x|\mathrm{e}^{-\mathrm{i}sh}\varrho_{\mathscr{R}}^{\boldsymbol{\beta},\boldsymbol{\mu}}\mathrm{e}^{\mathrm{i}sh}|y\rangle\langle y|\mathrm{e}^{-\mathrm{i}sh}\varrho_{\mathscr{R}}^{\boldsymbol{\beta},\boldsymbol{\mu}}\mathrm{e}^{\mathrm{i}s'h_{\mathscr{R}}}h_T|x'\rangle \\
&\quad -\langle x|\mathrm{e}^{-\mathrm{i}sh}\varrho_{\mathscr{R}}^{\boldsymbol{\beta},\boldsymbol{\mu}}\mathrm{e}^{\mathrm{i}s'h_{\mathscr{R}}}h_T|x'\rangle\langle y|\mathrm{e}^{-\mathrm{i}sh}\varrho_{\mathscr{R}}^{\boldsymbol{\beta},\boldsymbol{\mu}}\mathrm{e}^{\mathrm{i}sh}|y\rangle\Big) \\
&+ w(x',y)\Big(\langle x|h_T\mathrm{e}^{-\mathrm{i}sh_{\mathscr{R}}}\varrho_{\mathscr{R}}^{\boldsymbol{\beta},\boldsymbol{\mu}}\mathrm{e}^{\mathrm{i}s'h}|y\rangle\langle y|\mathrm{e}^{-\mathrm{i}s'h}\varrho_{\mathscr{R}}^{\boldsymbol{\beta},\boldsymbol{\mu}}\mathrm{e}^{\mathrm{i}s'h}|x'\rangle \\
&\quad -\langle x|h_T\mathrm{e}^{-\mathrm{i}sh_{\mathscr{R}}}\varrho_{\mathscr{R}}^{\boldsymbol{\beta},\boldsymbol{\mu}}\mathrm{e}^{\mathrm{i}s'h}|x'\rangle\langle y|\mathrm{e}^{-\mathrm{i}s'h}\varrho_{\mathscr{R}}^{\boldsymbol{\beta},\boldsymbol{\mu}}\mathrm{e}^{\mathrm{i}s'h}|y\rangle\Big)\Big].
\end{aligned}$$

The 'true' Keldysh identity appearing in the physics literature differs from (3.7) in that it involves the interacting retarded/advanced GF's, $G^{A/R}$, instead of the non-interacting ones $G_0^{A/R}$. The argument leading to such a relation relies on a Dyson type equation connecting $G^{A/R}$ to $G_0^{A/R}$ through the so-called advanced/retarded self-energies. In the physics literature, the derivation of these Dyson equations usually rests on formal analogies with zero temperature and/or diagrammatic perturbative techniques for the contour ordered GFs. The next two results stated in Proposition 3.7 and Proposition 3.8 are non-perturbative and provide a rigorous mathematical foundation to these relations.

3.5 Dyson equations

Given the construction in the beginning of this section relating the retarded and advanced Green's functions to boundary values of resolvent operators, it is clear that the Green's functions $G_v^{R/A}$ of a time-independent perturbation v of the one-body Hamiltonian, where $v \in \mathscr{B}(\mathscr{H})$, are related to the unperturbed Green's functions $G_0^{R/A}$ by the second resolvent equation, i.e.,

$$G_v^R(E|s,s') = G_0^R(E|s,s') + \int_{s'}^s G_0^R(E|s,r)\; v\; G_v^R(E|r,s')\mathrm{d}r,$$

$$G_v^A(E|s,s') = G_0^A(E|s,s') + \int_s^{s'} G_0^A(E|s,r)\; v\; G_v^A(E|r,s')\mathrm{d}r,$$

which we write as

$$G_\nu^{R/A} = G_0^{R/A} + G_0^{R/A}\nu G_\nu^{R/A} = G_0^{R/A} + G_\nu^{R/A}\nu G_0^{R/A}. \tag{3.8}$$

We now state our second result concerning the existence of interacting proper self-energies and formulate the Dyson equations, similar to (3.8), obeyed by the interacting advanced/retarded Green functions.

Proposition 3.7 (The advanced/retarded Dyson equation)**.** *Let $\langle\cdot\rangle$ be an arbitrary state on* CAR($\mathfrak{h}$)*. There exists continuous functions*

$$\mathbb{R}_+\times\mathbb{R}_+ \ni (s,s') \mapsto \Sigma^{A/R}(s,s') = \sum_{x,x'\in\mathscr{S}} |x\rangle \Sigma^{A/R}_{xx'}(s,s')\,\langle x'| \in \mathscr{B}(\mathfrak{h}_{\mathscr{S}})$$

such that for every $s,s'\geq 0$ we have:

$$\begin{aligned} G^{A/R}(E|s,s') &= G_0^{A/R}(E|s,s') + \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r'\, G_0^{A/R}(E|s,r)\Sigma^{A/R}(E|r,r')G^{A/R}(E|r',s') \\ &= G_0^{A/R}(E|s,s') + \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r'\, G^{A/R}(E|s,r)\Sigma^{A/R}(E|r,r')G_0^{A/R}(E|r',s'). \end{aligned} \tag{3.9}$$

Moreover, the map $\xi\mapsto\Sigma^{A/R}\in\mathscr{B}(\mathfrak{h}_{\mathscr{S}})$ which defines the irreducible advanced/retarded self-energy is entire analytic.

3.6 The Keldysh identity

We note an important feature of the above Dyson equations. Due to the special structure of the self-energy $\Sigma^{A/R}$ (which only lives in the sample), we see that the finite dimensional restriction of $G^{A/R}(E|s,s')$ to the small sample obeys the same equation.

Also, by isolating $G_0^{A/R}$ from (3.9) and introducing it in (3.7) we immediately obtain the following result:

Proposition 3.8 (The Keldysh identity)**.** *If the initial state $\langle\cdot\rangle$ is $(\boldsymbol{\beta},\boldsymbol{\mu})$-KMS and if its restriction to* CAR($\mathfrak{h}_{\mathscr{S}}$) *is the vacuum state, then there exists a continuous function*

$$\mathbb{R}_+\times\mathbb{R}_+ \ni (s,s') \mapsto \Sigma^{<}(s,s') = \sum_{x,x'\in\mathscr{S}} |x\rangle \Sigma^{<}_{xx'}(s,s')\,\langle x'| \in \mathscr{B}(\mathfrak{h}_{\mathscr{S}})$$

such that

$$\langle\phi|G^<(t,t')|\phi'\rangle = \int_0^\infty \mathrm{d}s \int_0^\infty \mathrm{d}s' \langle\phi|G^R(t,s)\Sigma^<(s,s')G^A(s',t')|\phi'\rangle, \tag{3.10}$$

for $\phi,\phi'\in\mathfrak{h}_{\mathscr{S}}$ and $t,t'\geq 0$.

4 Proofs

4.1 Proof of Proposition 3.4

One main ingredient of the proof is the following Duhamel formula

$$\tau_K^{t'}(A) = \tau_{K_D}^{t'}(A) + \int_0^{t'} \tau_K^s(\mathrm{i}[H_T, \tau_{K_D}^{t'-s}(A)])\,\mathrm{d}s, \tag{4.1}$$

which is obtained by differentiating $\tau_K^{-s}\circ\tau_{K_D}^{s}(A)$, then integrating back from 0 to t', and finally changing the integration variable from s to $t'-s$. Applying it to $A=a^*(\psi_j)$ we infer

$$\langle\phi_j|G^<(t,t')|\psi_j\rangle = \mathrm{i}\left\langle\tau_{K_D}^{t'}(a^*(\psi_j))\tau_K^t(a(\phi_j))\right\rangle + \int_0^{t'}\mathrm{i}\left\langle\tau_K^s(\mathrm{i}[H_T,\tau_{K_D}^{t'-s}(a^*(\psi_j))])\tau_K^t(a(\phi_j))\right\rangle\mathrm{d}s. \tag{4.2}$$

For $t'-s\geq 0$ we have

$$\begin{aligned}\mathrm{i}[H_T,\tau_{K_D}^{t'-s}(a^*(\psi_j))] &= \mathrm{i}[\mathrm{d}\Gamma(h_T),a^*(\mathrm{e}^{\mathrm{i}(t'-s)h_j}\psi_j)] = a^*(\mathrm{i}h_T\mathrm{e}^{\mathrm{i}(t'-s)h_j}\psi_j)\\ &= \mathrm{i}\,d_j\langle\psi_j|\mathrm{e}^{\mathrm{i}(t'-s)h_j}|\psi_j\rangle a^*(\phi_j) = d_j\langle\psi_j|G_D^A(s,t')|\psi_j\rangle a^*(\phi_j),\end{aligned}$$

and (4.2) becomes

$$\langle\phi_j|G^<(t,t')|\psi_j\rangle = \mathrm{i}\left\langle\tau_{K_D}^{t'}(a^*(\psi_j))\tau_K^t(a(\phi_j))\right\rangle + d_j\int_0^\infty\langle\phi_j|G^<(t,s)|\phi_j\rangle\langle\psi_j|G_D^A(s,t')|\psi_j\rangle\mathrm{d}s. \tag{4.3}$$

We see that the second term on the right hand side coincides with the second term on the rhs of (3.6). The rest of this proof will deal with the first term on the rhs of (4.3).

