Open Quantum Systems with the Kadanoff-Baym Approach

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Introduction

- the binding energies of light nuclei are much smaller than the 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 Green’s functions
  $\rightarrow$ Schwinger-Keldysh Contour
- Open bosonic systems from Lindblad equation

Schwinger-Keldysh Contour

- The one-particle Green's function 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 Green's function and assume $t > t'$

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

Schwinger-Keldysh Contour

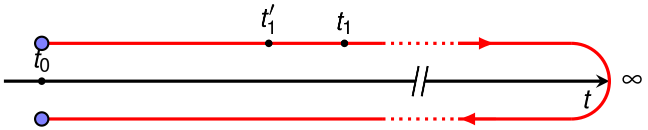
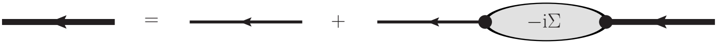


Figure: The closed-time path C. Thanks to David Wagner

- in “real” simulations, one can not start at $t_0 = -\infty$ and switch on the coupling adiabatically
- for a generall corrolated initial state, an imaginary time evolution would be needed
- because we couple to a heatbath later, there is no need for this and the temperature will be well defined

Kadanoff-Baym equations



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

- by multiplying with the (free) inverse propagator and integrating over $\bar{1}$

$$\int_C d\bar{1}\, G_0^{-1}(1,\bar{1})G(\bar{1},1') = \underbrace{\int_C d\bar{1}\, G_0^{-1}(1,\bar{1})G_0(\bar{1},1')}_{\delta_c(1,1')=\delta_c(t-t')\delta(x_1-x_{1'})}$$
$$+ \int_C d\bar{1} \int_C d2 \int_C d3 G_0^{-1}(1,\bar{1})G_0(\bar{1},2)\Sigma(2,3)G(3,1')$$

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

$$G_0^{-1}(1,\bar{1}) = \left(i\frac{\partial}{\partial t_1} + \frac{\Delta_1}{2m_f} - V(r_1)\right)\delta_c(1,\bar{1})$$

Kadanoff-Baym equations

- the equation for t' can be obtained similarly:

$$G(1,1')\left(-i\frac{\partial}{\partial t_1'}+\frac{\Delta_{1'}}{2m_f}-V(r_1')\right)=\delta_c(1,1')+\int_C d3G(1,3)\Sigma(3,1')$$

- Σ denotes the self-energy, an 1PI part of the Green's function, which is introduced by variational principle
- 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 completely, we need to propagate $G^{>}$ and $G^{<}$ for t and t'

1+1 dim test model

- The Hamiltonian should describe a system of (heavier) fermions scattering with free "heat-bath" bosons

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

$$+ \underbrace{\lambda \int dr\, \hat{\psi}(r,t)^\dagger \hat{\phi}(r,t)^\dagger \hat{\psi}(r,t) \hat{\phi}(r,t)}_{\hat{H}_{\mathrm{int}}(t)}$$

$$V(r) \begin{cases} -V_0 & \text{if } |r| \leq \frac{a}{2} \\ 0 & \text{if } |r| > \frac{a}{2} \\ \infty & \text{if } |r| > \frac{L}{2}, \end{cases}$$

- "heat-bath" means, that the bosons are kept always in equilibrium

1+1 dim test model

- the fermionic Green's functions are expanded in a set of eigenfunctions of the free Hamiltonian

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

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

- similar to the bosons

$$D_0^{>}(1,1') = -i \sum_{n}^{B} e^{-i\varepsilon_n(t-t')}(1+n_B(\varepsilon_n))\tilde{\phi}_n(r)\tilde{\phi}^*_n(r')$$

$$D_0^{<}(1,1') = -i \sum_{n}^{B} e^{-i\varepsilon_n(t-t')} n_B(\varepsilon_n)\tilde{\phi}_n(r)\tilde{\phi}^*_n(r')$$

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

1+1 dim test model

- Kadanoff-Baym equations:

$$\left(i\frac{\partial}{\partial t}+\frac{\Delta_1}{2m_f}-V_{\text{eff}}(1)\right)S^{\gtrless}(1,1')=I^{\gtrless}_{\text{coll}_1}(t,t')$$

$$\left(-i\frac{\partial}{\partial t'}+\frac{\Delta_{1'}}{2m_f}-V_{\text{eff}}(1')\right)S^{\gtrless}(1,1')=I^{\gtrless}_{\text{coll}_2}(t,t')$$

