Nonequilibrium Green's Functions for Mathematicians

A joint work with Horia Cornean and Valeriu Moldoveanu

Claude-Alain Pillet

Analytical & Numerical Methods in Quantum Transport
Aalborg — 28–30 May 2018

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thanks to long and lively discussions with N. Angelescu, J. Dereziński, P. Duclos, P. Gartner, V. Jakšić, G. Nenciu, G. Stefanucci, and V. Zagrebnov

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Introduction

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- ... and fashionable!

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Mathematics

- Steady state transport well understood in absence of interactions (Landauer-Büttiker regime): Cornean–Jensen–Moldoveanu (2005), Aschbacher–Jakšić–Pautrat–P and Nenciu (2007), Cornean–Duclos–Nenciu-Purice (2008), ...

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  - Linear response theory: Jakšić–Ogata–P (2006)
  - Steady state limit of 2-points functions: Cornean–(P)–Moldoveanu (2011)

What is the mathematical status of NEGF's formalism ?

At equilibrium

- Green (Schwinger, Wightman) functions have been widely and successfully used in constructive and axiomatic QFT: Haag-Kastler (1964), Osterwalder-Schrader (1973), Fröhlich (1977),...,

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- Mathematical foundations of NEGF's formalism still missing.
- Keldysh path-ordering replaces usual time-ordering.
  - Easy to formulate rigorously (but I won't do it).
  - Turns out to be a mere convenience tool to make non-equilibrium "look like" equilibrium.
  - Should be substituted by modular structure.
  - So called "analytic continuation" is needed to convert Keldysh ordered expressions to "real-time" ones. Misleading to mathematicians since this has nothing to do with what they call analytic continuation.

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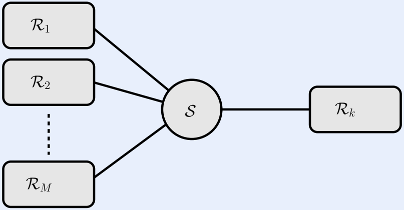
- Integral equations again play a central role.
  - Self-energies encode the effects of interactions.
  - Dyson type equations are either assumed or derived by diagrammatic arguments.

Setup



One particle setup

The Sample

With $\mathcal{S}$ a finite set: the sample Hamiltonian $h_{\mathcal{S}}$ acts on the Hilbert space $\mathfrak{h}_{\mathcal{S}} = \ell^2(\mathcal{S})$

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The Hamiltonian of the j-the reservoir is h_j acting on $\mathfrak{h}_j$. Set

$$h_{\mathcal{R}} = \bigoplus_{j=1}^{M} h_j, \qquad \mathfrak{h}_{\mathcal{R}} = \bigoplus_{j=1}^{M} \mathfrak{h}_j$$

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The Coupling

$$\mathfrak{h} = \mathfrak{h}_{\mathcal{S}} \oplus \mathfrak{h}_{\mathcal{R}}, \qquad h = (h_{\mathcal{S}} \oplus h_{\mathcal{R}}) + h_T$$

with the Tunneling Hamiltonian

$$h_T = \sum_{j=1}^{M} d_j \left(|\psi_j\rangle\langle\phi_j| + |\phi_j\rangle\langle\psi_j| \right)$$

and unit vectors $\phi_j \in \mathfrak{h}_{\mathcal{S}}$, $\psi_j \in \mathfrak{h}_j$.

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WLOG: $\mathfrak{h}_j = L^2(\mathbb{R}, d\nu_j(E))$, $h_j = E$, $\psi_j = 1$

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Second quantization $\Longrightarrow$ Quasi-free electronic gas

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- Initial state $\langle \cdot \rangle_{\beta,\mu}$ on $\mathrm{CAR}(\mathfrak{h})$ with $\beta = (\beta_j)$, $\mu = (\mu_j)$ and
  - $\langle \cdot \rangle_{\beta,\mu}|_{\mathrm{CAR}(\mathfrak{h}_j)}$ is τ_{H_j}-KMS at temperature β_j^{-1} and chemical potential μ_j.
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Interactions

Two-body potential ($w(x,y) = w(y,x)$, $w(x,x) = 0$, $\max w(x,y) = 1$)

$$W = \frac{1}{2} \sum_{x,y \in \mathcal{S}} w(x,y) a_x^* a_x a_y^* a_y$$

Interacting Hamiltonian $K = H + \xi W$ and dynamics $\tau_K^t(A) = \mathrm{e}^{\mathrm{i}tK} A \mathrm{e}^{-\mathrm{i}tK}$