Since h_T is finite rank, $H_T=\mathrm{d}\Gamma(h_T)$ is a self-adjoint element of CAR($\mathfrak{h}$). This allows us to introduce the *interaction representation* of the full dynamics: for any $A\in\mathrm{CAR}(\mathfrak{h})$ and $t\in\mathbb{R}$,

$$\tau_K^t(A)=\Gamma_t^*\tau_{K_D}^t(A)\Gamma_t,$$

where the cocycle $\Gamma_t=\mathrm{e}^{\mathrm{i}tK_D}\mathrm{e}^{-\mathrm{i}tK}$ satisfies the Cauchy problem

$$\mathrm{i}\partial_t\Gamma_t=\tau_{K_D}^t(H_T)\Gamma_t,\qquad \Gamma_0=\mathbb{1},$$

and takes its values in the unitary elements of CAR($\mathfrak{h}$). It follows that

$$\mathrm{i}\left\langle\tau_{K_D}^{t'}(a^*(\psi_j))\tau_K^t(a(\phi_j))\right\rangle = \mathrm{i}\left\langle\tau_{K_D}^{t'}(a^*(\psi_j))\Gamma_t^*\tau_{K_D}^t(a(\phi_j))\Gamma_t\right\rangle = \mathrm{i}\left\langle a^*(\mathrm{e}^{\mathrm{i}t'h_j}\psi_j)\Gamma_t^*\tau_{K_D}^t(a(\phi_j))\Gamma_t\right\rangle. \tag{4.4}$$

We shall now consider the expression $\mathrm{i}\langle a^*(\tilde\psi_j)\Gamma_t^*\tau_{K_D}^t(a(\phi_j))\Gamma_t\rangle$ for arbitrary $\tilde\psi_j\in\mathfrak{h}_j$. Using the canonical anti-commutation relations which implies

$$\{a^*(\tilde\psi_j),\tau_{K_D}^t(a(\phi_j))\}=\tau_{K_D}^t(\{a^*(\mathrm{e}^{-\mathrm{i}th_j}\tilde\psi_j),a(\phi_j)\})=0, \tag{4.5}$$

we commute the creation operator to the right, getting

$$\begin{aligned}\mathrm{i}\left\langle a^*(\tilde\psi_j)\Gamma_t^*\ \tau_{K_D}^t(a(\phi_j))\Gamma_t\right\rangle &= \mathrm{i}\left\langle\Gamma_t^*a^*(\tilde\psi_j)\tau_{K_D}^t(a(\phi_j))\Gamma_t+[a^*(\tilde\psi_j),\Gamma_t^*]\tau_{K_D}^t(a(\phi_j))\Gamma_t\right\rangle\\ &= \mathrm{i}\left\langle-\Gamma_t^*\tau_{K_D}^t(a(\phi_j))a^*(\tilde\psi_j)\Gamma_t+[a^*(\tilde\psi_j),\Gamma_t^*]\tau_{K_D}^t(a(\phi_j))\Gamma_t\right\rangle\\ &= \mathrm{i}\left\langle-\Gamma_t^*\tau_{K_D}^t(a(\phi_j))\Gamma_ta^*(\tilde\psi_j)-\Gamma_t^*\tau_{K_D}^t(a(\phi_j))[a^*(\tilde\psi_j),\Gamma_t]+[a^*(\tilde\psi_j),\Gamma_t^*]\tau_{K_D}^t(a(\phi_j))\Gamma_t\right\rangle.\end{aligned} \tag{4.6}$$

Since the initial state is $(\boldsymbol{\beta},\boldsymbol{\mu})$-KMS, the KMS condition (2.3) implies

$$\left\langle\Gamma_t^*\tau_{K_D}^t(a(\phi_j))\Gamma_ta^*(\tilde\psi_j)\right\rangle=\left\langle a^*(\mathrm{e}^{\beta_j(h_j-\mu_j)}\tilde\psi_j)\Gamma_t^*\tau_{K_D}^t(a(\phi_j))\Gamma_t\right\rangle,$$

which, combined with (4.6), yields

$$\mathrm{i}\left\langle a^*([1+\mathrm{e}^{\beta_j(h_j-\mu_j)}]\tilde\psi_j)\Gamma_t^*\tau_{K_D}^t(a(\phi_j))\Gamma_t\right\rangle=\mathrm{i}\left\langle-\Gamma_t^*\tau_{K_D}^t(a(\phi_j))[a^*(\tilde\psi_j),\Gamma_t]+[a^*(\tilde\psi_j),\Gamma_t^*]\tau_{K_D}^t(a(\phi_j))\Gamma_t\right\rangle.$$

Setting $\tilde{\psi}_j = [1+\mathrm{e}^{\beta_j(h_j-\mu_j)}]^{-1}\mathrm{e}^{\mathrm{i}t'h_j}\psi_j$ we can thus rewrite (4.4) as

$$\mathrm{i}\left\langle \tau^{t'}_{K_D}(a^*(\psi_j))\tau^t_K(a(\phi_j))\right\rangle = \mathrm{i}\left\langle -\Gamma^*_t\tau^t_{K_D}(a(\phi_j))[a^*(\tilde{\psi}_j),\Gamma_t] + [a^*(\tilde{\psi}_j),\Gamma^*_t]\tau^t_{K_D}(a(\phi_j))\Gamma_t\right\rangle.$$

We now undo the commutators and obtain four terms, two of them forming an anti-commutator equal to zero due to (4.5). This leads to

$$\mathrm{i}\left\langle \tau^{t'}_{K_D}(a^*(\psi_j))\tau^t_K(a(\phi_j))\right\rangle = \mathrm{i}\left\langle\{a^*(\tilde{\psi}_j),\tau^t_K(a(\phi_j))\}\right\rangle = \mathrm{i}\left\langle\tau^t_K\left(\{\tau^{-t}_K(a^*(\tilde{\psi}_j)),a(\phi_j)\}\right)\right\rangle. \tag{4.7}$$

Another application of a slightly modified version of the Duhamel formula in (4.1) further gives:

$$\begin{aligned}\{\tau^{-t}_K(a^*(\tilde{\psi}_j)),a(\phi_j)\} &= \{\tau^{-t}_{K_D}(a^*(\tilde{\psi}_j)),a(\phi_j)\} - \int_0^t\left\{\tau^{-(t-s)}_K(\mathrm{i}[H_T,\tau^{-s}_{K_D}(a^*(\tilde{\psi}_j))]),a(\phi_j)\right\}\mathrm{d}s\\ &= -d_j\int_0^t\{\tau^{-(t-s)}_K(a^*(\phi_j)),a(\phi_j)\}\mathrm{i}\langle\psi_j|\mathrm{e}^{-\mathrm{i}sh_j}|\tilde{\psi}_j\rangle\mathrm{d}s\\ &= -d_j\int_0^t\{\tau^{-(t-s)}_K(a^*(\phi_j)),a(\phi_j)\}\langle\psi_j|G^<_D(s,t')|\psi_j\rangle\mathrm{d}s,\end{aligned}$$

The anti-commutator on the rhs of the first equality equals zero as in (4.5). Inserting this relation into (4.7) we finally get

$$\begin{aligned}\mathrm{i}\left\langle \tau^{t'}_{K_D}(a^*(\psi_j))\tau^t_K(a(\phi_j))\right\rangle &= -d_j\int_0^t\mathrm{i}\left\langle\{\tau^s_K(a^*(\phi_j)),\tau^t_K(a(\phi_j))\}\right\rangle\langle\psi_j|G^<_D(s,t')|\psi_j\rangle\mathrm{d}s\\ &= d_j\int_0^\infty\langle\phi_j|G^R(t,s)|\phi_j\rangle\langle\psi_j|G^<_D(s,t')|\psi_j\rangle\mathrm{d}s,\end{aligned}$$

which, together with (4.3) yields the result.

4.2 Proof of Proposition 3.6

Recall that $N_{\mathscr{S}}$ denotes the particle number operator of the sample $\mathscr{S}$. For any $A\in\mathrm{CAR}(\mathfrak{h})$ and any unit vector $\phi\in\mathfrak{h}_{\mathscr{S}}$ one has

$$|\left\langle a^*(\phi)A\right\rangle| \le \left\langle a^*(\phi)a(\phi)\right\rangle^{1/2}\left\langle A^*A\right\rangle^{1/2} \le \langle N_{\mathscr{S}}\rangle^{1/2}\left\langle A^*A\right\rangle^{1/2}.$$

Since in this proposition we assume that the restriction of $\langle\cdot\rangle$ to $\mathrm{CAR}(\mathfrak{h}_{\mathscr{S}})$ is the vacuum state, one has $\langle N_{\mathscr{S}}\rangle = 0$ and hence $\left\langle a^*(\phi)A\right\rangle = 0$ for all $A\in\mathrm{CAR}(\mathfrak{h})$. In the following, we shall write $A\sim B$ whenever $A,B\in\mathrm{CAR}(\mathfrak{h})$ are such that

$$\left\langle (A-B)^*(A-B)\right\rangle = 0,$$

and hence $\langle CA\rangle = \langle CB\rangle$ for all $C\in\mathrm{CAR}(\mathfrak{h})$.