- with shortcuts

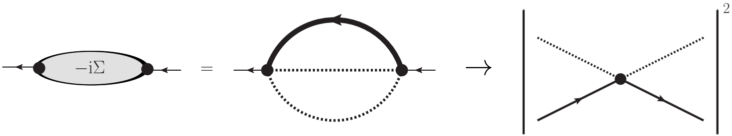
$$V_{\text{eff}}(1)=V(1)+\Sigma_H(1),$$

$$I^{\gtrless}_{\text{coll}_1}(t,t')=\int_{t_0}^{t}d\bar{1}\left[\Sigma^{>}(1,\bar{1})-\Sigma^{<}(1,\bar{1})\right]S^{\gtrless}(\bar{1},1')-\int_{t_0}^{t'}d\bar{1}\Sigma^{\gtrless}(1,\bar{1})\left[S^{>}(\bar{1},1')-S^{<}(\bar{1},1')\right]$$

$$I^{\gtrless}_{\text{coll}_2}(t,t')=\int_{t_0}^{t}d\bar{1}\left[S^{>}(1,\bar{1})-S^{<}(1,\bar{1})\right]\Sigma^{\gtrless}(\bar{1},1')-\int_{t_0}^{t'}d\bar{1}S^{\gtrless}(1,\bar{1})\left[\Sigma^{>}(\bar{1},1')-\Sigma^{<}(\bar{1},1')\right]$$

1+1 dim test model

- The lowest-order contributions to the self energy are given by the tadpole- and the sunset-diagram



- which will also be expanded in the same basis

$$\Sigma^{\gtrless}_{b,a}(t,t') = \lambda^2 \sum_{n,m}^{F} \Big(\sum_{j,k}^{B} e^{\mp i(\varepsilon_j - \varepsilon_k)(t-t')} \left(1 + n_B(\varepsilon_j)\right) n_B(\varepsilon_k)$$

$$\underbrace{\int dr \phi^*_b(r)\phi_n(r)\tilde{\phi}_j(r)\tilde{\phi}^*_k(r)}_{V_{b,n,j,k}} c^{\gtrless}_{n,m}(t,t')\, V_{m,a,k,j} \Big)$$

$$\Sigma_{H_{b,a}}(t) = \lambda \sum_{j}^{B} e^{-i\varepsilon_j(t-t^+)} n_B(\varepsilon_j) V_{b,a,j,j}$$

Spectral properties

- the two-time propagation allows to extract not only statistical but also spectral information of the system
- we introduce central time $\bar{T} = \frac{t+t'}{2}$ and relative time $\Delta t = t - t'$
- the spectral function is defined as the fourier transform in relative time of a

$$a_{n,m}(t,t') = c^{>}_{n,m}(t,t') + c^{<}_{n,m}(t,t')$$
$$\tilde{a}_{n,m}(\omega,\bar{T}) = \int d\Delta t \, e^{i\omega\Delta t} a_{n,m}(\bar{T} + \frac{\Delta t}{2}, \bar{T} - \frac{\Delta t}{2})$$

- for non-interacting systems, we see just a δ-peak at the "on-shell" frequency $\omega = \varepsilon_n$

Spectral properties

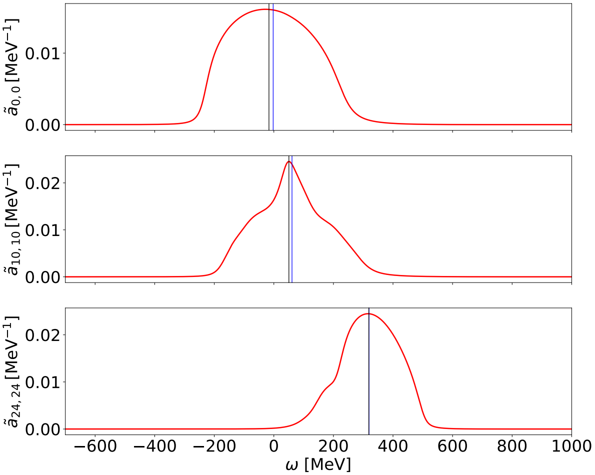


Figure: Spectral functions $\tilde{a}_{0,0}(\omega, \bar{T} = 52\text{fm})$, $\tilde{a}_{10,10}(\omega, \bar{T} = 52\text{fm})$ and $\tilde{a}_{24,24}(\omega, \bar{T} = 52\text{fm})$.

