Open Quantum Systems with Kadanoff-Baym Equations

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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

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 Greensfunction, 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

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

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

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

- "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

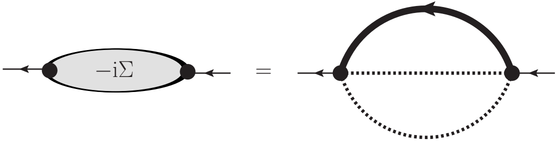
$$V_{\text{eff}}(1) = V(1) + \Sigma_H(1),$$

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

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

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

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

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

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

1+1 dim test model

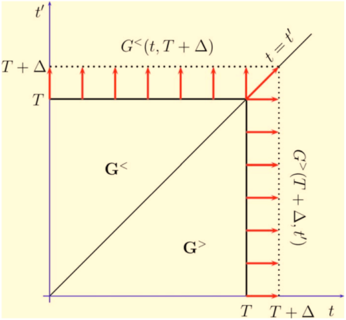


Figure: Stan et al,Time propagation of the KadanoffBaym equations for inhomogeneous systems, The Journal of Chemical Physics, 2009

- 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 $S^>$

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

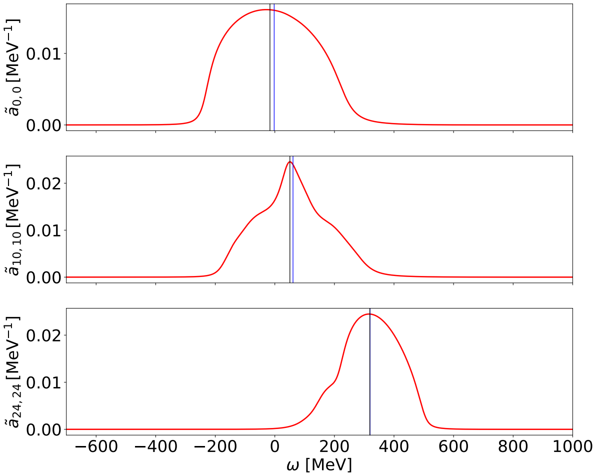


Figure: Spectral functions $\tilde{a}_{0,0}(\omega, \bar{T} = 52\mathrm{fm})$, $\tilde{a}_{10,10}(\omega, \bar{T} = 52\mathrm{fm})$ and $\tilde{a}_{24,24}(\omega, \bar{T} = 52\mathrm{fm})$.

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

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

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

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

Spectral properties

- the peak is shifted to

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

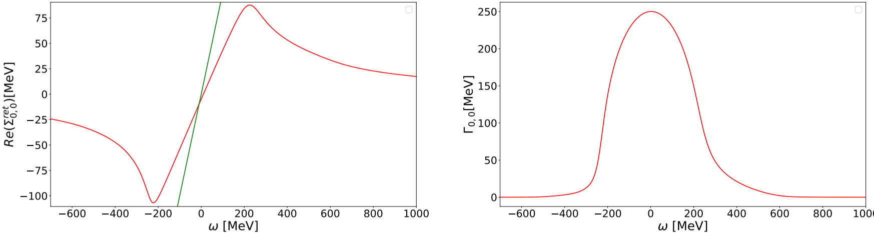


Figure: real part and imaginary part of the retarded self energy of the ground state for $\bar{T} = 52\mathrm{fm}$

Spectral properties

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

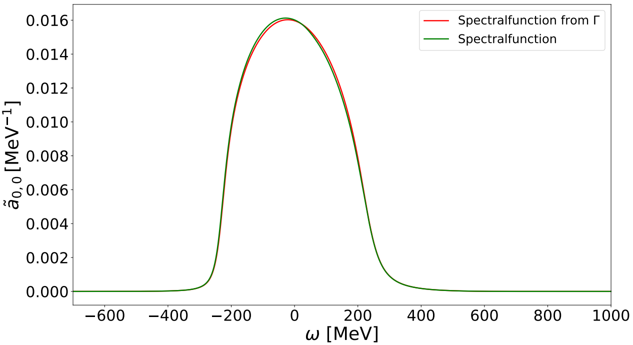


Figure: Spectral functions compared for $\bar{T} = 52\text{fm}$.