Starting with Duhamel's formula for the pair (K,H):

$$\tau^t_K(a(\phi)) = \tau^t_H(a(\phi)) + \xi\int_0^t\tau^s_K\left(\mathrm{i}[W,\tau^{t-s}_H(a(\phi))]\right)\mathrm{d}s,$$

we note that

$$\begin{aligned}\tau^t_H(a(\phi)) &= \tau^t_{H_D}(a(\phi)) + \int_0^t\tau^s_{H_D}\left(\mathrm{i}[H_T,\tau^{t-s}_H(a(\phi))]\right)\mathrm{d}s\\ &= a(\mathrm{e}^{\mathrm{i}th_D}\phi) + \int_0^t a(\mathrm{e}^{\mathrm{i}sh_D}\mathrm{i}h_T\mathrm{e}^{\mathrm{i}(t-s)h}\phi)\mathrm{d}s\\ &= a(\mathrm{e}^{\mathrm{i}th_D}\phi) + \int_0^\infty\sum_j d_j\left(\langle\phi|G^R_0(t,s)|\psi_j\rangle a(\mathrm{e}^{\mathrm{i}sh_D}\phi_j) + \langle\phi|G^R_0(t,s)|\phi_j\rangle a(\mathrm{e}^{\mathrm{i}sh_D}\psi_j)\right)\mathrm{d}s,\end{aligned}$$

from which we deduce

$$\tau_H^t(a(\phi)) \sim \int_0^\infty \sum_j d_j \langle \phi | G_0^R(t,s) | \phi_j \rangle a(\mathrm{e}^{\mathrm{i}sh_D}\psi_j)\mathrm{d}s.$$

Setting

$$V_x := \sum_{y\in\mathscr{S}} w(x,y)N_y,$$

we further write, for $t > s$,

$$\begin{aligned}
\mathrm{i}[W, \tau_H^{t-s}(a(\phi))] &= \frac{1}{2}\sum_{x,y\in\mathscr{S}} w(x,y)\mathrm{i}[N_xN_y, a(\mathrm{e}^{\mathrm{i}(t-s)h}\phi)] \\
&= \frac{1}{2}\sum_{x,y\in\mathscr{S}} w(x,y)\left(N_x\mathrm{i}[N_y, a(\mathrm{e}^{\mathrm{i}(t-s)h}\phi)] + \mathrm{i}[N_x, a(\mathrm{e}^{\mathrm{i}(t-s)h}\phi)]N_y\right) \\
&= \frac{1}{2}\sum_{x,y\in\mathscr{S}} w(x,y)\left(N_x\langle\phi|G_0^R(t,s)|y\rangle a_y + \langle\phi|G_0^R(t,s)|x\rangle a_xN_y\right) \\
&= \sum_{x\in\mathscr{S}} \langle\phi|G_0^R(t,s)|x\rangle a_xV_x.
\end{aligned}$$

Thus,

$$\begin{aligned}
\tau_K^t(a(\phi)) &\sim \int_0^\infty \sum_j d_j\langle\phi|G_0^R(t,s)|\phi_j\rangle a(\mathrm{e}^{\mathrm{i}sh_D}\psi_j)\mathrm{d}s + \xi\int_0^\infty\sum_{x\in\mathscr{S}}\langle\phi|G_0^R(t,s)|x\rangle\tau_K^s(a_xV_x)\mathrm{d}s \\
&\sim \int_0^\infty\sum_{x\in\mathscr{S}}\langle\phi|G_0^R(t,s)|x\rangle\mathscr{T}_x(s)\mathrm{d}s
\end{aligned}$$

where we have set

$$\mathscr{T}_x(s) := a(\mathrm{e}^{\mathrm{i}sh_D}h_T\delta_x) + \xi\tau_K^s(a_xV_x).$$

Since $G_0^R(t,s)^* = G_0^A(s,t)$, we can write

$$\langle\phi|G^<(t,t')|\phi'\rangle = \sum_{x,x'\in\mathscr{S}}\int_0^\infty \mathrm{d}s\int_0^\infty \mathrm{d}s'\langle\phi|G_0^R(t,s)|x\rangle S^<_{xx'}(s,s')\langle x'|G_0^A(s',t')|\phi'\rangle$$

with

$$S^<_{xx'}(s,s') = \mathrm{i}\left\langle\mathscr{T}^*_{x'}(s')\mathscr{T}_x(s)\right\rangle.$$

Note that $S^<(s,s')$, as an operator on $\mathfrak{h}_\mathscr{S}$, is real analytic and extends to an entire function of ξ. The first terms of its Taylor expansion around $\xi = 0$

$$S^<(s,s') = \sum_{n=0}^\infty \xi^n S^{<(n)}(s,s'),$$

are easily generated by iterating the Duhamel formula

$$\mathscr{T}_x(s) = a(\mathrm{e}^{\mathrm{i}sh_D}h_T\delta_x) + \xi\tau_H^s(a_xV_x) + \xi^2\int_0^s \mathrm{i}[\tau_H^r(W), \tau_H^s(a_xV_x)]\mathrm{d}r + \mathscr{O}(\xi^3).$$

5 Proof of Proposition 3.7

5.1 Functional setup

In this section we introduce a few function spaces which provide a convenient framework for the study of various GFs.

We identify $\mathscr{H}_\pm = L^2(\mathbb{R}_\pm, \mathrm{d}s) \otimes \mathfrak{h}$ with subspaces of

$$\mathscr{H} = L^2(\mathbb{R}, \mathrm{d}s) \otimes \mathfrak{h} = \mathscr{H}_- \oplus \mathscr{H}_+.$$

The Fourier transform $\hat{\varphi}(\omega) = \int_{\mathbb{R}} \varphi(s) \mathrm{e}^{-\mathrm{i}\omega s} \mathrm{d}s$ maps $\mathscr{H}$ to $L^2(\mathbb{R}, \mathrm{d}\omega) \otimes \mathfrak{h}$ and $\mathscr{H}_\pm$ to $\mathfrak{H}^2(\mathbb{C}_\mp) \otimes \mathfrak{h}$, the Hardy space of $\mathfrak{h}$-valued analytic functions on the half-plane $\mathbb{C}_\mp = \{z \in \mathbb{C} \,|\, \mp \mathrm{Im}\,(z) > 0\}$ with the norm

$$\|\varphi\|^2 = \int_{\mathbb{R}_\pm} \|\varphi(s)\|^2 \mathrm{d}s = \int_{\mathbb{R}} \|\hat{\varphi}(E \mp \mathrm{i}0)\|^2 \frac{\mathrm{d}E}{2\pi} = \sup_{\eta > 0} \int_{\mathbb{R}} \|\hat{\varphi}(E \mp \mathrm{i}\eta)\|^2 \frac{\mathrm{d}E}{2\pi}.$$

The Sobolev space $\mathscr{H}^1 = H^1(\mathbb{R}) \otimes \mathfrak{h}$ (see (3.1)) is a subset of $C(\mathbb{R}; \mathfrak{h})$, the Banach space of continuous $\mathfrak{h}$-valued functions on $\mathbb{R}$ equipped with the sup-norm. In fact elements of $\mathscr{H}^1$ are uniformly (Hölder) continuous

$$\|\varphi(s) - \varphi(s')\| \leq |s - s'|^{1/2} \|\varphi\|_{\mathscr{H}^1},$$

$$\sup_{s \in \mathbb{R}} \|\varphi(s)\| \leq \int_{\mathbb{R}} \|\hat{\varphi}(\omega)\| \frac{\mathrm{d}\omega}{2\pi} \leq 2^{-1/2} \|\varphi\|_{\mathscr{H}^1}.$$

We denote by $\mathscr{H}^1_0$ the closed subspace of $\mathscr{H}^1$ consisting of functions $\varphi : \mathbb{R} \to \mathfrak{h}$ such that $\varphi(0) = 0$.

