Nonrelat. inhomogenius Greensfunctions in open thermal systems via Kadanoff-Baym Equations

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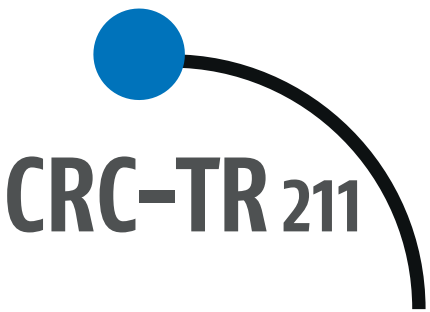

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Introduction

- the binding energies of light nuclei are much smaller then temperature of the environment (snowballs in hell)
- how fast do they form and how broad are they
- a quantum mechanical description of creation and decay of bound states (the nuclei) in an open thermal system (fireball) is needed
- use the framework of Kadanoff-Baym equations to analyse the time evolution of occupation numbers and spectral functions
- These are obtained via non-equilibrium Greensfunctions

Schwinger-Keldysh-Contour

- The one-particle Greensfunction is defined as a corrolation function i.e. an expectation value of two (Heisenberg) operators

$$G(1,1') = -i\left\langle T_c\left[\hat{\psi}(r,t)\hat{\psi}(r',t')^\dagger\right]\right\rangle$$

- Where T_c is the time ordering operator:

$$T_c = \begin{cases} \hat{\psi}(r,t)\hat{\psi}(r',t')^\dagger & \text{if } t > t' \\ \pm\hat{\psi}(r',t')^\dagger\hat{\psi}(r,t) & \text{if } t \leq t' \end{cases}$$

- the $\pm$ corresponds to bosons/fermions. The operators are defined as:

$$\hat{\psi}(r,t) = e^{i\hat{H}t}\underbrace{\sum_k \phi_k(r)\hat{c}_k}_{=\hat{\psi}(r)}e^{-i\hat{H}t}$$

Schwinger-Keldysh-Contour

- To ”see” the contour, we switch to the interaction representation:

$$\hat{\psi}(r,t) = \hat{U}_I(-\infty,t)\hat{\psi}_I(r,t)\hat{U}_I(t,-\infty)$$

- Where $\hat{U}_I(t,t_1)$ is the time evolution operator in this representation:

$$\hat{U}_I(t,t_1) = T_c\left[exp(-i\int_{t_1}^{t} dt'\,\hat{H}_{int}(t'))\right]$$

- substituting these expressions in the definition of the Greensfunction with Heienberg operators will lead us to the Schwinger-Keldysh-Contour! Assume $t > t'$

Schwinger-Keldysh-Contour

$$
\begin{aligned}
G^{>}(1,1') &= \frac{-i}{Z} Tr\left\{ e^{-\beta \hat{H}} \hat{\psi}(r,t) \hat{\psi}(r',t')^{\dagger} \right\} \\
&= \frac{-i}{Z} Tr\left\{ \hat{U}_I(-\infty,\infty) e^{-\beta \hat{H}} \hat{U}_I(\infty,-\infty) \hat{U}_I(-\infty,t) \hat{\psi}_I(r,t) \hat{U}_I(t,-\infty) \right. \\
&\quad \left. \hat{U}_I(-\infty,t') \hat{\psi}_I(r',t')^{\dagger} \hat{U}_I(t',-\infty) \right\} \\
&= \frac{-i}{Z} Tr\left\{ \hat{U}_I(-\infty,\infty) e^{-\beta \hat{H}} \hat{U}_I(\infty,t) \hat{\psi}_I(r,t) \right. \\
&\quad \left. \hat{U}_I(t,t') \hat{\psi}_I(r',t')^{\dagger} \hat{U}_I(t',-\infty) \right\} \\
&= \frac{-i}{Z} Tr\left\{ e^{-\beta \hat{H}} T_c\left[\hat{U}_C \hat{\psi}_I(r,t) \hat{\psi}_I(r',t')^{\dagger} \right] \right\}
\end{aligned}
$$

- in the last line the time-ordering operator was inserted to place the field operators at the right time point
- because of the time-ordering operator this works also for $t < t'$, so it works for the whole Greensfunction!

