Kadanoff-Baym Approach to Bound States in Open Quantum Systems

Hendrik van Hees

Goethe University Frankfurt

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GOETHE UNIVERSITÄT FRANKFURT AM MAIN

Institute for Theoretical Physics

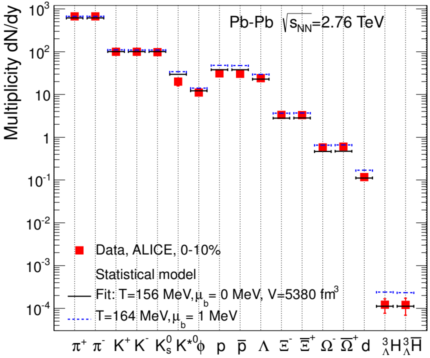
Helmholtz Forschungsakademie Hessen für FAIR

Outline

based on T. Neidig PhD Thesis, T. Neidig et al, Phys. Lett. B 851 (2024), Phys.Rev.C 112, 044007 (2025) [Nei25, NRB+24, NBHG25]

Motivation: “Snowballs in Hell”

- Motivation: Production of light nuclei in ultra-relativistic heavy-ion collisions
  - the “snowball-in hell puzzle”
  - Pb-Pb collisions at the LHC: chemical freeze-out at $T \simeq T_{\text{pc}} \simeq 155\,\text{MeV}$, $\mu_{\text{B}} \simeq 0$
  - close to confinement-deconfinement/chiral phase transition of QCD



  - light nuclei (particularly d with a binding energy of 2.224 MeV)

Open quantum-system approach I

- standard approach: “coalescence” in-medium p+n close in phase space form d according to some probability
  - violates energy conservation
  - violates H-theorem $\Rightarrow$ lack of equilibration with medium
- Kinetic theory
  - rate equations/Saha equation [NGG+22]
  - Transport simulations with multi-particle collisions like $N\mathrm{pn} \longleftrightarrow N\mathrm{d}$ [SOTRE21]
- here full “quantum dynamics”: Kadanoff-Baym approach
  - nonequilibrium QFT/Green’s function description
  - dynamical equations for one-body Green’s function derived from a Φ functional
  - guarantees conservation laws and thermodynamical consistency
  - correct long-time limit: equilibration with heat bath

Open quantum-system approach II

- QM toy model for in-medium bound-state formation
  - "System:" single non-relativistic particle in potential

$$\hat{h}_0 = -\frac{\Delta}{2\mu_S} + V_S(\vec{r})$$

  - in "second quantization" (Heisenberg picture)

$$\hat{H}(t) = \underbrace{\int \mathrm{d}r \, \hat{\psi}(r,t)^\dagger \underbrace{\left(-\frac{\Delta}{2\mu_S} + V_S(r)\right)}_{\hat{h}_0} \hat{\psi}(r,t)}_{\hat{H}_S(t)}$$

$$+ \underbrace{\int \mathrm{d}r \int \mathrm{d}r' \, \hat{\psi}(r,t)^\dagger \hat{\psi}(r,t) V_{\text{int}}(|r-r'|) \hat{\phi}(r',t)^\dagger \hat{\phi}(r',t)}_{\hat{H}_{SB}(t)}$$

Open quantum-system approach III

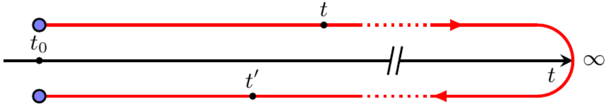
- potentials:

$$V(r) = \begin{cases} -V_0 & \text{if } |r| \leq \frac{a}{2}, \\ 0 & \text{if } |r| > \frac{a}{2}, \\ \infty & \text{if } |r| > \frac{L}{2}. \end{cases} \qquad V_{\text{int}}(|r - r'|) = \lambda \delta(|r - r'|)$$

Extended Schwinger-Keldysh real-time contour

- state: statistical operator $\hat{\rho} = \hat{\rho}_{\text{initial}}$
- expectation values

$$\langle O(t)\rangle = \mathrm{Tr}\left[\hat{\rho}\,\hat{U}(t,t_0)\hat{O}(t)\hat{U}(t,t_0)\right]$$



- for Green's functions

$$\mathrm{i}S_n(1,\ldots,n;1',\ldots,n') = \left\langle \mathcal{T}_C\left[\hat{\psi}(1)\cdots\hat{\psi}(n)\hat{\psi}^\dagger(n')\cdots\hat{\psi}^\dagger(1')\right]\right\rangle$$