We also introduce $\mathscr{H}_{\mathrm{loc}} = L^2_{\mathrm{loc}}(\mathbb{R}, \mathrm{d}s) \otimes \mathfrak{h}$, the Fréchet space of all locally square integrable functions $\varphi : \mathbb{R} \to \mathfrak{h}$ with the seminorms

$$\|\varphi\|_T^2 = \int_{-T}^{T} \|\varphi(s)\|^2 \mathrm{d}s,$$

and we set

$$\mathscr{H}_{\mathrm{loc}\pm} = \{\varphi \in \mathscr{H}_{\mathrm{loc}} \,|\, \mathrm{supp}\,\varphi \subset \mathbb{R}_\pm\}.$$

We consider the subspaces

$$\mathscr{H}^1_{\mathrm{loc}} = \{\varphi \in \mathscr{H}_{\mathrm{loc}} \,|\, \chi\varphi \in \mathscr{H}^1 \text{ for all } \chi \in C_0^\infty(\mathbb{R})\},$$

and

$$\mathscr{H}^1_{0,\mathrm{loc}} = \{\varphi \in \mathscr{H}_{\mathrm{loc}} \,|\, \chi\varphi \in \mathscr{H}^1_0 \text{ for all } \chi \in C_0^\infty(\mathbb{R})\},$$

$$\mathscr{H}^1_{0,\mathrm{loc}\pm} = \mathscr{H}^1_{0,\mathrm{loc}} \cap \mathscr{H}_{\mathrm{loc}\pm}.$$

We shall say that a linear operator $M : \mathscr{H}_{\mathrm{loc}\pm} \to \mathscr{H}_{\mathrm{loc}\pm}$ is non-negative, and write $M \geq 0$, whenever

$$\chi_K M \chi_K \geq 0,$$

holds as an operator on $\mathscr{H}$ for all compact interval $K \subset \mathbb{R}_\pm$, where χ_K denotes the operator of multiplication with the characteristic function of K.

5.2 Volterra operators

Let $\Delta = \{(s, s') \in \mathbb{R}^2 | 0 \leq s' \leq s < \infty\}$ and $\Delta \ni (s, s') \mapsto B(s, s') \in \mathscr{B}(\mathfrak{h})$ a continuous function such that

$$\|B(s, s')\| \leq b \mathrm{e}^{\gamma(s - s')}$$

for some constants $b > 0$ and $\gamma \in \mathbb{R}$. The Volterra operator with kernel B is the map

$$(V\varphi)(s) = \varphi(s) - \int_0^s B(s, s') \varphi(s') \mathrm{d}s',$$

on $\mathscr{H}_{\mathrm{loc}+}$. We shall denote it by $V = I - B$. One easily checks that (by estimating the Hilbert-Schmidt norm)

$$\|(I-V)\varphi\|_T \leq \frac{b}{2|\gamma|}(\mathrm{e}^{2\gamma T} - 1 - 2\gamma T)^{1/2}\|\varphi\|_T,$$

so that $V : \mathscr{H}_{\mathrm{loc}+} \to \mathscr{H}_{\mathrm{loc}+}$ is continuous. Moreover, the set of Volterra operators on $\mathscr{H}_{\mathrm{loc}+}$ form a group. The inverse of $V = I - B$ is the Volterra operator $V^{-1} = I + R$ where

$$R(s,s') = B(s,s') + \sum_{n=2}^{\infty} \int_{s'\leq s_1 \leq \cdots \leq s_{n-1} \leq s} B(s,s_{n-1}) \cdots B(s_2,s_1)B(s_1,s')\mathrm{d}s_1 \cdots \mathrm{d}s_{n-1},$$

is such that

$$\|R(s,s')\| \leq b\mathrm{e}^{(\gamma+b)(s-s')}.$$

In particular $\mathrm{Ran}\, V = \mathscr{H}_{\mathrm{loc}+}$ and $\mathrm{Ker}\, V = \{0\}$. Volterra operators on $\mathscr{H}_{\mathrm{loc}-}$ are defined in a similar way.

5.3 More on the non-interacting advanced/retarded Green's functions

The operators $G_0^{\pm}(z) : \mathscr{H} \to \mathscr{H}$ defined in (3.2) satisfy $G_0^{\pm}(z)^* = G_0^{\mp}(\bar{z})$ and

$$G_0^{\pm}(z) - G_0^{\pm}(z)^* = (z - \bar{z})G_0^{\pm}(z)^* G_0^{\pm}(z)$$

so that, in particular,

$$\pm \mathrm{Im}\, G_0^{\pm}(z) = \pm \mathrm{Im}\,(z) G_0^{\pm}(z)^* G_0^{\pm}(z) > 0.$$

In the Fourier representation $G_0^{\pm}(z)$ acts as multiplication with $(-\omega - h - z)^{-1}$ which is bounded on $\mathfrak{H}^2(\mathbb{C}_{\pm}) \otimes \mathfrak{h}$. It follows that

$$G_0^{\pm}(z)\mathscr{H}_{\mp} \subset \mathscr{H}_{\mp}.$$

In fact the causality/anti-causality relations

$$\mathrm{supp}\,\varphi \subset [T,\infty[\Longrightarrow \mathrm{supp}\, G_0^-(z)\varphi \subset [T,\infty[,$$

$$\mathrm{supp}\,\varphi \subset]-\infty,T] \Longrightarrow \mathrm{supp}\, G_0^+(z)\varphi \subset]-\infty,T],$$

hold for all $T > 0$ and justify the name advanced/retarded Green's function given to the integral kernel of $G_0^{\mp}$. Since $\mathrm{Ran}\, G_0^{\pm}(z) = \mathscr{H}^1$ for $z \in \mathbb{C}_{\pm}$, if

$$\langle \psi | G_0^{\pm}(z)\varphi \rangle = 0,$$

for all $\varphi \in \mathscr{H}_{\mp}$, then

$$\langle G_0^{\mp}(\bar{z})\psi | \varphi \rangle = \langle \psi | G_0^{\pm}(z)\varphi \rangle = 0$$

and it follows that $G_0^{\mp}(\bar{z})\psi \in \mathscr{H}_{\pm} \cap \mathscr{H}^1$. Since $(\Omega - \bar{z})G_0^{\mp}(\bar{z})\psi = \psi$ the locality of Ω implies that $\psi \in \mathscr{H}_{\pm}$. Thus $(G_0^{\pm}(z)\mathscr{H}_{\mp})^{\perp} \subset \mathscr{H}_{\pm}$ and hence $\mathscr{H}_{\mp} = \mathscr{H}_{\pm}^{\perp} \subset (G_0^{\pm}(z)\mathscr{H}_{\mp})^{\perp\perp}$. This means that $G_0^{\pm}(z)\mathscr{H}_{\mp}$ is dense in $\mathscr{H}_{\mp}$. In fact one has $G_0^{\pm}(z)\mathscr{H}_{\mp} = \mathscr{H}_0^1 \cap \mathscr{H}_{\mp}$.

We also observe that the boundary values $G_0^{\pm}(E \pm \mathrm{i}0)$ are well defined as maps from $\mathscr{H}_{\mathrm{loc}\mp}$ to $\mathscr{H}_{\mathrm{loc}\mp}$ with the estimate

$$\|G_0^{\pm}(E \pm \mathrm{i}0)\varphi\|_T \leq T\|\varphi\|_T,$$

for all $T > 0$ and $\varphi \in \mathscr{H}_{\mathrm{loc}\mp}$. In fact $G_0^{\pm}(E \pm \mathrm{i}0) : \mathscr{H}_{\mathrm{loc}\mp} \to \mathscr{H}^1_{0,\mathrm{loc}\mp}$.

As an application of the above results, let us consider the inhomogeneous Schrödinger equation

$$\mathrm{i}\partial_s \varphi(s) = (h+z)\varphi(s) + \psi(s), \qquad \varphi(0) = f \in \mathfrak{h},$$

for $\mathrm{Im}\, z \leq 0$ and $\psi \in \mathscr{H}_{\mathrm{loc}+}$. By Duhamel's formula, the solution for $s \geq 0$ is given by

$$\varphi(s) = \mathrm{e}^{-\mathrm{i}s(h+z)} f + (G_0^-(z)\psi)(s),$$

and thus belongs to $\mathscr{H}_{\mathrm{loc}+}$.

5.4 More on the interacting advanced/retarded Green's functions

Starting from (3.3) we can also associate integral operators on $\mathscr{H}$ to the interacting advanced/retarded GFs. We define $G^{\pm}(z)$ by

$$\langle\psi|G^{\pm}(z)\varphi\rangle = \pm\mathrm{i}\int_{-\infty}^{\infty}\mathrm{d}s\int_{\pm(s'-s)>0}\mathrm{d}s'\mathrm{e}^{\mathrm{i}(s'-s)z}\langle\{\tau_K^s(a(\psi(s))),\tau_K^{s'}(a^*(\varphi(s')))\}\rangle,$$

for $\pm\mathrm{Im}\,z>0$, so that

$$\begin{aligned}|\langle\psi|G^{\pm}(z)\varphi\rangle| &\leq 2\int_{-\infty}^{\infty}\mathrm{d}s\int_0^{\infty}\mathrm{d}r\|\psi(s)\|\|\varphi(s\pm r)\|\mathrm{e}^{-r|\mathrm{Im}\,z|}\\ &\leq 2\int_0^{\infty}\mathrm{d}r\mathrm{e}^{-r|\mathrm{Im}\,z|}\int_{-\infty}^{\infty}\mathrm{d}s\|\psi(s)\|\|\varphi(s\pm r)\|\\ &\leq 2\int_0^{\infty}\mathrm{d}r\mathrm{e}^{-r|\mathrm{Im}\,z|}\|\psi\|\|\varphi\| \leq \frac{2}{|\mathrm{Im}\,z|}\|\psi\|\|\varphi\|,\end{aligned}$$