Schwinger-Keldysh-Contour

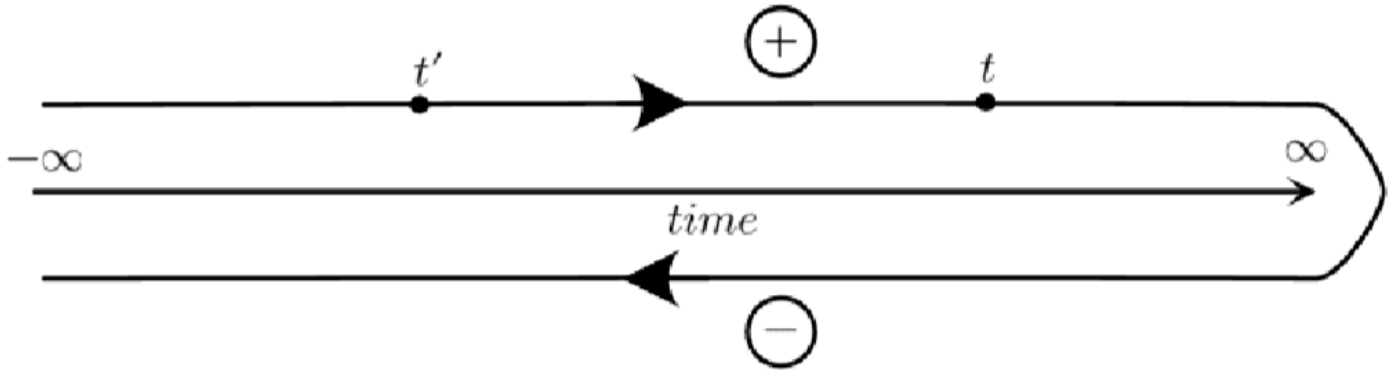

Figure: Taken from ”Advanced Statistical Physics: Many-Body out of equilibrium” by Oleksandr Tsyplyatyev

- the upper contour is going from $-\infty$ to ∞ representing the time ordering of the field operators
- the lower part going the reverse way outside of the time ordering operator
- in general there are three other Greensfunction (upper-lower, lower-upper and lower-lower)

Kadanoff-Baym equations

- The Kadanoff-Baym equations are equation of motion for the Greensfunction, obtained from the Dyson equation by multiplying with the invers propagator

$$G(\bar{1},1') = G_0(\bar{1},1') + \int_C d2 \int_C d3 G_0(\bar{1},2)\Sigma(2,3)G(3,1')$$

$$G_0^{-1}(1,\bar{1})G(\bar{1},1') = \underbrace{G_0^{-1}(1,\bar{1})G_0(\bar{1},1')}_{\delta_c(1,1')=\delta_c(t-t')\delta(x_1-x_{1'})} + \int_C d3\Sigma(1,3)G(3,1')$$

- Where $G_0^{-1}(1,\bar{1})$ is:

$$G_0^{-1}(1,\bar{1}) = \left(i\frac{\partial}{\partial t_1} + \frac{\Delta_1}{2m_f} - V(r)\right)\delta_c(1,\bar{1})$$

Kadanoff-Baym equations

- the equation for t' can be obtained similar:

$$G(1,\bar{1})G_0^{\dagger\,-1}(\bar{1},1') = \delta_c(1,1') + \int_C d3\, G(1,3)\Sigma(3,1')$$

- Σ denotes the self-energy, an irreducible part of the Greensfunction, which is often introduced variationally
- the general form contains also singular (in time) contributions on the contour: (P. Danielewicz, Ann. Phys. (N.Y.) 152, 239 (1984))

$$\Sigma(1,1') = \underbrace{\Sigma^{\delta}(1,1')}_{\propto\delta_c(t_1-t_{1'})} + \Theta_c(t_1,t_{1'})\Sigma^{>}(1,1') + \Theta_c(t_{1'},t_1)\Sigma^{<}(1,1')$$

- To solve a system completly, we need to propagate $G^{>}$ and $G^{<}$ for t and t'