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

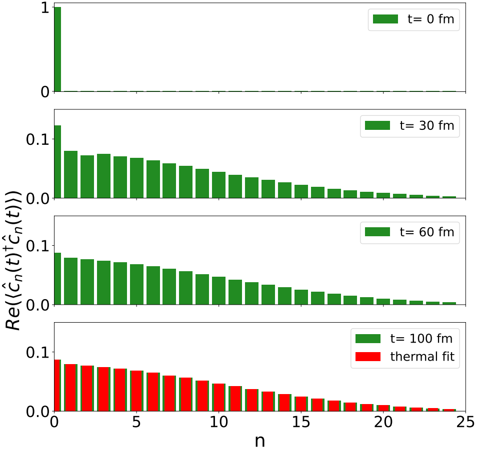


Figure: $c^{<}_{n,n}(t,t)$ plotted for different times. The occupation number of the final states ($t = 100\mathrm{fm}$) was fitted to a Fermi-Dirac distribution yield $T_{\mathrm{system}} \approx 100.133\,\mathrm{MeV}$ and $\mu_{\mathrm{system}} \approx -298.125\,\mathrm{MeV}$.

Kubo-Martin-Schwinger boundary condition

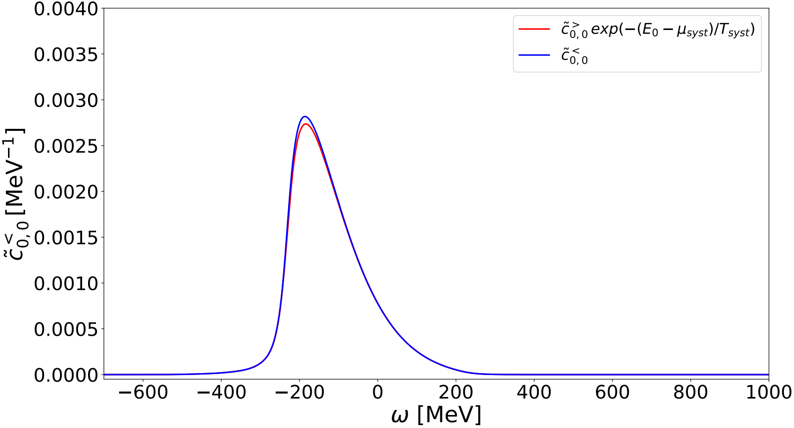


Figure: KMS - condition checked. For the derivation: ”Quantum Statistical Mechanics” by L. Kadanoff and G. Baym.

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

$$|\Psi\rangle_{\text{super}} = \frac{1}{\sqrt{2}}|10\rangle + \frac{1}{\sqrt{2}}|15\rangle$$

$$\rightarrow \hat{\rho}_{\text{super}} = 0.5 \cdot (|10\rangle\langle 10| + |10\rangle\langle 15| + |15\rangle\langle 10| + |15\rangle\langle 15|)$$

$$\hat{\rho}_{\text{pure}} = 1.0 \cdot |0\rangle\langle 0|$$

Decoherence

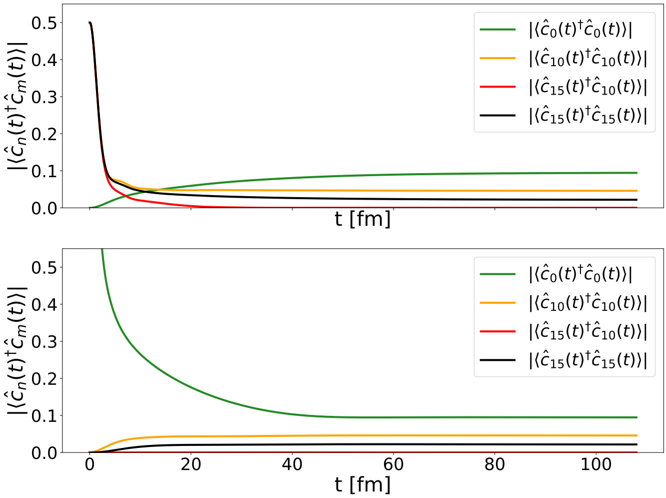


Figure: **Top:** The initial superimposed and **Bottom:** the initial pure state.

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

Outlook:

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

Back up: 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:

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

Back up: 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 $t > t'$

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

Back up: Schwinger-Keldysh Contour

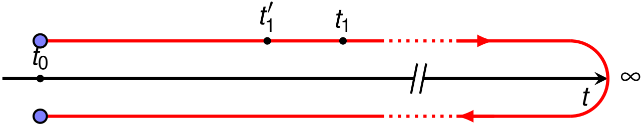


Figure: The closed-time path $\mathscr{C}$. Thanks to David Wagner

- 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 ”anti-time ordering” operator
- in general there are three other Green’s function (upper-lower, lower-upper and lower-lower)