i.e. $\|G^{\pm}(z)\|\leq\frac{2}{|\mathrm{Im}(z)|}$. Clearly, the map $z\mapsto G^{\pm}(z)\in\mathscr{B}(\mathscr{H})$ is analytic in $\mathbb{C}_{\pm}$. Moreover, for $z\in\mathbb{C}_+$ one has

$$\begin{aligned}\langle\psi|G^{+}(z)\varphi\rangle &= \mathrm{i}\int_{-\infty}^{\infty}\mathrm{d}s\int_s^{\infty}\mathrm{d}s'\,\mathrm{e}^{\mathrm{i}(s'-s)z}\langle\{\tau_K^s(a(\psi(s))),\tau_K^{s'}(a^*(\varphi(s')))\}\rangle\\ &= \mathrm{i}\int_{-\infty}^{\infty}\mathrm{d}s'\int_{-\infty}^{s'}\mathrm{d}s\,\mathrm{e}^{\mathrm{i}(s'-s)z}\langle\{\tau_K^s(a(\psi(s))),\tau_K^{s'}(a^*(\varphi(s')))\}\rangle\\ &= \mathrm{i}\int_{-\infty}^{\infty}\mathrm{d}s\int_{-\infty}^{s}\mathrm{d}s'\,\mathrm{e}^{-\mathrm{i}(s'-s)z}\langle\{\tau_K^{s'}(a(\psi(s'))),\tau_K^{s}(a^*(\varphi(s)))\}\rangle\\ &= \overline{\left[-\mathrm{i}\int_{-\infty}^{\infty}\mathrm{d}s\int_{-\infty}^{s}\mathrm{d}s'\,\mathrm{e}^{\mathrm{i}(s'-s)\bar{z}}\langle\{\tau_K^{s'}(a^*(\psi(s'))),\tau_K^{s}(a(\varphi(s)))\}\rangle\right]}\\ &= \overline{\langle\varphi|G^{-}(\bar{z})\psi\rangle} = \langle G^{-}(\bar{z})\psi|\varphi\rangle,\end{aligned}$$

hence

$$G^{\pm}(z)^* = G^{\mp}(\bar{z}). \tag{5.1}$$

Finally, it immediately follows from its definition that $G^{\pm}(z)$ satisfies the same causality/anti-causality relations than $G_0^{\pm}(z)$, and in particular that

$$G^{\pm}(z)\mathscr{H}_{\mp}\subset\mathscr{H}_{\mp}.$$

5.5 The reducible self-energy

For $\varphi\in\mathscr{H}^1$, we can write

$$\langle\psi|G^{\pm}(z)(\Omega-z)\varphi\rangle = \pm\mathrm{i}\int_{-\infty}^{\infty}\mathrm{d}s\int_0^{\infty}\mathrm{d}r\langle\{\tau_K^s(a(\mathrm{e}^{\mathrm{i}s\bar{z}}\psi(s))),\tau_K^{s\pm r}(a^*(\tilde{\varphi}(s\pm r)))\}\rangle$$

where $\tilde{\varphi}(s')=\mathrm{e}^{\mathrm{i}s'z}((\Omega-z)\varphi)(s')$. Let us define $b(f):=\mathrm{i}\xi[W,a(f)]$, so that $b^*(f)=\mathrm{i}\xi[W,a^*(f)]$ and

$$\mathrm{i}[K,a^{\#}(f)] = \partial_s\tau_K^s(a^{\#}(f))|_{s=0} = a^{\#}(\mathrm{i}hf)+b^{\#}(f).$$

One easily derives the relations

$$\tau_K^t(a^*(\tilde{\varphi}(t))) = \mathrm{i}\partial_t\tau_K^t(a^*(\mathrm{e}^{\mathrm{i}tz}\varphi(t)))-\mathrm{i}\tau_K^t(b^*(\mathrm{e}^{\mathrm{i}tz}\varphi(t))) \tag{5.2}$$

which leads to:

$$\tau_K^{s\pm r}(a^*(\tilde{\varphi}(s\pm r))) = \pm \mathrm{i}\partial_r \tau_K^{s\pm r}(a^*(\mathrm{e}^{\mathrm{i}(s\pm r)z}\varphi(s\pm r))) - \mathrm{i}\tau_K^{s\pm r}(b^*(\mathrm{e}^{\mathrm{i}(s\pm r)z}\varphi(s\pm r))).$$

Integration by parts with respect to r yields:

$$\langle\psi|G^{\pm}(z)(\Omega - z)\varphi\rangle = \langle\psi|\varphi\rangle \pm \int_{-\infty}^{\infty}\mathrm{d}s\int_0^{\infty}\mathrm{d}r\,\langle\{\tau_K^s(a(\mathrm{e}^{\mathrm{i}s\bar{z}}\psi(s))), \tau_K^{s\pm r}(b^*(\mathrm{e}^{\mathrm{i}(s\pm r)z}\varphi(s\pm r))\}\rangle,$$

which we can rewrite as

$$G^{\pm}(z)(\Omega - z) = I + F^{\pm}(z),$$

where $F^{\pm}(z)$ extends to a bounded operator on $\mathscr{H}$ with

$$\|F^{\pm}(z)\| \leq \frac{4|\xi|\|W\|}{|\mathrm{Im}\, z|}.$$

Using this together with (5.1), by duality it follows that $\mathrm{Ran}\, G^{\pm}(z) \subset \mathscr{H}^1$. For $\psi \in \mathscr{H}^1$, we further have

$$\langle(\Omega - \bar{z})\psi|F^{\pm}(z)\varphi\rangle = \pm\int_{-\infty}^{\infty}\mathrm{d}s\int_{\pm(s'-s)>0}\mathrm{d}s'\,\langle\{\tau_K^s(a(\tilde{\psi}(s))), \tau_K^{s'}(b^*(\mathrm{e}^{\mathrm{i}s'z}\varphi(s'))\}\rangle,$$

where

$$\tilde{\psi}(s) = \mathrm{e}^{\mathrm{i}s\bar{z}}((\Omega - \bar{z})\psi)(s).$$

Using the adjoint of (5.2):

$$\tau_K^s(a(\tilde{\psi}(s))) = -\mathrm{i}\partial_s\tau_K^s(a(\mathrm{e}^{\mathrm{i}s\bar{z}}\psi(s))) + \mathrm{i}\tau_K^s(b(\mathrm{e}^{\mathrm{i}s\bar{z}}\psi(s)),$$

interchanging the s and s' integrals and then integrating by parts with respect to s, yields

$$\langle(\Omega - \bar{z})\psi|F^{\pm}(z)\varphi\rangle = \langle\psi|\widetilde{\Sigma}^{\pm}(z)\varphi\rangle,$$

where

$$\widetilde{\Sigma}^{\pm}(z) = v_{\mathrm{HF}} + \mathfrak{S}^{\pm}(z),$$

with

$$(v_{\mathrm{HF}}\varphi)(s) = v_{\mathrm{HF}}(s)\varphi(s)$$

the Hartree-Fock energy

$$(v_{\mathrm{HF}}(s)f)(x) = -\mathrm{i}\langle\tau_K^s(\{a_x, b^*(f)\})\rangle, \quad \langle\delta_y|v_{\mathrm{HF}}(s)\delta_x\rangle = \xi\langle\tau_K^s(\{a_y, [W, a_x^*]\})\rangle,$$

and

$$\langle\psi|\mathfrak{S}^{\pm}(z)|\varphi\rangle = \pm\mathrm{i}\int_{-\infty}^{\infty}\mathrm{d}s\int_{\pm(s'-s)>0}\mathrm{d}s'\,\langle\{\tau_K^s(b(\mathrm{e}^{\mathrm{i}s\bar{z}}\psi(s))), \tau_K^{s'}(b^*(\mathrm{e}^{\mathrm{i}s'z}\varphi(s'))\}\rangle.$$

We note that $v_{\mathrm{HF}}(s)$ is a finite rank operator on $\mathfrak{h}$ with $\mathrm{Ran}\, v_{\mathrm{HF}}(s) \subset \mathfrak{h}_{\mathscr{S}}$, and an entire analytic function of s. In the NESS, it is independent of s. Let us show that it is self-adjoint. We have:

$$\langle y|v_{\mathrm{HF}}(s)|x\rangle = \xi\langle\tau_K^s(a_yWa_x^* - a_ya_x^*W + Wa_x^*a_y - a_x^*Wa_y)\rangle$$

and

$$\overline{\langle y|v_{\mathrm{HF}}(s)|x\rangle} = \xi\langle\tau_K^s(a_xWa_y^* - Wa_xa_y^* + a_y^*a_xW - a_y^*Wa_x)\rangle.$$

Using that $\{a_x, a_y^*\} = \{a_x^*, a_y\} = \delta_{xy}$ we obtain $\langle y|v_{\mathrm{HF}}(s)|x\rangle = \overline{\langle x|v_{\mathrm{HF}}(s)|y\rangle}$ and we are done.