1+1 dim Testmodel

- The Hamiltonian should describe a system of (heavier) fermions scattering with free ”heatbath” bosons

$$\hat{H}(t) = \underbrace{\int dr \hat{\psi}(r,t)^\dagger \underbrace{\left(-\frac{\Delta}{2m_f} + V(r)\right)}_{=h_0} \hat{\psi}(r,t)}_{=\hat{H}_0(t)} + \underbrace{\lambda \int dr \hat{\psi}(r,t)^\dagger \hat{\phi}(r,t)^\dagger \hat{\psi}(r,t) \hat{\phi}(r,t)}_{=\hat{H}_{int}(t)}$$

- ”heatbath” means, that the bosons are kept always in equilibrium and therefore do not need to be evolved in time by Kadanoff-Baym equ.
- The lowest contributions to the Selfenergy are given by the Hartree- and the (direct) Born-diagram

1+1 dim Testmodel

- we do not assume homogeneity in our model, so the Greensfunction does not only depend on relative differences!
- this is different to the state of the art in the past, where these equations were transformed in momentum space and solved via FFT (H. S. Koehler, N. H. Kwong, and H. A. Yousif, Comput. Phys. Commun. 123, 123 1999)
- the fermionic Greensfunctions are expanded in a set of eigenfunctions of the Hamiltonian, e.g DFT-orbitals in atomic-theory (Stan et al,Time propagation of the KadanoffBaym equations for inhomogeneous systems, The Journal of Chemical Physics, AIP Publishing, 2009, 130, 224101) or as in this test case free particles

$$S^{>}(1,1') = -i \sum_{n,m=1} \langle \hat{c}_n(t) \hat{c}_m(t')^{\dagger} \rangle \phi_n(r) \phi_m(r')^{*}$$

$$S^{<}(1,1') = i \sum_{n,m=1} \langle \hat{c}_m(t')^{\dagger} \hat{c}_n(t) \rangle \phi_n(r) \phi_m(r')^{*}$$

$$h_0 \phi_n(r) = E_n \phi_n(r)$$

1+1 dim Testmodel

- obtain (ordinary) integro-differential equ. for the time dependent matrix-valued coefficients of $S^{>}$ in t direction and neglect the Hartree-Term for simplicity

$$\left(i\frac{\partial}{\partial t}+\frac{\Delta_1}{2m_f}-V(1)\right)S^{>}(1,1')=\int_{t_0}^{t}d\bar{1}\left[\Sigma^{>}(1,\bar{1})-\Sigma^{<}(1,\bar{1})\right]S^{>}(\bar{1},1')$$
$$-\int_{t_0}^{t'}d\bar{1}\Sigma^{>}(1,\bar{1})\left[S^{>}(\bar{1},1')-S^{<}(\bar{1},1')\right]$$

$$\Sigma^{>}(1,1')=(i\lambda)^2S^{>}(1,1')D_0^{>}(1,1')D_0^{<}(1',1)$$
$$\Sigma^{<}(1,1')=(i\lambda)^2S^{<}(1,1')D_0^{<}(1,1')D_0^{>}(1',1)$$

- Here D_0 represents the Greensfunction of the ”heatbath” bosons

1+1 dim Testmodel

- As mentioned, we assume, that these bosons stay in equilibrium (even after scattering)
- for the 1+1 dim case in a testbox:

$$D_0^{>}(1,1') = -i \sum_{n=1} \exp(-i\varepsilon_n(t-t'))(1+n_B(\varepsilon_n))\sin(k_n r)\sin(k_n r')$$
$$D_0^{<}(1,1') = -i \sum_{n=1} \exp(-i\varepsilon_n(t-t'))n_B(\varepsilon_n)\sin(k_n r)\sin(k_n r')$$

- were $k_n = \frac{\pi n}{L_{bath}}$, $\varepsilon_n = \frac{k_n^2}{2m_b} - \mu$ and $n_B(\varepsilon_n) = \frac{1}{\exp(\varepsilon_n/T)-1}$