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Decoupled interacting Hamiltonian $K_D = H - H_T = (H_{\mathcal{S}} + \xi W) + H_{\mathcal{R}}$

Green's functions

Motivation: non-interacting advanced/retarded Green's functions

Inhomogeneous time-dependent Schrödinger equation in $\mathcal{K} = L^2(\mathbb{R}, \mathrm{d}s) \otimes \mathfrak{h}$

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

has resolvent $G_0(z) = (\Omega - z)^{-1}$ with integral kernel

$$(G_0(z)\varphi)(s) = \pm\mathrm{i}\int \theta(\pm(s' - s))\mathrm{e}^{\mathrm{i}(s'-s)(h+z)}\varphi(s')\mathrm{d}s'$$

for $z \in \mathbb{C}_\pm = \{\pm\mathrm{Im}(z) > 0\}$.

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$$G_0^{a/r}(E) = G_0(E \pm \mathrm{i}0)$$

exist as continuous operator on $\mathcal{K}^{\mp}_{\mathrm{loc}} = L^2_{\mathrm{loc}}(\mathbb{R}_\mp, \mathrm{d}s) \otimes \mathfrak{h}$.

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Non-interacting advanced/retarded Green's functions $\equiv$ integral kernels of $G_0^{a/r}$

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has resolver

For $\psi \in \mathcal{K}^{\mp}_{\mathrm{loc}}$ the unique anti-causal/causal solution $\varphi \in \mathcal{K}^{\mp}_{\mathrm{loc}}$ is

$$\varphi(s) = (G_0^{a/r}\psi)(s) = \int G_0^{a/r}(s, s')\psi(s')\mathrm{d}s'$$

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Keldysh Green's function & spectral function

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

$$\begin{aligned}\langle f|A(s,s')g\rangle &= \mathrm{i}\langle f|G^{r}(s,s')-G^{a}(s,s')|g\rangle\\ &= \mathrm{i}\langle f|G^{>}(s,s')-G^{<}(s,s')|g\rangle = \mathrm{i}\left\langle\{\tau_K^{s'}(a^*(g)),\tau_K^{s}(a(f))\}\right\rangle_{\beta,\mu}\end{aligned}$$

The Langreth identity & the Jauho–Meir–Wingreen formula

The Langreth identity

Decoupled reservoir Green's functions are **one-particle** objects

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Decoupled reservoir Green's functions are **one-particle** objects

For $f, g \in \mathfrak{h}_j$:

$$\begin{aligned}
\langle f | G_D^{a/r}(s,s') g \rangle &= \pm \mathrm{i}\theta(\pm(s-s')) \left\langle \{ \tau_{K_D}^{s'}(a^*(g)), \tau_{K_D}^{s}(a(f)) \} \right\rangle_{\beta,\mu} \\
&= \pm \mathrm{i}\theta(\pm(s-s')) \langle f | \mathrm{e}^{\mathrm{i}(s'-s)h_j} g \rangle \\
\langle f | G_D^{<}(s,s') g \rangle &= +\mathrm{i} \left\langle \tau_{K_D}^{s'}(a^*(g)) \tau_{K_D}^{s}(a(f)) \right\rangle_{\beta,\mu} \\
&= +\mathrm{i} \langle f | \mathrm{e}^{\mathrm{i}(s'-s)h_j} (1 + \mathrm{e}^{\beta_j(h_j-\mu_j)})^{-1} g \rangle \\
\langle f | G_D^{>}(s,s') g \rangle &= -\mathrm{i} \left\langle \tau_{K_D}^{s}(a(f)) \tau_{K_D}^{s'}(a^*(g)) \right\rangle_{\beta,\mu} \\
&= -\mathrm{i} \langle f | \mathrm{e}^{\mathrm{i}(s'-s)h_j} (1 + \mathrm{e}^{-\beta_j(h_j-\mu_j)})^{-1} g \rangle
\end{aligned}$$

The Langreth identity

Decoupled reservoir Green's functions are **one-particle** objects

Theorem 1

$$\langle \phi_j | G^<(t,t')\psi_j\rangle = d_j \int_0^\infty \Big(\langle \phi_j | G^r(t,s) | \phi_j \rangle \langle \psi_j | G_D^<(s,t')\psi_j \rangle + \langle \phi_j | G^<(t,s) | \phi_j \rangle \langle \psi_j | G_D^a(s,t')\psi_j \rangle \Big) \mathrm{d}s$$