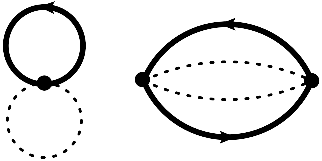
- "Wightman functions" (upper/lower signs: boson/fermions)

$$\mathrm{i}S^{21}(1,1') = \mathrm{i}S^{>}(1,1') = \left\langle\hat{\psi}(1)\hat{\psi}^\dagger(1')\right\rangle$$
$$\mathrm{i}S^{12}(1,1') = \mathrm{i}S^{<}(1,1') = \pm\left\langle\hat{\psi}^\dagger(1')\hat{\psi}(1)\right\rangle$$

- equations of motion: infinite tower of equations for n-point Green's functions (Martin-Schwinger hierarchy) $\Rightarrow$ need approximations

Φ-derivable approximations I

- Φ functional: all closed two-particle irreducible diagrams
- approximations: (finite) subset of Φ-functional diagrams
- full lines: self-consistent two-point (one-particle) Green's functions $S(1,1')$ for system particles
  at arbitrary nonequilibrium $\hat{\rho}_{\text{syst}}^{(\text{initial})}$
- dotted lines: free equilibrium propagator for bath particles
  $\hat{=}$ heat bath at fixed $(T_{\text{bath}}, \mu_{\text{bath}})$
- $\Phi = \Phi[S]$: (Hartree + Born collision term)

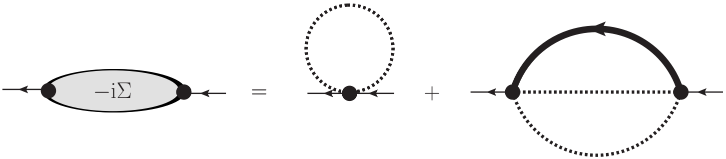


- neglects influence of the bath by the system!

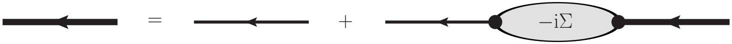
Φ-derivable approximations II

- Self energy: open one S-line of Φ functional

$$\Sigma(1;1') = \frac{\delta \Phi[s]}{\delta S(1',1)}$$



- Kadanoff-Baym equations $\hat{=}$ self-consistent Dyson equation



Φ-derivable approximations III

- expansion in $\hat{h}_0$ eigenfunctions $\phi_n(r)$:

$$\hat{\psi}(r,t) = \sum_{n=0}^{S} \hat{c}_n(t)\phi_n(r),$$

$$S^{>}(1,1') = -\mathrm{i} \sum_{n,m=0}^{S} \underbrace{\langle \hat{c}_n(t)\hat{c}_m(t')^\dagger \rangle}_{c^{>}_{n,m}(t,t')} \phi_n(r)\phi^*_m(r'),$$

$$S^{<}(1,1') = \mp\mathrm{i} \sum_{n,m=0}^{S} \underbrace{\langle \hat{c}_m(t')^\dagger \hat{c}_n(t) \rangle}_{c^{<}_{n,m}(t,t')} \phi_n(r)\phi^*_m(r').$$

Φ-derivable approximations IV

- Kadanoff-Baym (KB) equations ⇔ set of coupled integro-differential equations (upper/lower signs: bosons/fermions)

$$\frac{\partial}{\partial t} c^{>}_{n,m}(t,t') + \mathrm{i} \sum_{i}^{S} V_{\text{eff}\,n,i}(t) c^{>}_{i,m}(t,t') = I^{>}_{n,m1}(t,t'),$$

$$\mp \frac{\partial}{\partial t'} c^{<}_{n,m}(t,t') \pm \mathrm{i} \sum_{i}^{S} c^{<}_{n,i}(t,t') V_{\text{eff}\,i,m}(t') = I^{<}_{n,m2}(t,t'),$$

$$\pm \frac{\partial}{\partial t} c^{<}_{n,m}(t,t) \mp \mathrm{i} [c^{<}, V_{\text{eff}}]_{n,m}(t) = I^{<}_{n,m1}(t,t) - I^{<}_{n,m2}(t,t)$$

- with Hartree (one-point) parts...

$$V_{\text{eff}\,n,m}(t) = E_n \delta_{n,m} + \Sigma_{H\,n,m},$$

$$[c^{<}, V_{\text{eff}}]_{n,m}(t) = \sum_{i}^{S} c^{<}_{n,i}(t,t) V_{\text{eff}\,i,m}(t) - V_{\text{eff}\,n,i}(t) c^{<}_{i,m}(t,t),$$