The operators $\mathfrak{S}^{\pm}(z)$ define functions $(s,s')\mapsto\mathfrak{S}^{\pm}(z|s,s')\in\mathscr{B}(\mathfrak{h}_{\mathscr{S}})$ which, up to a factor of $\theta(\pm(s'-s))$ are also entire analytic in both variables

$$\langle g|\mathfrak{S}^{\pm}(z|s,s')|f\rangle=\pm\mathrm{i}\theta(\pm(s'-s))\mathrm{e}^{\mathrm{i}(s'-s)z}\langle\{\tau_K^s(b(g)),\tau_K^{s'}(b^*(f))\}\rangle.$$

These operators are also finite rank with

$$\mathrm{Ran}\,\mathfrak{S}^{\pm}(z|s,s')\subset\mathfrak{h}_{\mathscr{S}},\qquad\mathfrak{h}_{\mathscr{R}}\subset\mathrm{Ker}\,\mathfrak{S}^{\pm}(z|s,s'),$$

and

$$\langle\psi|\mathfrak{S}^{\pm}(z)|\varphi\rangle=\int_{-\infty}^{\infty}\mathrm{d}s\int_{-\infty}^{\infty}\mathrm{d}s'\langle\psi(s)|\mathfrak{S}^{\pm}(z|s,s')|\varphi(s')\rangle.$$

The relation

$$\mathfrak{S}^{+}(z)^*=\mathfrak{S}^{-}(\bar z),$$

can be proved following the same idea as in (5.1). In the NESS, $\mathfrak{S}^{\pm}(z|s,s')=\mathfrak{S}^{\pm}(z|s-s')$.

Summarizing, we have shown that $G^{\pm}(s)(\Omega-z)=I+F^{\pm}(z)$ and $(\Omega-z)F^{\pm}(z)=\widetilde{\Sigma}^{\pm}(z)$ which can be rewritten as $G^{\pm}(z)=G_0^{\pm}(z)+F^{\pm}(z)G_0^{\pm}(z)$ and $F^{\pm}(z)=G_0^{\pm}(z)\widetilde{\Sigma}^{\pm}(z)$. The operator $\widetilde{\Sigma}^{\pm}(z)$ is called *reducible advanced/retarded self-energy*. Thus, we have proved

Lemma 5.1. *For $\pm\mathrm{Im}\,z>0$ the advanced/retarded interacting Green's function satisfies the equation*

$$G^{\pm}(z)=G_0^{\pm}(z)+G_0^{\pm}(z)\widetilde{\Sigma}^{\pm}(z)G_0^{\pm}(z),\tag{5.3}$$

where $\widetilde{\Sigma}^{\pm}(z)$ is the reducible self-energy, an operator acting on $L^2(\mathbb{R},\mathrm{d}s)\otimes\mathfrak{h}_{\mathscr{S}}$ as

$$(\widetilde{\Sigma}^{\pm}(z)\varphi)(s)=v_{\mathrm{HF}}(s)\varphi(s)+\int\mathfrak{S}^{\pm}(z|s,s')\varphi(s')\mathrm{d}s',$$

with

$$\langle y|v_{\mathrm{HF}}(s)|x\rangle=\xi\langle\tau_K^s(\{a_y,[W,a_x^*]\})\rangle,$$

and

$$\langle y|\mathfrak{S}^{\pm}(z|s,s')|x\rangle=\mp\mathrm{i}\xi^2\theta(\pm(s'-s))\mathrm{e}^{\mathrm{i}(s'-s)z}\langle\{\tau_K^s([W,a_y]),\tau_K^{s'}([W,a_x^*])\}\rangle.$$

We observe that the boundary values of all these advanced/retarded operators $G_0^{\pm}(E\pm\mathrm{i}0)$, $G^{\pm}(E\pm\mathrm{i}0)$ and $\tilde\Sigma^{\pm}(E\pm\mathrm{i}0)$ are well defined as operators on $\mathscr{H}_{\mathrm{loc}\mp}$, by the same estimate as for the free Green's functions. It follows that relation (5.3) remains valid on $\mathscr{H}_{\mathrm{loc}\mp}$ for $z=E\pm\mathrm{i}0$. In particular

$$\langle x|G^{A/R}(s,s')|x'\rangle=\langle x|G_0^{A/R}(s,s')|x'\rangle+\sum_{y,z\in\mathscr{S}}\int\mathrm{d}u\int\mathrm{d}v\,\langle x|G_0^{A/R}(s,u)|y\rangle\widetilde{\Sigma}^{\pm}_{yz}(0\pm\mathrm{i}0|u,v)\langle z|G_0^{A/R}(v,s')|x'\rangle.$$

Remark 5.2. The self-energy $\widetilde{\Sigma}^{\pm}(z)$ has an important property related to dissipation. As already noticed, the Hartree-Fock part is self-adjoint, thus, for $z=E-\mathrm{i}\eta$, $\eta>0$ and $\varphi\in\mathscr{H}_+$, one has

$$(\tilde\Sigma^{-}(z)\varphi)(s)=v_{\mathrm{HF}}(s)\varphi(s)+\int_0^s\mathfrak{S}^{-}(z|s,s')\varphi(s')\mathrm{d}s',$$

and hence, with $B_s=\tau_K^s(b(\mathrm{e}^{\mathrm{i}sE}\varphi(s)))$ and invoking Lemma A.1,

$$\begin{aligned}\mathrm{Im}\int_0^T\langle\varphi(s)|(\tilde\Sigma^{-}(z)\varphi)(s)\rangle\mathrm{d}s&=\mathrm{Im}\int_0^T\mathrm{d}s\int_0^s\mathrm{d}s'\langle\varphi(s)|\mathfrak{S}^{-}(z|s,s')|\varphi(s')\rangle\\&=-\mathrm{Re}\int_0^T\mathrm{d}s\int_0^s\mathrm{d}s'\langle\{\tau_K^s(b(\mathrm{e}^{\mathrm{i}s\bar z}\varphi(s))),\tau_K^{s'}(b^*(\mathrm{e}^{\mathrm{i}s'z}\varphi(s')))\}\rangle\\&=-\mathrm{Re}\int_0^T\mathrm{d}s\int_0^s\mathrm{d}s'\mathrm{e}^{-\eta(s-s')}\langle\{B_s,B_{s'}^*\}\rangle\le0.\end{aligned}\tag{5.4}$$

5.6 The irreducible advanced/retarded self-energy

Considering $G_0^\pm$ and $G^\pm$ as operators on $\mathscr{H}_{\mathrm{loc}\mp}$, the relation

$$G^\pm(z) = G_0^\pm(z) + G_0^\pm(z)\widetilde{\Sigma}^\pm(z)G_0^\pm(z), \tag{5.5}$$

can be rewritten as

$$G^\pm(z) = \left(I + G_0^\pm(z)\widetilde{\Sigma}^\pm(z)\right)G_0^\pm(z),$$

and since $I + G_0^\pm(z)\widetilde{\Sigma}^\pm(z)$ is a Volterra operator on $\mathscr{H}_{\mathrm{loc}\mp}$, the last relation leads to

$$G_0^\pm(z) = \left(I + G_0^\pm(z)\widetilde{\Sigma}^\pm(z)\right)^{-1} G^\pm(z),$$

which, inserted into (5.5), yields

$$G^\pm(z) = G_0^\pm(z) + G_0^\pm(z)\Sigma^\pm(z)G^\pm(z), \tag{5.6}$$

with

$$\Sigma^\pm(z) = \widetilde{\Sigma}^\pm(z)\left(I + G_0^\pm(z)\widetilde{\Sigma}^\pm(z)\right)^{-1}, \tag{5.7}$$

a Volterra kernel. The operator $\Sigma^\pm(z)$ is the *irreducible self-energy* announced in (3.9). This ends the proof of Proposition 3.7.