1+1 dim Testmodel

- now we insert this Ansatz in the Kadanoff-Baym equations and use the eigenvalue equation on the lhs
- in the next step the orthogonality of the eigenfunction is used to integrate out the position dependency which yields the lhs:

$$\frac{\partial}{\partial t} c^{>}_{b,a}(t,t') + iE_b c^{>}_{b,a}(t,t')$$

- the rhs looks a bit more complicated after this manipulations. only for the first term:

$$-\lambda^2 \int_{t_0}^{t} d\bar{t} \sum_{m,n,i}^{f} \Big(\sum_{j,k}^{b} \exp\big(-\mathrm{i}(\varepsilon_\mathrm{j} - \varepsilon_\mathrm{k})(\mathrm{t} - \bar{\mathrm{t}})\big) \left(1 + \mathrm{n_B}(\varepsilon_\mathrm{j})\right) \mathrm{n_B}(\varepsilon_\mathrm{k}) \underbrace{\int dr \phi_b(r)^* \phi_n(r) \sin(\mathrm{k_j r}) \sin(\mathrm{k_k r})}_{= V_{b,n,j,k}} c^{>}_{n,m}(t,\bar{t})\, V_{m,i,k,j}\, c^{>}_{i,a}(\bar{t},t') \Big)$$

1+1 dim Testmodel

- The Algorithm used to solve these highly coupled system of equations is a Predictor-Corrector tandem of explicit and implicit linear multistep methods (Adams-Bashforth-Moulten)
- explicit methods are faster, but become very fast unstable
- implicit methods are highly stable and accurate, but become very slow because of the need to solve a huge system of nonlinear equations
- the method used here is also more practical than standard Runge-Kutta Methods, because you need less function evaluation there

1+1 dim Testmodel

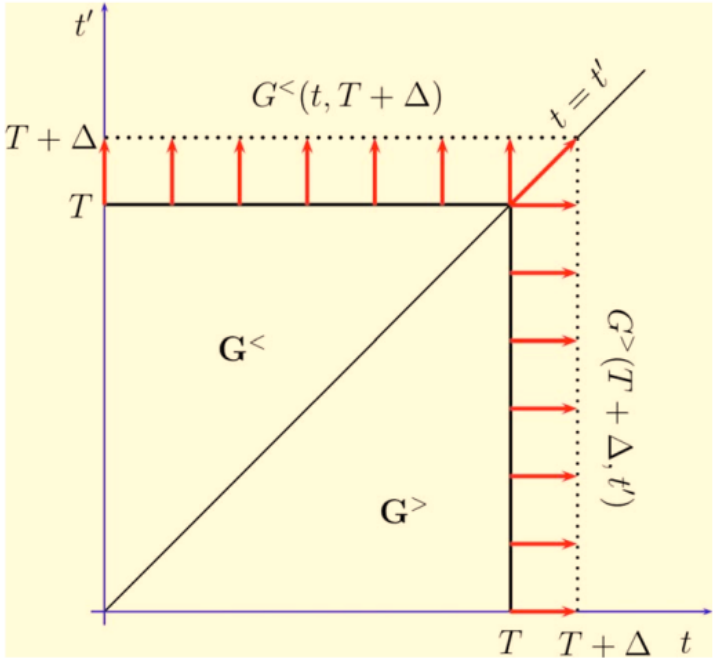

Figure: Stan et al,Time propagation of the KadanoffBaym equations for inhomogeneous systems, The Journal of Chemical Physics, 2009

- the corresponding values of the functions on the other triangle are obtained by symmetry relations: $-S^{\gtrless}(1,1')^{\dagger} = S^{\gtrless}(1',1)$
- on the time diagonal only the ”lesser” function is propagated and the equal-time commutation relation is used for the ”greater” part