Spectral properties

- non-vanishing self energies will lead to a shift of the peak (real part of the retarded self energy) and a broadening of the delta-type (imaginary part of the retarded self energy) of the spectral function

$$Re(\Sigma^{\mathrm{ret}}_{n,m}(\bar{T},\omega)) = \frac{-i}{2}\int d\Delta t\, e^{i\omega\Delta t}\Big[sign(\Delta t)$$
$$\left(\Sigma^{>}_{n,m}\left(\bar{T}+\frac{\Delta t}{2},\bar{T}-\frac{\Delta t}{2}\right)+\Sigma^{<}_{n,m}\left(\bar{T}+\frac{\Delta t}{2},\bar{T}-\frac{\Delta t}{2}\right)\right)\Big]$$

$$\Gamma_{n,m}(\bar{T},\omega) = -2\,Im(\Sigma^{\mathrm{ret}}_{n,m}(\bar{T},\omega)) = \int d\Delta t\, e^{i\omega\Delta t}$$
$$\left[\left(\Sigma^{>}_{n,m}\left(\bar{T}+\frac{\Delta t}{2},\bar{T}-\frac{\Delta t}{2}\right)+\Sigma^{<}_{n,m}\left(\bar{T}+\frac{\Delta t}{2},\bar{T}-\frac{\Delta t}{2}\right)\right)\right]$$

- the width can be understood as an inverse life time of the state

Spectral properties

- the peak is shifted to

$$E_{\text{medium}} - E_n = \mathrm{Re}(\Sigma^{\text{ret}}_{n,n}(T, \omega = E_{\text{medium}}))$$

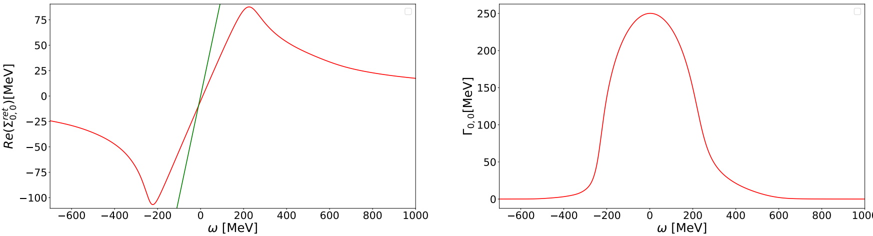


Figure: real part and imaginary part of the retarded self energy of the ground state for $\bar{T} = 52\mathrm{fm}$

Spectral properties

$$\tilde{a}_{0,0}(\omega,\bar{T}) = \frac{\Gamma_{0,0}(\omega,\bar{T})}{\left[\omega - E_0 - Re(\Sigma^{\mathrm{ret}}_{0,0}(\bar{T},\omega))\right]^2 + \left[\frac{\Gamma_{0,0}(\omega,\bar{T})}{2}\right]^2}$$

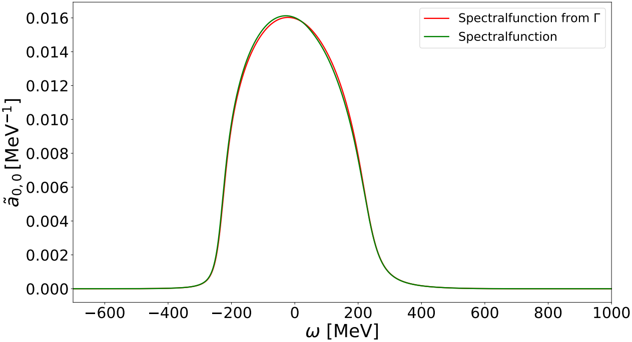


Figure: Spectral functions compared for $\bar{T} = 52\mathrm{fm}$.

