Time-dependent adiabatic *GW*

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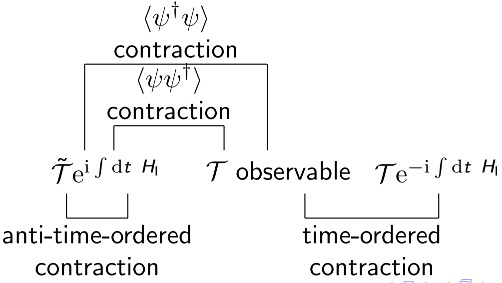
Non-equilibrium Green function

Motivation

$$\langle A \rangle = \langle S^{-1} \mathcal{T}_t (S A_\mathrm{I}(t)) \rangle \,, \quad S = U(\infty, -\infty) \tag{1}$$

Non-equilibrium state: not pure; contains excited state components; $|\Psi_n\rangle$ is excited state $\Rightarrow S|\Psi_n\rangle \neq \mathrm{e}^{\mathrm{i}\,\alpha}|\Psi_n\rangle \Rightarrow$ we can't peel the S^{-1} off!!

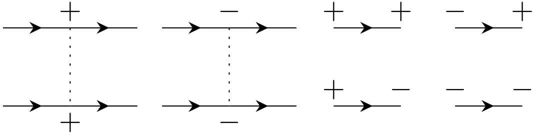
Solution Four (instead of one) types of propagators: (note S^{-1} is *anti*-time ordered)



Four types of (fermionic) propagators

$$
\begin{aligned}
\mathrm{i}\, G^{--} &= \mathrm{i}\, G^{\mathrm{c}} = \langle \mathcal{T}\, \psi_1 \psi_2^\dagger \rangle\,, \quad \mathrm{i}\, G^{++} = \mathrm{i}\, G^{\mathrm{a}} = \langle \tilde{\mathcal{T}} \psi_1 \psi_2^\dagger \rangle\,, \\
\mathrm{i}\, G^{+-} &= \mathrm{i}\, G^{>} = \langle \psi_1 \psi_2^\dagger \rangle\,, \quad \mathrm{i}\, G^{-+} = \mathrm{i}\, G^{<} = - \langle \psi_2^\dagger \psi_1 \rangle\,.
\end{aligned} \tag{2}
$$

Diagrams

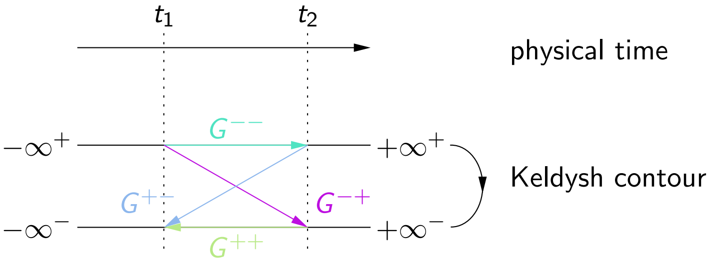


Self-energy

$$
G = \begin{pmatrix} G^{--} & G^{-+} \\ G^{+-} & G^{++} \end{pmatrix}, \quad \Sigma = \begin{pmatrix} \Sigma^{--} & \Sigma^{-+} \\ \Sigma^{+-} & \Sigma^{++} \end{pmatrix}, \quad G = G_0 + G_0 \Sigma G. \tag{3}
$$

Alternative formulation: Keldysh contour

Keldysh contour The information in the G matrix can be alternatively stored in a time-ordered Green function on *Keldysh contour*



Green function EOM

From Keldysh contour to physical contour Lengreth theorem:

$$
\begin{aligned}
(AB)^< = A^{\mathrm{R}} B^< + A^< B^{\mathrm{A}}, \quad (AB)^> = A^{\mathrm{R}} B^> + A^> B^{\mathrm{A}}, \\
(AB)^{\mathrm{R}} = A^{\mathrm{R}} B^{\mathrm{R}}, \quad (AB)^{\mathrm{A}} = A^{\mathrm{A}} B^{\mathrm{A}},
\end{aligned} \tag{4}
$$

where

$$
\begin{aligned}
A^>(t_1, t_2) = A(t_1^+, t_2^-), \quad A^<(t_1, t_2) = A(t_1^-, t_2^+), \\
A^{\mathrm{R}}(t_1, t_2) = \theta(t_1 - t_2)(A^> - A^<).
\end{aligned} \tag{5}
$$

Mapping an equation on Keldysh contour to its counterpart on the physical time axis!