5.7 Some dissipative properties of the irreducible self-energy

Since $I - \Sigma^\pm(z)G^\pm(z)$ is a Volterra operator, (5.6) implies that $G^\pm(z)\mathscr{H}_\mp$ is dense in $\mathscr{H}_\mp$. Multiplying (5.6) on the left by $\Omega - z$ further gives

$$\left(\Omega - \Sigma^\pm(z) - z\right)G^\pm(z) = I,$$

so that

$$G^\pm(z) = (\Omega - \Sigma^\pm(z) - z)^{-1}.$$

Reasoning like in (5.4) we obtain $\mathrm{Im}\,(G^-(z)) \le 0$. Using this in the 'resolvent identity'

$$G^-(z) - G^-(z)^* = G^-(z)^*(z - \bar{z} + \Sigma^-(z) - \Sigma^-(z)^*)G^-(z)$$

one deduces

$$\mathrm{Im}\,(z + \Sigma^-(z)) \le 0 \tag{5.8}$$

and in particular, in the limit $\mathrm{Im}\,z \to 0$,

$$\mathrm{Im}\,(\Sigma^-(E - \mathrm{i}0)) \le 0.$$

Let us consider the Schrödinger equation

$$\mathrm{i}\partial_s\varphi(s) = (h + z)\varphi(s) + (\Sigma^-(z)\varphi)(s)$$

with the initial condition $\varphi(0)$ for $\mathrm{Im}\,z \le 0$. The dissipative property (5.8) ensures that the solution satisfies $\|\varphi(s)\| \le \|\varphi(0)\|$ for $s \ge 0$:

$$\frac{1}{2}\partial_s\|\varphi(s)\|^2 = \mathrm{Im}\,\langle\varphi(s)|\mathrm{i}\partial_s\varphi(s)\rangle = \mathrm{Im}\,\langle\varphi(s)|(z + \Sigma^-(z)\varphi)(s)\rangle$$

so

$$\frac{1}{2}(\|\varphi(T)\|^2 - \|\varphi(0)\|^2) = \mathrm{Im}\int_0^T \mathrm{d}s\int_0^s \mathrm{d}s'\,\langle\varphi(s)|\Sigma^-(z|s,s')|\varphi(s')\rangle + \mathrm{Im}\,z\int_0^T \|\varphi(s)\|^2\mathrm{d}s \le 0.$$

It follows that the equation has a contractive propagator $\varphi(s) = U(s,s')\varphi(s')$. By Duhamel's formula, the initial value problem is equivalent to the integral equation

$$\begin{aligned}\varphi(s) &= \mathrm{e}^{-\mathrm{i}s(h+z)}\varphi(0) + (G_0^-(z)\Sigma^-(z)\varphi)(s)\\ &= \mathrm{e}^{-\mathrm{i}s(h+z)}\varphi(0) - \mathrm{i}\int_0^s \mathrm{d}r\,\mathrm{e}^{-\mathrm{i}(s-r)(h+z)}\int_0^r \mathrm{d}s'\Sigma^-(r,s')\varphi(s').\end{aligned}$$

Since $G_0^-(z)\Sigma^-(z)$ is a Volterra kernel, this equation is solved by setting

$$\varphi(s) = ((I - G_0^-(z)\Sigma^-(z))^{-1}\psi)(s),$$

with

$$\psi(s) = \theta(s)\mathrm{e}^{-\mathrm{i}s(h+z)}\varphi(0) = \mathrm{i}G_0^-(z)\delta_0\otimes\varphi,$$

where $\delta_0\otimes\varphi \in \mathscr{H}^{-1}$, δ_0 denoting the Dirac mass at $s=0$. By (5.7)

$$\begin{aligned}I - G_0^-(z)\Sigma^-(z) &= I - G_0^-(z)\widetilde{\Sigma}^-(z)(I + G_0^-(z)\widetilde{\Sigma}^-(z))^{-1}\\ &= (I + G_0^-(z)\widetilde{\Sigma}^-(z))^{-1}\\ \varphi(s) &= (I + G_0^-(z)\widetilde{\Sigma}^-(z))\psi\\ &= \mathrm{i}(I + G_0^-(z)\widetilde{\Sigma}^-(z))G_0^-(z)\delta_0\otimes\varphi\\ &= \mathrm{i}G^-(z)\delta_0\otimes\varphi.\end{aligned}$$

Thus we have the following formula for the interacting Green's function

$$(G^-(z)\varphi)(s) = -\mathrm{i}\int_{-\infty}^s U(s,s')\varphi(s')\mathrm{d}s'.$$

6 Concluding remarks and open problems

We established the first systematic mathematical approach to the non-equilibrium Green's function formalism for interacting transport in open systems. Rather than introducing the textbook Keldysh contours and contour-ordering operators we follow a three-step bottom-up strategy only using real-time GFs (i.e., retarded, advanced and lesser):

1. We relate the time-dependent current to a fully interacting lesser GF $\langle\phi_j|G^<(t,t)|\psi_j\rangle$ associated with a pair of states from a given lead j and the sample.
2. Using the KMS condition and Duhamel identities we show that $\langle\phi_j|G^<(t,t)|\psi_j\rangle$ obeys a Langreth-type identity which immediately implies the JMW formula.
3. We derive the Keldysh equation for the lesser GF restricted to the sample in terms of a lesser interaction self-energy for which we provide explicit expressions.

Last but not least we rely on the theory of Volterra operators to rigorously define the irreducible retarded self-energy via its Dyson equation. This is a mandatory back-up for practical diagrammatic recipes (e.g., Hartree-Fock, self-consistent Born approximation, GW). For completeness and comparison we recall here that in the standard top-down way to the JMW formula one rather takes for granted a Dyson equation for contour-ordered GFs and then uses the formal Langreth rules to come back to real-time quantities.

Let us also point out some open problems related to the NEGF formalism for interacting systems:

• *Initial correlations.* We recall that the Keldysh identity (3.10) requires that the initial state of the sample is the vacuum. From a physical point of view, this means that there are no initial correlations due to the Coulomb interaction between particles before the coupling to the leads is established. If the initial state can have particles in the sample before the coupling, the Keldysh equation acquires a more complicated form [HJ, SvL].

• *The partition-free setting.* This alternative transport scenario has been put forward a long time ago by Cini [Ci] and goes as follows: i) the initial state describes a coupled but unbiased system where all the chemical potentials μ_j are equal, i.e., the initial state $\langle\cdot\rangle^{\beta,\mu}$ is the thermodinamic limit of the grand canonical Gibbs state associated with the restriction of K to finitely extended reservoirs; ii) at some instant t_0 one adds a potential bias on the leads and a current is established. Later on, Stefanucci and Almbladh [SA] adapted the Keldysh formalism for the partition-free scenario. They found in particular that the Keldysh equation for the lesser interaction self-energy is far more complicated. In fact, they argue that in this case the Keldysh equation should only be used to describe the long-time response of the interacting system. They also derive a generalized JMW formula (see Eq. (16.7) in [SvL]). Although we [CMP1, CMP2] were able to establish the existence of a NESS *in the fully resonant case* for the free-partition setting as well, a 'contourless' derivation of a JMW-type formula and its corresponding Langreth-like identities is still missing.

A A positivity lemma

Lemma A.1. *Let* $[0,T] \ni s \mapsto A_s \in \mathscr{B}(\mathfrak{h})$ *be a continuous map such that* $\sup_{s\in[0,T]} \|A_s\| < \infty$. *Then for any* $\eta \geq 0$ *one has*

$$\mathrm{Re}\int_0^T \mathrm{d}s \int_0^s \mathrm{d}s' \mathrm{e}^{-\eta(s-s')} A_s^* A_{s'} \geq 0.$$

Proof. It suffices to show that for any $f \in \mathfrak{h}$

$$\mathrm{Re}\int_0^T \mathrm{d}s \int_0^s \mathrm{d}s' \mathrm{e}^{-\eta(s-s')} \langle f_s | f_{s'}\rangle \geq 0,$$

where $f_s = A_s f$. Extending $s \mapsto f_s$ by zero on $\mathbb{R}\setminus[0,T]$ yields a strongly measurable $\mathfrak{h}$-valued function which belongs to $L^1(\mathbb{R};\mathfrak{h})$. Set

$$f_{s,\epsilon} = \int_0^T \mathrm{e}^{-(s-s')^2/2\epsilon} f_{s'} \frac{\mathrm{d}s'}{\sqrt{2\pi\epsilon}},$$

so that $f_{s,\epsilon} \to f_s$ in $L^1(\mathbb{R};\mathfrak{h})$ as $\epsilon \downarrow 0$. It follows from the dominated convergence theorem that

$$\mathrm{Re}\int_0^T \mathrm{d}s \int_0^s \mathrm{d}s' \mathrm{e}^{-\eta(s-s')} \langle f_s | f_{s'}\rangle = \lim_{\epsilon\downarrow 0} \mathrm{Re}\int_{-\infty}^{\infty} \mathrm{d}s \int_{-\infty}^s \mathrm{d}s' \mathrm{e}^{-\eta(s-s')} \langle f_{s,\epsilon} | f_{s',\epsilon}\rangle.$$

The Fourier transform of $f_{s,\epsilon}$ is given by $\mathrm{e}^{-\epsilon\omega^2/2}\widehat{f}_\omega$ with

$$\widehat{f}_\omega = \int_0^T \mathrm{e}^{-\mathrm{i}\omega s} f_s \mathrm{d}s.$$

It follows that $(\nu,\omega) \mapsto \langle \widehat{f}_{\nu,\epsilon} | \widehat{f}_{\omega,\epsilon}\rangle$ is a Schwartz function and an explicit calculation yields

$$\int_{-\infty}^{\infty} \mathrm{d}s \int_{-\infty}^s \mathrm{d}s' \mathrm{e}^{-\eta(s-s')} \langle f_{s,\epsilon} | f_{s',\epsilon}\rangle = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \frac{1}{\eta - \mathrm{i}\omega} \|\widehat{f}_{\omega,\epsilon}\|^2,$$

so that

$$\mathrm{Re}\int_{-\infty}^{\infty} \mathrm{d}s \int_{-\infty}^s \mathrm{d}s' \mathrm{e}^{-\eta(s-s')} \langle f_{s,\epsilon} | f_{s',\epsilon}\rangle = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \frac{\eta}{\eta^2+\omega^2} \|\widehat{f}_{\omega,\epsilon}\|^2 \geq 0.$$

References

[AH] Araki, H., and Ho, T.G.: Asymptotic time evolution of a partitioned infinite two-sided isotropic XY-chain. Proc. Steklov Inst. Math. **228**,191–204 (2000).