Equilibration and Thermalization

- in the long-time limit the system should approach a thermal equilibration fixed point at temperature T_{bath}
- the diagonal elements $c^{<}_{n,n}(t,t)$ should approach the Fermi-Dirac distribution

$$\lim_{t\to\infty} c^{<}_{n,n}(t,t) = \int d\omega\, n_F(T_{\mathrm{syst}}, \mu_{\mathrm{syst}}, \omega)\, \tilde{a}_{n,n}(\omega, T)$$

- T_{syst} and μ_{syst} are extracted via a fit to all n under the constrains, that the trace of $c^{<}_{n,m}(t,t)$ is constant

Equilibration and Thermalization

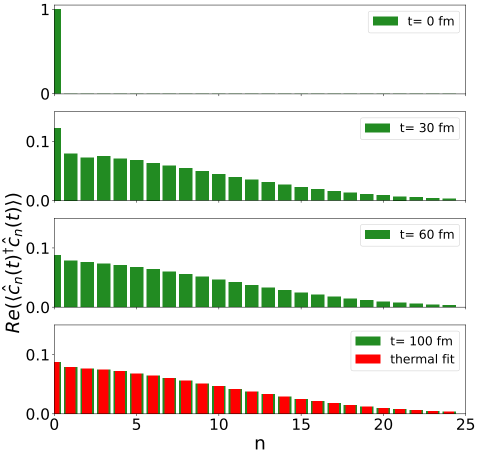


Figure: $c^{<}_{n,n}(t,t)$ plotted for different times. The occupation number of the final states ($t = 100\mathrm{fm}$) was fitted to a Fermi-Dirac distribution yield $T_{\text{system}} \approx 100.133\,\mathrm{MeV}$ and $\mu_{\text{system}} \approx -298.125\,\mathrm{MeV}$.

Kubo-Martin-Schwinger boundary condition

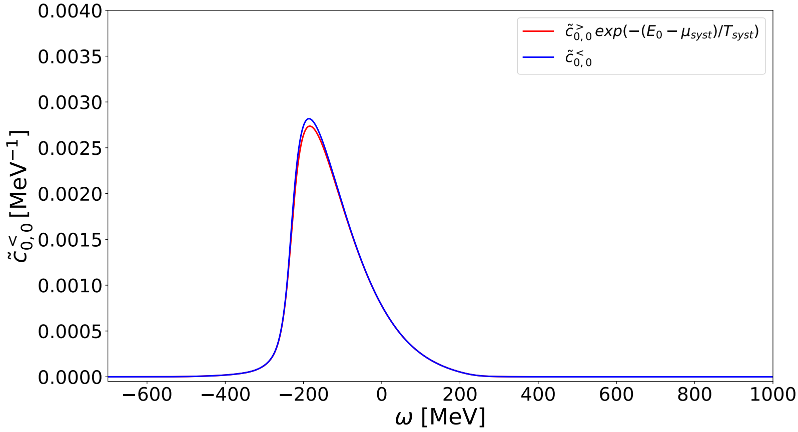


Figure: KMS - condition checked. For the derivation: ”Quantum Statistical Mechanics” by L. Kadanoff and G. Baym.

Decoherence

- density matrix of a pure state

$$\hat{\rho} = |\Psi\rangle\langle\Psi|$$

- density matrix of a mixed state

$$\hat{\rho} = \sum_i p_i \cdot |\psi_i\rangle\langle\psi_i| \quad ; \quad \sum_i p_i = N_{tot}(1)$$

- for an explicit example, we choose for the initial conditions

$$\begin{aligned} |\Psi\rangle_{\text{super}} &= \frac{1}{\sqrt{2}}|10\rangle + \frac{1}{\sqrt{2}}|15\rangle \\ \rightarrow \hat{\rho}_{\text{super}} &= 0.5 \cdot (|10\rangle\langle 10| + |10\rangle\langle 15| + |15\rangle\langle 10| + |15\rangle\langle 15|) \\ \hat{\rho}_{\text{pure}} &= 1.0 \cdot |0\rangle\langle 0| \end{aligned}$$