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Using the Duhamel formula

$$\tau_K^t(A) = \tau_{K_D}^t(A) + \int_0^t \tau_K^s(\mathrm{i}[H_T, \tau_{K_D}^{t-s}(A)])\mathrm{d}s$$

the interaction picture

$$\tau_K^t(A) = \Gamma_t^* \tau_{K_D}^t(A)\Gamma_t, \qquad \mathrm{i}\partial_t \Gamma_t = \tau_{K_D}(H_T)\Gamma_t$$

the anti-commutation relations and the KMS property, the proof reduces to some elementary algebra (no Keldysh contour integral nor "analytic continuation" needed).

The Jauho–Meir–Wingreen formula

Both the local carrier density in the sample and the current from the reservoirs are easily expressed in terms of interacting lesser Green's functions

$$\rho(x,t) = \left\langle \tau_K^t(a_x^* a_x) \right\rangle_{\beta,\mu} = \mathrm{Im}\langle x | G^<(t,t) x \rangle$$

$$I_j(t) = \mathrm{i} d_j \left\langle \tau_K^t(a^*(\psi_j) a(\phi_j) - a^*(\phi_j) a(\psi_j)) \right\rangle_{\beta,\mu} = 2 d_j \mathrm{Re}\langle \phi_j | G^<(t,t) \psi_j \rangle$$

The Jauho–Meir–Wingreen formula

Both the local carrier density in the sample and the current from the reservoirs are easily expressed in terms of interacting lesser Green's functions

$$\rho(x,t) = \left\langle \tau_K^t(a_x^* a_x) \right\rangle_{\beta,\mu} = \mathrm{Im}\langle x|G^<(t,t)x\rangle$$

$$I_j(t) = \mathrm{i}d_j \left\langle \tau_K^t(a^*(\psi_j)a(\phi_j) - a^*(\phi_j)a(\psi_j)) \right\rangle_{\beta,\mu} = 2d_j \mathrm{Re}\langle\phi_j|G^<(t,t)\psi_j\rangle$$

Theorem 1 then immediately yields

The JMW Transient Current Formula

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

The calculation of transient density and currents is thus reduced to that of the interacting sample Green's functions matrices

$$[\langle x|G^{r/<}(s,s')|y\rangle]_{x,y\in\mathcal{S}}$$

Nonequilibrium self-energies & Dyson equations

Advanced/Retarded Dyson Equations

Theorem 2

There exists continuous maps

$$\mathbb{R}_+ \times \mathbb{R}_+ \ni (s, s') \mapsto \Sigma^{a/r}(s, s') \in \mathcal{L}(\mathfrak{h}_{\mathcal{S}})$$

such that the following Dyson equations hold

$$\begin{aligned} G^{a/r}(t, t') &= G_0^{a/r}(t, t') + \int_0^\infty \mathrm{d}s \int_0^\infty \mathrm{d}s'\, G_0^{a/r}(t, s)\Sigma^{a/r}(s, s')G^{a/r}(s', t') \\ &= G_0^{a/r}(t, t') + \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r'\, G^{a/r}(t, s)\Sigma^{a/r}(s, s')G_0^{a/r}(s', t') \end{aligned}$$

Moreover the irreducible self-energy $\Sigma^{a/r}(s, s')$ is an entire analytic function of the coupling constant ξ.

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Observe that these Dyson equations can be restricted to the sample. So, for given self-energy they give a finite dimensional integral equation for the sample interacting r/a-Green's functions. This equation can be solved by geometric series

$$G = G_0 + G_0\Sigma G \quad \Longrightarrow \quad G = \sum_{N \geq 0} G_0(\Sigma G_0)^N = G_0(I - \Sigma G_0)^{-1}$$