Derivation of EOM of $G^{<,>}$ and G^{A} I

Recommended references The following series:

- Václav Špička, Bedřich Velickỳ, and Anděla Kalvová. "Long and short time quantum dynamics: I. Between Green's functions and transport equations". In: *Physica E: Low-dimensional Systems and Nanostructures* 29.1-2 (2005), pp. 154–174
- Jørgen Rammer and H Smith. "Quantum field-theoretical methods in transport theory of metals". In: *Reviews of modern physics* 58.2 (1986), p. 323

From self-energy correction to EOM From Lengreth theorem:

$$G = G_0 + G_0 \Sigma G \Rightarrow G^< = G_0^< + G_0^< \Sigma^{\mathrm{A}} G^{\mathrm{A}} + G_0^{\mathrm{R}} \Sigma^{\mathrm{R}} G^< + G_0^{\mathrm{R}} \Sigma^< G^{\mathrm{A}}, \quad (6)$$

$$G = G_0 + G \Sigma G_0 \Rightarrow G^< = G_0^< + G_0^{\mathrm{R}} \Sigma^{\mathrm{R}} G_0^< + G^{\mathrm{R}} \Sigma^< G_0^{\mathrm{A}} + G^< \Sigma^{\mathrm{A}} G^{\mathrm{A}}, \quad (7)$$

$$G^{\mathrm{A}} = G_0^{\mathrm{A}} + G_0^{\mathrm{A}} \Sigma^{\mathrm{A}} G^{\mathrm{A}}, \quad G^{\mathrm{R}} = G_0^{\mathrm{R}} + G_0^{\mathrm{R}} \Sigma^{\mathrm{R}} G^{\mathrm{R}}. \quad (8)$$

Getting rid of G_0 We define

$$G_0^{-1} := \mathrm{i}\, \partial_t - H_0, \quad (9)$$

and

$$G_0^{-1} G_0^{\mathrm{A,R}} = I, \quad G_0^{-1} G_0^{<,>} = 0. \quad (10)$$

Taking complex conjugate of the def. of $G_0^{<,>}$ we find (left arrow = apply ∂_t and H_0 to the second index of $G_0^{<,>}$)

$$G_0^{<,>} (-\mathrm{i}\, \overleftarrow{\partial_{t_2}} - H_0) = 0. \quad (11)$$

The Schrödinger-like EOM Applying G_0^{-1} to the left of (6) and to the right of (7):

$$(\mathrm{i}\,\partial_{t_1} - H_0)G^<(1,2) = \Sigma^{\mathrm{R}} G^< + \Sigma^< G^{\mathrm{A}}, \tag{12}$$

$$-\mathrm{i}\,\partial_{t_2} G^<(1,2) - G^< H_0 = G^{\mathrm{R}}\Sigma^< + G^<\Sigma^{\mathrm{A}}, \tag{13}$$

$$\Rightarrow \mathrm{i}(\partial_{t_1} + \partial_{t_2})G^< - [H_0, G^<] = \Sigma^{\mathrm{R}} G^< + \Sigma^< G^{\mathrm{A}} - G^{\mathrm{R}}\Sigma^< - G^<\Sigma^{\mathrm{A}}. \tag{14}$$

Mixed coordinates We define "average time" and "relative time":

$$T = \frac{t_1 + t_2}{2}, \quad t = t_1 - t_2, \tag{15}$$

$$\Rightarrow \frac{\partial}{\partial T} = \frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2}. \tag{16}$$

We then do Fourier transform over t: similar to the equilibrium case. ($T \simeq$ driving, $t \simeq$ internal time evolution)

Towards a single-time formalism

Summary up to now

- *Accurate* EOMs about $G^{\mathrm{A,R}}$, and EOM of $G^{<}$:

$$\mathrm{i}\,\partial_T G^{<} - [H_0, G^{<}] = \Sigma^{\mathrm{R}} G^{<} + \Sigma^{<} G^{\mathrm{A}} - G^{\mathrm{R}} \Sigma^{<} - G^{<} \Sigma^{\mathrm{A}}. \tag{17}$$

  The RHS contains t (or ω) and $G^{<}$.

- Note: we can actually put the $t = 0$ part of Σ into H_0! $\Rightarrow$ Example: COHSEX TD-aGW

Goal Obtaining quantum kinetics:

- Quantum master equation (QME), i.e. EOM of $\rho(\boldsymbol{r}_1, \boldsymbol{r}_2, t)$,
- and its long wave length limit, the quantum Boltzmann equation (QBE)

Problem Both LHS and RHS contain ω: problem too large.
What we want Obtaining a close form EOM about $G^{<}(T, t = 0)$

Reconstruction of $G^<$

Reduced density matrix Single-electron density matrix:

$$\mathrm{i}\,\rho(T) = G^<(T, t=0) = \int \frac{\mathrm{d}\omega}{2\pi} G^<(T, \omega) \tag{18}$$

What we want Two types of reduction:

- Reducing Σ to an easy function of G, ideally $G^<$
- Reducing $G^<$ to $\rho(T)$

Reducing Σ

Gradient expansion: from QME to QBE

Approximations leading to QBE

- Gradient expansion: smooth U_{ext}:

$$[H_0, \rho] \tag{19}$$

- Quasiparticle approx.

$$G^{<}(\boldsymbol{x}, \boldsymbol{p}, T, \omega) = 2\pi\delta(\omega -) \tag{20}$$

Immediate problem:

TODO: how to get the Fermi golden rule???

Example: TODO