Decoherence

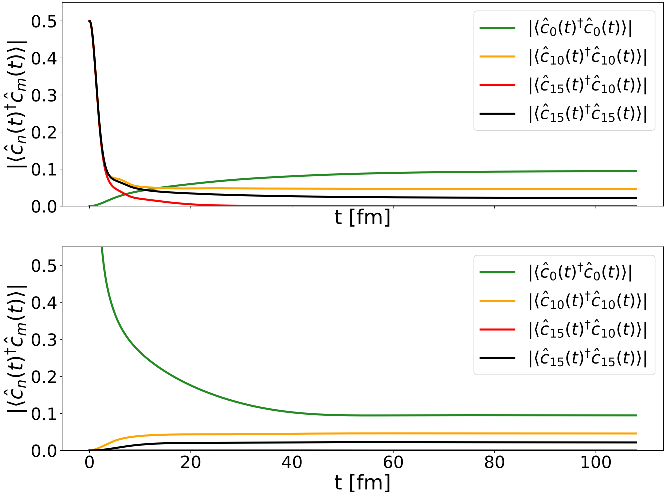


Figure: **Top:** The initial superimposed and **Bottom:** the initial pure state.

Entropy

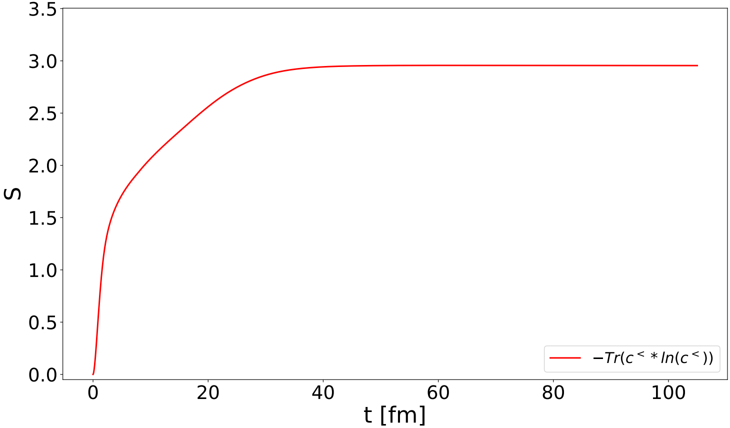


Figure: Von Neumann entropy from the equal time Green's function.

From Lindblad to Kadanoff-Baym in open bosonic systems

- The Lindblad equation is given as:

$$\frac{\partial}{\partial t}\rho(t) = \mathscr{L}[\rho] = -i\left[H', \rho\right] + \frac{1}{2}\sum_{i=1}^{\infty}\left(\left[V_i\rho, V_i^\dagger\right] + \left[V_i^\dagger, \rho V_i\right]\right)$$

- its formal solution can be written as

$$\rho(t) = e^{(t-t_0)\mathscr{L}}\rho(t_0)$$

- which is very similar to the time evolution operator in standard QM, when switching $\mathscr{L} \leftrightarrow H$
- the Keldysh partition function $Z = tr\rho(t)$ kann now be written as a path integral by Trotter decomposition and inserting unities of coherent states

$$Z = \int \mathscr{D}[\phi_+, \phi_+^*, \phi_-, \phi_-^*] e^{iS} \langle\phi_+(t_0)|\,\rho(t_0)\,|\phi_-(t_0)\rangle$$

$$S = \int dt\left(\phi_+^* i\partial_t\phi_+ - \phi_-^* i\partial_t\phi_- - i\mathscr{L}(\phi_+, \phi_+^*, \phi_-, \phi_-^*)\right)$$

An specific example: Bose-polymer

- The Lindblad equation is :

$$\frac{\partial}{\partial t}\hat{\rho}(t) = -i[\hat{H}\hat{\rho} - \hat{\rho}\hat{H}^{\dagger}] + \lambda \sum_{i=1}^{L}[(N_i+1)\hat{a}_i\hat{\rho}(t)\hat{a}_i^{\dagger} + N_i\hat{a}_i^{\dagger}\hat{\rho}(t)\hat{a}_i]$$

- L bosonic modes in with energies ω_i coupled to markovian reservoirs at inverse temperature β_i with occupation number $N_i = \frac{1}{\exp(\omega_i\beta_i)-1}$ and system Hamiltonian $\hat{H}$ given as

$$\hat{H} = \sum_{i,j=1}^{L} \underbrace{\delta_{i,j}(\omega_i - i\lambda(N_i+0.5)) + (1-\delta_{i,j})J]}_{h_{i,j}}\hat{a}_i^{\dagger}\hat{a}_j$$