[AJPP1] Aschbacher, W., Jakšić, V., Pautrat, Y., and Pillet, C.-A.: Topics in non-equilibrium quantum statistical mechanics. In *Open Quantum Systems III. Recent Developments*. S. Attal, A. Joye and C.-A. Pillet editors. Lecture Notes in Mathematics **1882**. Springer, Berlin, 2006.

[AJPP2] Aschbacher, W., Jakšić, V., Pautrat, Y., and Pillet, C.-A.: Transport properties of quasi-free Fermions. J. Math. Phys. **48**, 032101-1–28 (2007).

[AM] Araki, H., and Moriya, H.: Joint extension of states of subsystems for a CAR system. Commun. Math. Phys. **237**, 105–122 (2003).

[AP] Aschbacher, W., and Pillet, C.-A.: Non-equilibrium steady states of the XY chain. J. Stat. Phys. **112**, 1153–1175 (2003).

[BP] Ben Sâad, R., and Pillet, C.-A.: A geometric approach to the Landauer-Büttiker formula. J. Math. Phys. 55, 075202 (2014).

[BR2] Bratelli, O., and Robinson, D.W.: *Operator Algebras and Quantum Statistical Mechanics 2*. Second Edition. Springer, New York,1997.

[Ca1] Caroli, C., Combescot, R., Nozières, P., and Saint-James, D.: Direct calculation of the tunneling current. J. Phys. C: Solid State Phys. **4**, 916–929 (1971).

[Ca2] Caroli, C., Combescot, R., Lederer, D., Nozières, P., and Saint-James, D.: A direct calculation of the tunneling current II. Free electron description. J. Phys. C: Solid State Phys. **4**, 2598–2610 (1971).

[Ca3] Caroli, C., Combescot, R., Nozières, P., and Saint-James, D.: A direct calculation of the tunneling current IV. Electron-phonon interaction effects. J. Phys. C: Solid State Phys. **5**, 21–42 (1972).

[CDNP] Cornean, H.D., Duclos, P., Nenciu, G., and Purice, R.: Adiabatically switched-on electrical bias and the Landauer-Büttiker formula. J. Math. Phys. **49**, 102106 (2008).

[Ci] Cini, M.: Time-dependent approach to electron transport through junctions: General theory and simple applications. Phys. Rev. B **22**, 5887–5899 (1980).

[CJM] Cornean, H.D., Jensen, A., and Moldoveanu, V.: A rigorous proof of the Landauer-Büttiker formula. J. Math. Phys. **46**, 042106 (2005).

[CM] Cornean, H.D., and Moldoveanu, V.: On the cotunneling regime of interacting quantum dots. J. Phys. A: Math. Theor. **44**, 305002, (2011).

[CMP1] Cornean, H.D., Moldoveanu, V., and Pillet, C.-A.: Nonequilibrium steady states for interacting open systems: Exact results. Phys. Rev. B **84**, 075464 (2011).

[CMP2] Cornean, H.D., Moldoveanu, V., and Pillet, C.-A.: On the steady state correlation functions of open interacting systems. Commun. Math. Phys. **331**, 261–295 (2014).

[Co] Combescot, R.: A direct calculation of the tunneling current III. Effect of localized impurity states in the barrier. J. Phys. C: Solid State Phys. **4**, 2611–2622 (1971).

[Cr] Craig, R.A.: Perturbation expansion for real-time Green's functions. J. Math. Phys. **9**, 605–611 (1968).

[Da] Danielewicz, P.: Quantum theory of nonequilibrium processes I. Ann. Phys. **152**, 239–304 (1984).

[DeGe] Dereziński, J., and Gérard, C.: *Mathematics of Quantization and Quantum Fields.* Cambridge University Press, Cambridge, UK, 2013.

[FMU] Fröhlich, J., Merkli, M., and Ueltschi, D.: Dissipative transport: thermal contacts and tunneling junctions. Ann. Henri Poincaré **4**, 897–945 (2004).

[Fu] Fujita, S.: Partial self-energy parts of Kadanoff-Baym. Physica **30**, 848–856 (1964).

[FVA] von Friesen, P.M., Verdozzi, V., and Almbladh, C.-O.: Kadanoff-Baym dynamics of Hubbard clusters: Performance of many-body schemes, correlation-induced damping and multiple steady and quasi-steady states. Phys. Rev. B **82**, 155108 (2010).

[FW] Fetter, A.L., and Walecka, J.D.: *Quantum Theory of Many-Particle Systems.* Dover Publications, New York, 2003.

[GML] Gell-Mann, M., and Low, F.: Bound states in quantum field theory. Phys. Rev. **84**, 350–354 (1951).

[HJ] Haugh, H., and Jauho A.-P..: *Quantum Kinetics in Transport and Optics of Semiconductors.* Springer Series in Solid State Sciences **123**, 2nd Edition. Springer, Berlin, 2007.

[Im] Imry, Y.: *Introduction to Mesoscopic Physics.* Oxford University Press, Oxford, 1997.

[JOP1] Jakšić, V., Ogata, Y., and Pillet, C.-A.: The Green-Kubo formula and the Onsager reciprocity relations in quantum statistical mechanics. Commun. Math. Phys. **265**, 721–738 (2006).

[JOP2] Jakšić, V., Ogata, Y., and Pillet, C.-A.: Linear response theory for thermally driven quantum open systems. J. Stat. Phys. **123**, 547–569 (2006).

[JOP3] Jakšić, V., Ogata, Y., and Pillet, C.-A.: The Green-Kubo formula for locally interacting fermionic open systems. Ann. Henri Poincaré **8**, 1013–1036 (2007).

[JP1] Jakšić, V., and Pillet, C.-A.: Non-equilibrium steady states of finite quantum systems coupled to thermal reservoirs. Commun. Math. Phys. **226**, 131–162 (2002).

[JWM] Jauho, A.-P., Wingreen, N.S., and Meir, Y.: Time-dependent transport in interacting and noninteracting resonant-tunneling systems. Phys. Rev. B **50**, 5528–5544 (1994).

[KB] Kadanoff, L.P., and Baym, G.: *Quantum Statistical Mechanics.* Benjamin, New York, 1962.

[Ke] Keldysh, L.V.: Diagram technique for nonequilibrium processes. Zh. Eksp. Teor. Fiz. **47**, 1515 (1964). English translation in Sov. Phys. JETP **20**, 1018–1026 (1965).

[Ku] Kubo, R., Toda, M., and Hashitsume, N.: *Statistical Physics II. Nonequilibrium Statistical Mechanics.* Springer, Berlin, 1985.

[La] Langreth, D.C.: Linear and nonlinear response theory with applications. In *Linear and Nonlinear Electron Transport in Solids.* J.T. Devreese and V.E. van Doren editors. NATO Advanced Study Institute, Series B: Physics **17**. Plenum Press, New York, 1976.

[MMS] Merkli, M., Mück, M., and Sigal, I.M.: Theory of non-equilibrium stationary states as a theory of resonances. Ann. Henri Poincaré **8**, 1539–1593 (2007).

[MSSL] Myohanen, P., Stan, A., Stefanucci, G., and van Leeuwen, R.: Kadanoff-Baym approach to quantum transport through interacting nanoscale systems: From the transient to the steady-state regime. Phys. Rev. B **80**, 115107 (2009).

[MW] Meir, Y., and Wingreen, N.S.: Landauer formula for the current through an interacting electron region. Phys. Rev. Lett. **68**, 2512–2515 (1992).

[N] Nenciu, G.: Independent electrons model for open quantum systems: Landauer-Büttiker formula and strict positivity of the entropy production. J. Math. Phys. **48**, 033302 (2007).

[ND] Ness, H., and Dash, L.K.: Dynamical equations for time-ordered Green's functions: from the Keldysh time-loop contour to equilibrium at finite and zero temperature. J. Phys.: Condens. Matter **24**, 505601 (2012).

[NDG] Ness, H., Dash, L.K., and Godby, R.W.: Generalization and applicability of the Landauer formula for nonequilibrium current in the presence of interactions. Phys. Rev. B **82**, 085426 (2010).

[Ne] Ness, H.: Nonequilibrium distribution functions for quantum transport: Universality and approximation for the steady state regime. Phys. Rev. B **89**, 045409 (2014).

[SA] Stefanucci, G., and Almbladh, C.-O.: Time-dependent partition-free approach in resonant tunneling systems. Phys. Rev. B **69**, 195318 (2004).

[Sc] Schwinger, J.: Brownian motion of a quantum oscillator. J. Math. Phys. **2**, 407–432 (1961).

[SvL] Stefanucci, G., and van Leeuwen, R.: *Nonequilibrium Many-Body Theory of Quantum System, A Modern Introduction.* Cambridge University Press, Cambridge, 2013.