Truncating the lesser Green's function

Using the Duhamel formulas

$$\tau_K^t(A) = \tau_H^t(A) + \xi \int_0^t \tau_K^s \left(\mathrm{i}[W, \tau_H^{t-s}(A)]\right) \mathrm{d}s$$

$$\tau_H^t(A) = \tau_{H_D}^t(A) + \int_0^t \tau_{H_D}^s \left(\mathrm{i}[H_T, \tau_H^{t-s}(A)]\right) \mathrm{d}s$$

one shows

Lemma

Assume that the restriction of the initial state to the sample is the vacuum state and define a linear operator on $\mathfrak{h}_{\mathcal{S}}$ by its matrix elements

$$S^<_{xx'}(s,s') = \mathrm{i}\left\langle \mathcal{T}^*_{x'}(s')\mathcal{T}_x(s)\right\rangle_{\beta,\mu}$$

where

$$\mathcal{T}_x(s) = a(\mathrm{e}^{\mathrm{i}sh_D} h_T \delta_x) + \xi \tau_K^s(a_x V_x), \qquad V_x = \sum_{y \in \mathcal{S}} w(x,y) a_y^* a_y$$

Then, for $\phi, \phi' \in \mathfrak{h}_{\mathcal{S}}$

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

Lesser Dyson Equation

Combining the Lemma with Theorem 2 one gets

Theorem 3

Assume that the restriction of the initial state to the sample is the vacuum state. There exists a continuous map

$$\mathbb{R}_+ \times \mathbb{R}_+ \ni (s, s') \mapsto \Sigma^<(s, s') \in \mathcal{L}(\mathfrak{h}_\mathcal{S})$$

such that, for $\phi, \phi' \in \mathfrak{h}_\mathcal{S}$,

$$\langle \phi | G^<(t, t') \phi' \rangle = \int_0^\infty \mathrm{d}s \int_0^\infty \mathrm{d}s' \langle \phi | G^r(t, s) \Sigma^<(s, s') G^a(s', t') \phi' \rangle$$

Moreover the irreducible self-energy $\Sigma^<(s, s')$ is an entire analytic function of the coupling constant ξ.

Ideas for the proof of Theorem 2

For $\pm\mathrm{Im} z > 0$

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

defines a bounded operator on $\mathcal{K} = L^2(\mathbb{R}, \mathrm{d}s) \otimes \mathfrak{h}$ such that

$$G^{\pm}(z)^* = G^{\mp}(\bar{z}), \qquad G^{\pm}(z)\mathcal{K}_{\mp} \subset \mathcal{K}_{\mp}$$

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By explicit calculation and some integration by parts, one shows that

$$(\Omega - z)G^{\pm}(z)(\Omega - z) = \Omega + \widetilde{\Sigma}^{\pm}(z) - z$$

where $\widetilde{\Sigma}^{\pm}(z)$ denotes the bounded operator on $\mathcal{K}_{\mathcal{S}} = L^2(\mathbb{R}, \mathrm{d}s) \otimes \mathfrak{h}_{\mathcal{S}}$ given by

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

with

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

and

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

Ideas for the proof of Theorem 2

It follows that

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

where $\widetilde{\Sigma}^{\pm}(z)$ is the **reducible** self-energy.

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The operator $I + G_0^{\pm}(z)\widetilde{\Sigma}^{\pm}(z)$ is of Volterra type II and hence invertible. Setting

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

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Letting $\mathrm{Im}(z) \to 0$ finally gives Theorem 2.

Outlook

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We provide a systematic mathematical approach to the non-equilibrium Green's function formalism for interacting transport in open systems. We follow a three-steps bottom-up strategy only using real-time GFs (i.e., retarded, advanced and lesser):

1. We relate the transient current $I_j(t)$ to the fully interacting GF $\langle \phi_j | G^<(t,t)\psi_j \rangle$.
2. Combining the available modular structure, i.e., the KMS conditions induced by the thermal states of the reservoirs, with Duhamel identities we show that $\langle \phi_j | G^<(t,t)\psi_j \rangle$ obeys a Langreth-type identity whose rhs involves only the interacting sample GF $\langle \phi_j | G^<(t,t)\phi_j \rangle$ and $\langle \phi_j | G^r(t,t)\phi_j \rangle$. This immediately implies the JMW formula
3. We construct a retarded self-energy operator Σ^r connecting $\langle \phi_j | G^r(t,t)\phi_j \rangle$ to its non-interacting counterpart through a Dyson equation. We then derive the Keldysh equation relating $\langle \phi_j | G^<(t,t)\phi_j \rangle$ to a lesser interaction self-energy $\Sigma^<$ for which we provide an explicit expression.

To be worked out in the future:

- Allowing initial correlations in the sample.
- Partition-free setting.
- Feynman rules for the self-energies.

Thank you !