Φ-derivable approximations V

- ...and "collision terms"

$$I^{>}_{n,m1}(t,t') = -\int_{t_0}^{t} \mathrm{d}\bar{t} \sum_i^S \left[\Sigma^{>}_{n,i}(t,\bar{t}) \mp \Sigma^{<}_{n,i}(t,\bar{t})\right] c^{>}_{i,m}(\bar{t},t')$$
$$+ \int_{t_0}^{t'} \mathrm{d}\bar{t} \sum_i^S \Sigma^{>}_{n,i}(t,\bar{t}) \left[c^{>}_{i,m}(\bar{t},t') \mp c^{<}_{i,m}(\bar{t},t')\right],$$
$$I^{<}_{n,m1}(t,t') = \mp \int_{t_0}^{t} d\bar{t} \sum_i^S \left[\Sigma^{>}_{n,i}(t,\bar{t}) \mp \Sigma^{<}_{n,i}(t,\bar{t})\right] c^{<}_{i,m}(\bar{t},t')$$
$$\pm \int_{t_0}^{t'} d\bar{t} \sum_i^S \Sigma^{<}_{n,i}(t,\bar{t}) \left[c^{>}_{i,m}(\bar{t},t') \mp c^{<}_{i,m}(\bar{t},t')\right],$$

Φ-derivable approximations VI

$$
\begin{aligned}
I^{<}_{n,m2}(t,t') = &\mp \int_{t_0}^{t} \mathrm{d}\bar{t} \sum_{i}^{S} \left[c^{>}_{n,i}(t,\bar{t}) \mp c^{<}_{n,i}(t,\bar{t}) \right] \Sigma^{<}_{i,m}(\bar{t},t') \\
&\pm \int_{t_0}^{t'} \mathrm{d}\bar{t} \sum_{i}^{S} c^{<}_{n,i}(t,\bar{t}) \left[\Sigma^{>}_{i,m}(\bar{t},t') \mp \Sigma^{<}_{i,m}(\bar{t},t') \right].
\end{aligned}
$$

Φ-derivable approximations VII

- Features of Kadanoff-Baym equations
  - conservation laws fulfilled (on expectation-value level)
  - KMS conditions of "bath Green's functions"
    $\Rightarrow$ occupation numbers of system particles approach correct equilibrium limit

$$\lim_{t \to \infty} c^{<}_{n,n}(t,t) = \int \frac{\mathrm{d}\omega}{2\pi} n_{\mathrm{B/F}}(T_{\mathrm{syst}}, \mu_{\mathrm{syst}}, \omega) \tilde{a}_{n,n}(\omega, \bar{t}).$$

    with $T_{\mathrm{syst}} = T_{\mathrm{bath}}$!
  - Green's function provides spectral properties via Wigner transformation

$$\tilde{a}_{n,m}(\omega, \bar{t}) = \int \mathrm{d}\Delta t \, e^{\mathrm{i}\omega\Delta t} a_{n,m}\left(\bar{t} + \frac{\Delta t}{2}, \bar{t} - \frac{\Delta t}{2}\right).$$

    with $a_{n,m}(t,t') = c^{>}_{nm}(t,t') \mp c^{<}_{nm}(t,t')$

Φ-derivable approximations VIII

- "thermodynamic consistency": direct calculation of occupation numbers $\tilde{a}_{n,n}(\omega,\bar{t})$ $\hat{=}$ coincides with (dynamically determined!) Green's function:

$$\tilde{a}(n,n)(\omega,\bar{t}) = -2\,\mathrm{Im}\,S^{(\mathrm{ret})}_{n,n}(\bar{t},\omega) = \frac{\Gamma_{n,n}(\omega,\bar{t})}{\left[\omega - E_n - \mathrm{Re}[\Sigma^{\mathrm{ret}}_{n,n}(\omega,\bar{t})]\right]^2 + \left[\frac{\Gamma_{n,n}(\omega,\bar{t})}{2}\right]^2},$$

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

- analytical properties of Green's functions:
  Kramers-Kronig relations/Källén-Lehmann representation
  $\Leftrightarrow$ fluctuation-dissipation relation

Open fermionic system I

- Bound-state formation, decoherence, and equilibration
  - system particles fermions
  - two initial conditions for two system particles
  - uncorrelated mixed initial state (dashed lines)