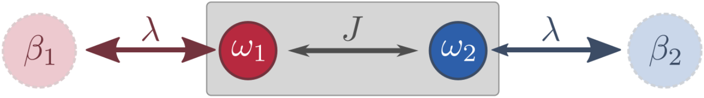


Figure: taken from 10.21468/SciPostPhysCore.5.2.030

An specific example: Bose-polymer

- the corresponding Keldysh - action reads

$$S = \sum_{i,j=1}^{L} \int dt \, (\phi^*_{i,+}, \phi^*_{i,-}) \underbrace{\begin{pmatrix} G^{-1\,++}_{i,j,0} & G^{-1\,+-}_{i,j,0} \\ G^{-1\,-+}_{i,j,0} & G^{-1\,--}_{i,j,0} \end{pmatrix}}_{\hat{G}^{-1}_{i,j,0}} (\phi_{j,+}, \phi_{j,-})^T$$

- with expressions:

$$\begin{aligned} G^{-1\,++}_{i,j,0} &= i\partial_t - h_{i,j} \\ G^{-1\,--}_{i,j,0} &= -(i\partial_t - h^*_{i,j}) \\ G^{-1\,-+}_{i,j,0} &= -i\lambda(N_i + 1)\delta_{i,j} \\ G^{-1\,+-}_{i,j,0} &= -i\lambda(N_i)\delta_{i,j} \end{aligned}$$

- there are no higher interaction terms, so the Kadanoff-Baym equ. do not contain any selfenergies. In Keldysh space the KBE

$$\begin{pmatrix} G^{-1\,++}_{i,j,0} & G^{-1\,+-}_{i,j,0} \\ G^{-1\,-+}_{i,j,0} & G^{-1\,--}_{i,j,0} \end{pmatrix} \begin{pmatrix} G^{++}_{i,j} & G^{+-}_{i,j} \\ G^{-+}_{i,j} & G^{--}_{i,j} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

An specific example: Bose-polymer

- the important equations are the off-diagonal ones, after inserting the explicit expressions

$$(i\partial_t - h_{i,j})G^{+-}_{i,j} - i\lambda(N_i)\delta_{i,j}G^{--}_{i,j} = 0$$
$$-(i\partial_t - h^*_{i,j})G^{-+}_{i,j} - i\lambda(N_i+1)\delta_{i,j}G^{++}_{i,j} = 0$$

- these equation and their complex conjugate are needed for the evolution in the two-time plane
- as a last step we want to translate it back to the usual ”greater/lesser” and (anti)-timeordered

$$G^{+-}_{i,j} = G^{<}_{i,j}$$
$$G^{-+}_{i,j} = G^{>}_{i,j}$$
$$G^{++}_{i,j} = G^{T}_{i,j} = \Theta_c(t-t')G^{<}_{i,j} + \Theta_c(t'-t)G^{<}_{i,j}$$
$$G^{--}_{i,j} = G^{\tilde{T}}_{i,j} = \Theta_c(t'-t)G^{<}_{i,j} + \Theta_c(t-t')G^{<}_{i,j}$$

An specific example: Bose-polymer

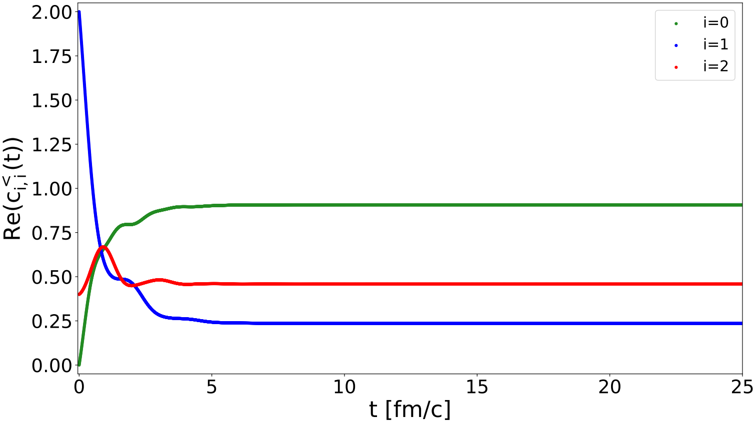


Figure: **Left:** Occupation number of the states for $L = 3$. For parameters: $\lambda = 1$, $J = \pi/4$, $\omega_i = 500 \cdot \mathrm{i}[\mathrm{MeV}]$, $N_0 = 1$,$N_1 = 0.1$, $N_2 = 0.5$