Results

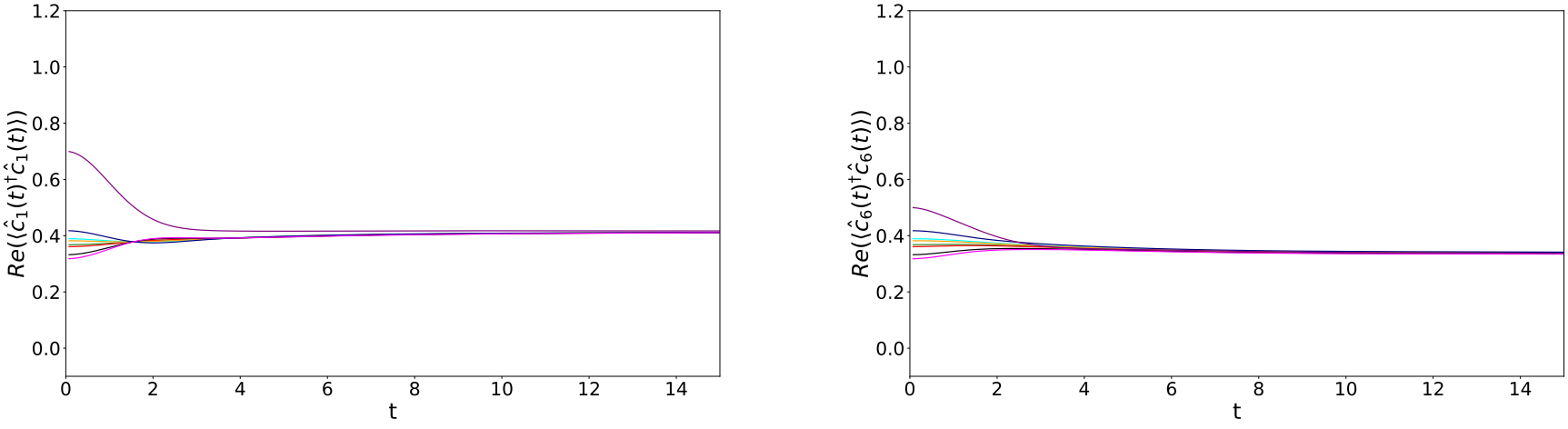

Figure: Equilibration of the 2. state with $E_1 \approx 2.04\mathrm{MeV}$ and the 6. state with $E_6 \approx 18.4\mathrm{MeV}$ in a Box with $L//L_{bath} = 20//200\mathrm{fm}$, Temperature $T = 20\mathrm{MeV}$ and a coupling $\lambda = 0.4$

Results

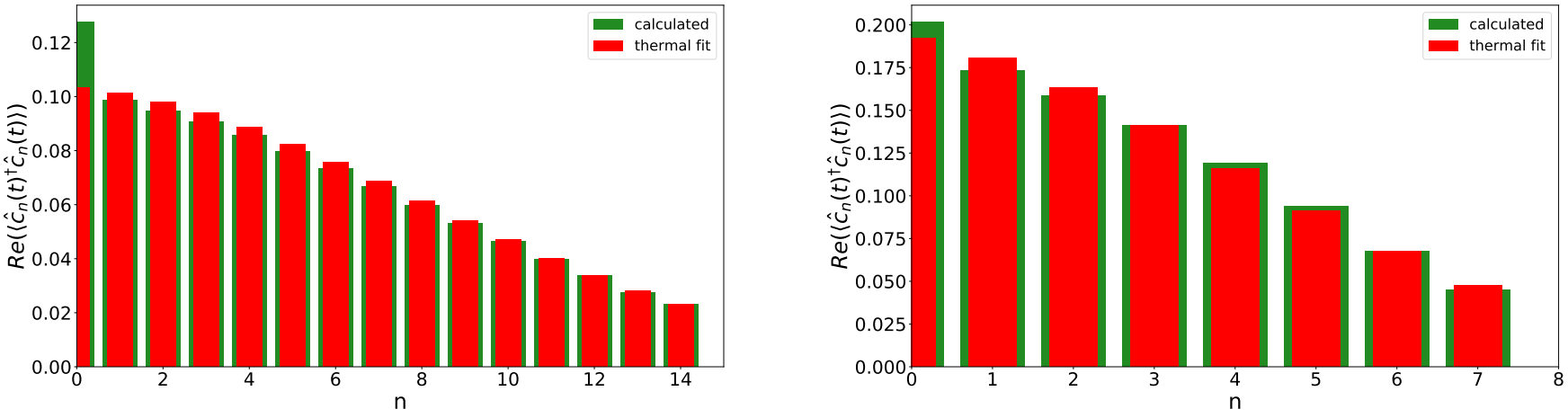

Figure: ”Final states” for different number of states fited to Fermi-Dirac distribution. Left $T \approx 52\mathrm{MeV}$, $\mu \approx -134\mathrm{MeV}$ and right $T \approx 71\mathrm{MeV}$, $\mu \approx -117\mathrm{MeV}$.