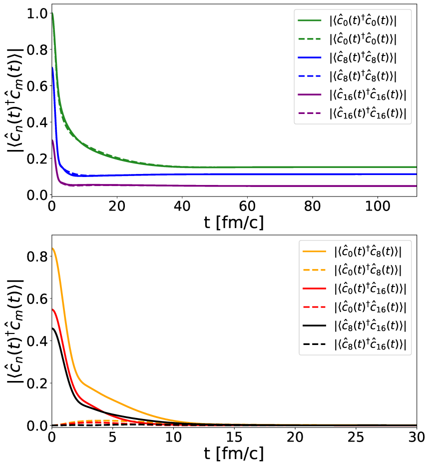
$$c^{<}_{0,0}(0,0) = 1.0,\; c^{<}_{8,8}(0,0) = 0.7,\; c^{<}_{16,16}(0,0) = 0.3,$$

  - pure state (solid lines)

$$\left|\phi\right\rangle = \left|\phi_0\right\rangle + \sqrt{0.7}\left|\phi_8\right\rangle + \sqrt{0.3}\left|\phi_{16}\right\rangle$$
$$\rightarrow c^{<}(0,0) = \left|\phi\right\rangle\left\langle\phi\right|$$

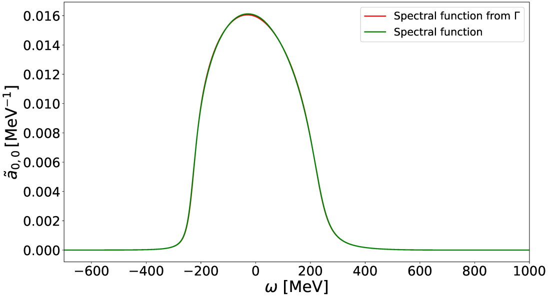
  - pure state: rather quick decoherence
  - mixed state: some “quantum correlations” build up first
  - same equilibrium state for $t \to \infty$

Open fermionic system II



Open fermionic system III

- Thermodynamic consistency check



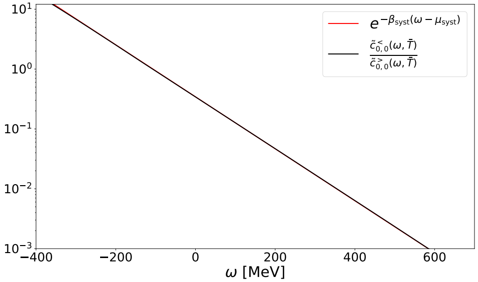
- spectral function (neglecting the Hartree term) from Wigner transformed $a_{n,m}$ vs. from retarded Green's function

Open fermionic system IV

- equilibration of "system" with "bath"
  - in equilibrium, i.e., for sufficiently large $\bar{t} \Rightarrow$ fit T_{syst} from KMS condition

$$\frac{c^{<}_{n,n}(\omega,\bar{t})}{c^{>}_{n,n}(\omega,\bar{t})} = \mathrm{e}^{-\beta_{\text{syst}}(\omega-\mu_{\text{syst}})},$$

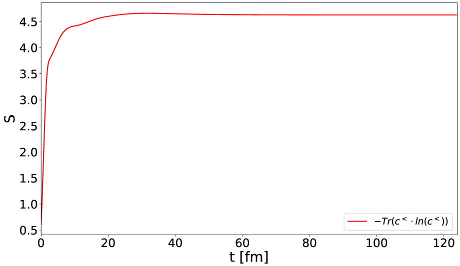
  - fit result $T_{\text{syst}} = 99.993$ MeV (vs. $T_{\text{bath}} = 100$ MeV



Open fermionic system V

- H-theorem
  - density matrix in $\hat{h}_0$-representation: $\rho_{n,m}(t) = c^{<}_{n,m}(t,t) \Rightarrow$ eigenvalues $\xi_n(t)$
  - entropy:

$$S(t) = -\mathrm{Tr}(\hat{\rho} \ln \hat{\rho}) = -\sum_n \xi_n(t) \ln \xi_n(t).$$