An specific example: Bose-polymer

- in the usual Lindblad equation the norm is conserved by construction (using the cyclicity of the trace)

$$tr\Big(\frac{\partial}{\partial t}\hat{\rho}(t)\Big) = 0$$

- for the KBE, the trace of the time diagonal is relevant (in this example for $J = 0$, because it would cancel anyway)

$$\begin{aligned}
\frac{\partial}{\partial t} G^{<}_{i,i}(t,t) &= -i[\delta_{i,j}(\omega_i - i\lambda(N_i + 0.5))G^{<}_{j,i}(t,t) - G^{<}_{i,j}(t,t) \\
&\quad \delta_{j,i}(\omega_i + i\lambda(N_i + 0.5))] + \lambda N_i(G^{<}_{i,i}(t,t) + \underbrace{G^{>}_{i,i}(t,t)}_{1+G^{<}_{i,i}(t,t)}) \\
&= -i[-2i\lambda(N_i + 0.5)G^{<}_{i,i}(t,t)] + \lambda N_i(2G^{<}_{i,i}(t,t) + 1) \\
&= \lambda(N_i - G^{<}_{i,i}(t,t))
\end{aligned}$$

An specific example: Bose-polymer

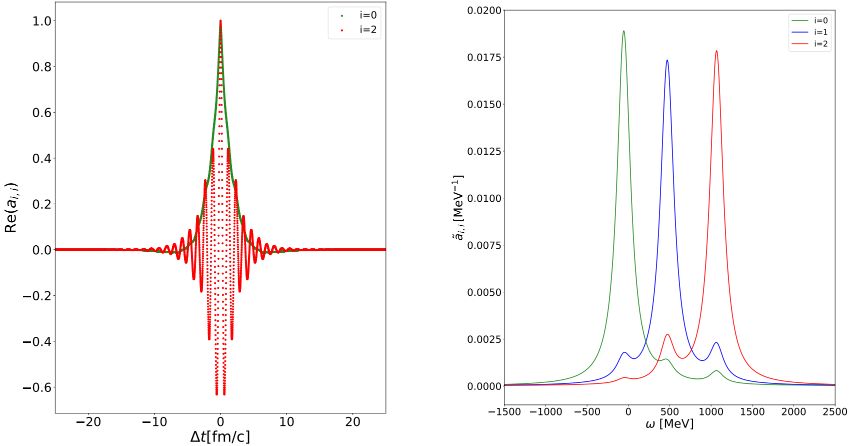


Figure: **Left:** Spectralfunctions of the three states for fixed $T = 25\,\mathrm{fm}$ and **right:** Fourier transform of the spectralfunctions.

Conclusions and Outlook

Conclusion:

- short introduction to non-relativistic, non-equilibrium Green's functions
- presentation of the used method to solve the coupled integro-differential equations for a simple testbox
- results for spectral properties, thermalisation and decoherence
- Lindblad to KBE - a quick introduction

Outlook:

- extend it to 3+1 dimensions is done
- spectral function of a Bose-Einstein condensate

Back up: Two-time plane

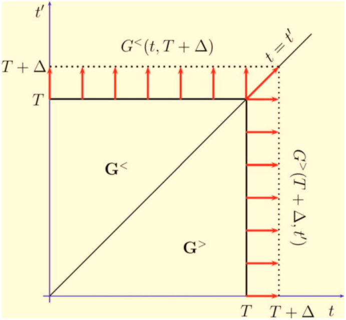


Figure: Stan et al,Time propagation of the Kadanoff-Baym equations for inhomogeneous systems, The Journal of Chemical Physics, 2009

- only 3 instead of 4 equations need to be solved because of symmetry relations: $-S^{\gtrless}(1,1')^\dagger = S^{\gtrless}(1',1)$
- on the time diagonal only $S^<$ is propagated and the equal-time commutation relation is used to obtain $S^>$