Results

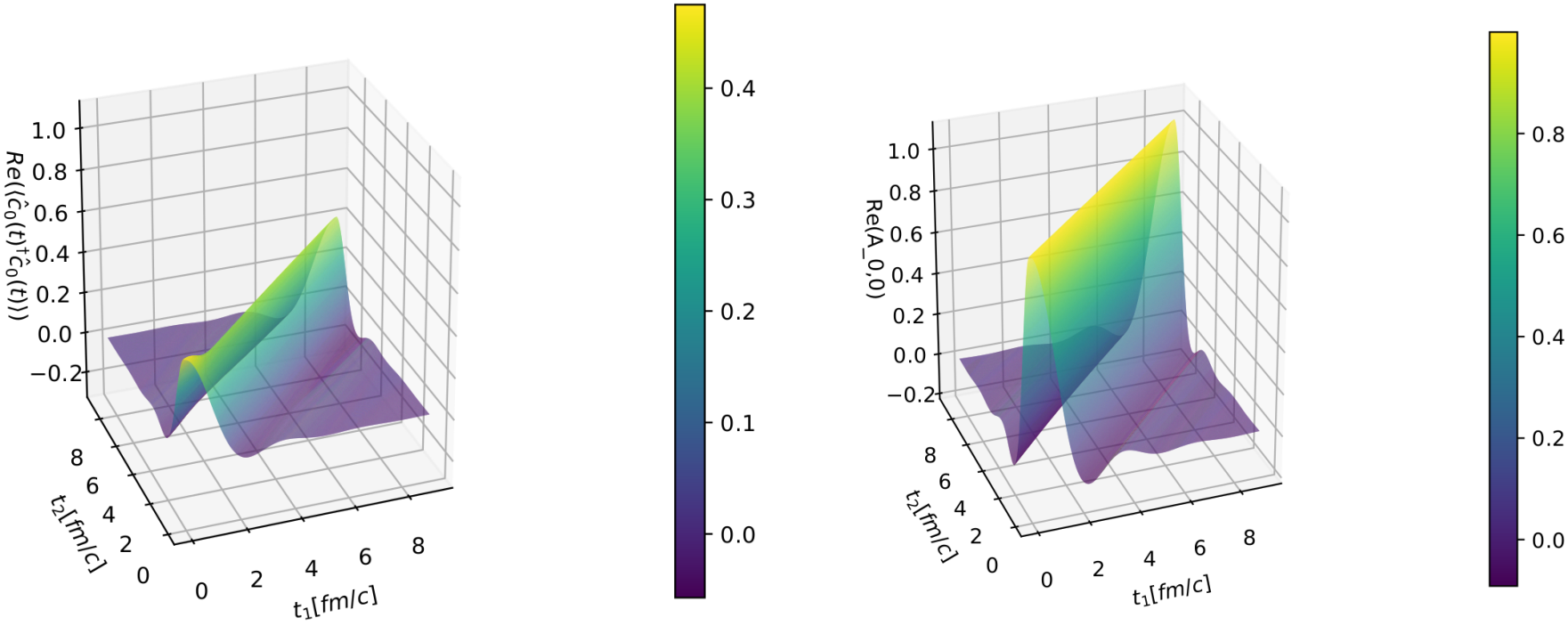

Figure: Real part of the (0,0) coefficient left and of the spectral function of this coefficient defined as: $A_{0,0}(t_1, t_2) = \left\langle [\hat{c}_0(t_1), \hat{c}_0(t_2)^\dagger]_+ \right\rangle$

Conclusions and Outlook

Conclusion:

- short introduction to non-relativistic, non-equilibrium Greensfunctions
- presentation of the used method to solve the coupled integro-differential equations for a simple testbox
- some preliminary results for equilibration of the sytem and problem of thermalisation

Outlook:

- compute spectral function in energy domain, to have an idea of the width (lifetime) of the states
- include potential to observe bound-state formation and decays
- extend it to 3+1 dimensions $\rightarrow$ OMP to MPI is necessary because of runtime