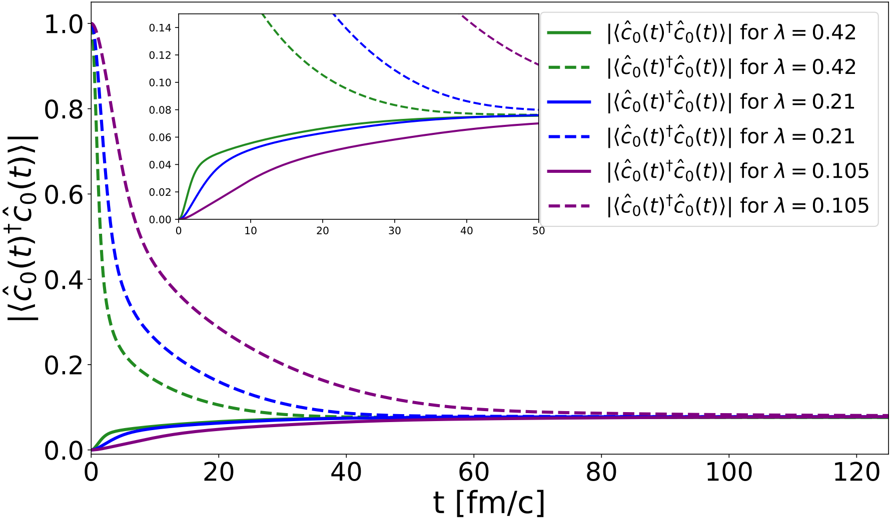


  - NB: slight non-monotony no contradiction to H-theorem: $S(t)$ is entropy of open system

Deuteron (toy) model I

- set $\mu_{\text{S}} = m_N/2$ (reduced mass), $T_{\text{bath}} = 120\,\text{MeV}$, box potential such that $E_{\text{bound}} \simeq 2.2\,\text{MeV}$
- two initial conditions (1 particle): $c^{<}_{0,0}(0,0) = 1$ (dashed lines) and $c^{<}_{8,8}(0,0) = 0.7$, $c^{<}_{16,16}(0,0) = 0.3$ (full lines)
- dependence on coupling λ to heat bath

Deuteron (toy) model II



Open bosonic system I

- system: bosons in a harmonic trap

$$V_{\mathrm{S/B}}(r) = \frac{1}{2}\Omega_{\mathrm{S/B}}^2 r^2$$

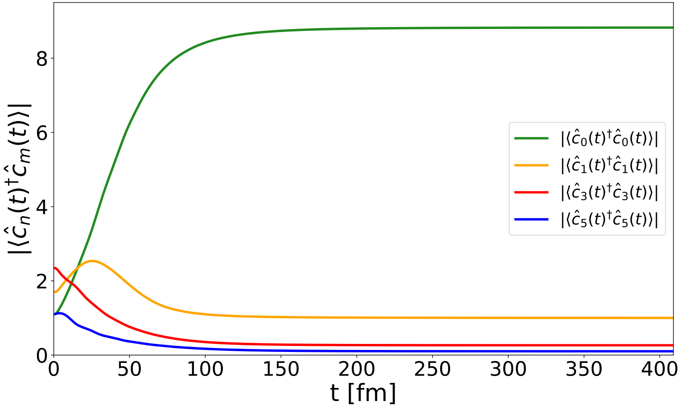
- simulate 11 system particles with $\Omega_{\mathrm{S/B}} = 39.46\ \mathrm{MeV}$, $T_{\mathrm{bath}} = 100\ \mathrm{MeV}$, $\mu_{\mathrm{bath}} = -3\ \mathrm{MeV}$, $\lambda = 0.2$
- interaction potential between system and bath

$$V_{\mathrm{int}}(|r - r'|) = \frac{\lambda}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(r - r')^2}{2\sigma^2}\right], \quad \sigma = 0.5\ \mathrm{fm}$$

- similar to Caldeira-Leggett model

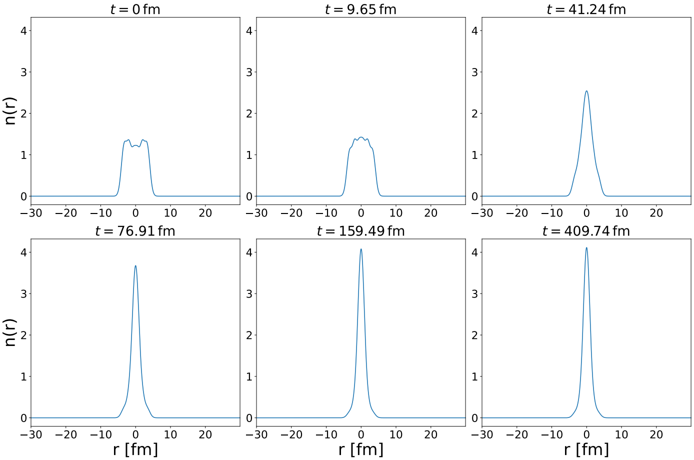
Open bosonic system II

- Time evolution of occupation numbers



Open bosonic system III

- Density: $n(r,t) = \mathrm{i}S^{<}(r,t;r,t)$



Open bosonic system IV

- Internal energy

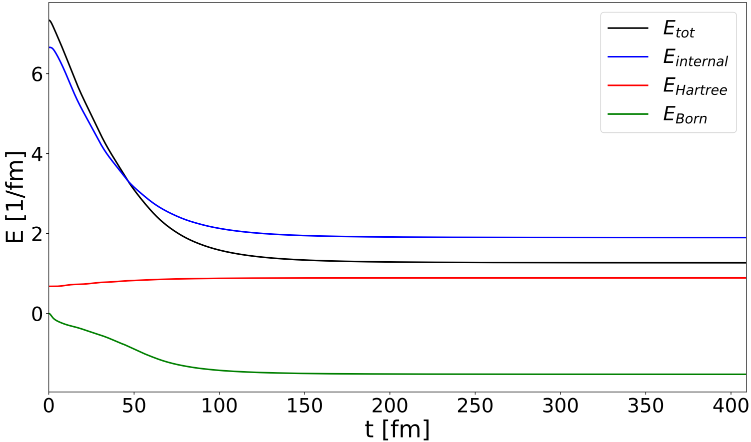
$$U(t) = \int \mathrm{d}r' \int \mathrm{d}r\, \rho(r, r', t)\, h_0(r, r') = \sum_i E_i\, c^<_{i,i}(t, t)$$

- Total energy (Galitskii-Migdal functional)

$$E = \pm \mathrm{i} \int \mathrm{d}r \left\{ \left[\int \mathrm{d}r' h_0(r, r') S^<(r', r, t, t^+) + \frac{1}{2} \Sigma_H(r, r') S^<(r', r, t, t^+) \right] + I^<_{\mathrm{coll}_1}(r, r, t, t^+) \right\}$$

$$= \sum_i^S \left[E_i \cdot c^<_{i,i}(t, t^+) + \left(\sum_j^S \frac{1}{2} \Sigma_{\mathrm{H}i,j} \cdot c^<_{j,i}(t, t^+) \right) \pm \mathrm{i} \frac{1}{2} I^<_{i,i1}(t, t^+) \right].$$

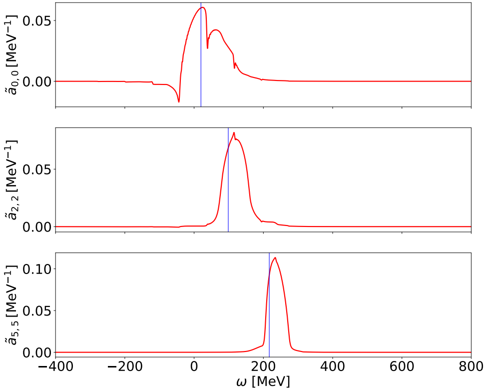
Open bosonic system V



- System cools down

Open bosonic system VI

- Spectral function
  - can become negative (zero at $\mu_{\text{syst}} \simeq -50$ MeV): “laser effect”



Conclusions I

- Kadanoff-Baym approach (Φ-derivable approximations/2PI)
  - guarantees conservation laws
  - thermodynamic consistency
  - system equilibrates with heat bath ($T_{\text{syst}} = T_{\text{bath}}$)
- Toy model for bound-state formation
  - "system:" 1D particles in an external potential (with 1 bound state) coupled to a fixed heat bath in thermal equilibrium
  - time scales: "short" decoherence time; "longer" equilibration time
- Bosons in a trap
  - additional phenomenon specific for bosons
    spectral functions can become negative ("laser effect")

Conclusions II

- further work (not shown here, see [Nei25, NRB+24, NBHG25])
  - extension to 3D
  - investigation of approximations: “diagonalized” KB equations: neglect “quantum correlations” by enforcing diagonal density matrix but still two-time formalism/memory
  - further simplification to quantum-kinetic master equation (Markov approximation) (one-time formalism)
  - numerics very demanding (see [NBHG25])
  - Lindblad approach to bound-state problem (PhD work by Jan Rais) $\longrightarrow$ [RKZG25, RHG25, Rai26]

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