Real-time methods for spectral functions II

Gaussian-state approximation

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Based on
J. V. Roth, D. Schweitzer, LS, L. von Smekal, *Real-time methods for spectral functions*, TBP

Motivation

Long-term goal

Study the QCD phase-diagram and its critical end point

- Classical-statistical simulations are *exact* near 2nd order phase transitions
- At finite 'distance' from the critical point quantum corrections may become important
  - e.g. in heavy-ion collisions concerned with the search of the critical point

$\Rightarrow$ Consider (quantum) corrections of Gaussian type to the classical-statistical dynamics

$\rightarrow$ 'Gaussian-state approximation' (GSA)

Introduction to the GSA

Simple benchmark system (anharmonic oscillator):

$$\hat{H} = \frac{\hat{p}^2}{2} + \frac{m^2}{2}\hat{x}^2 + \frac{\lambda}{4!}\hat{x}^4 \tag{1}$$

Equations of motion:

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\hat{x} = \hat{p}, \quad \frac{\mathrm{d}}{\mathrm{d}t}\,\hat{p} = -m^2\hat{x} - \frac{\lambda}{6}\hat{x}^3 \tag{2}$$

- E.o.m. for $\langle\hat{x}\rangle$, $\langle\hat{p}\rangle$ depend on $\langle\hat{x}^3\rangle$
- E.o.m. for $\langle\hat{x}^3\rangle$ depends on higher-order moments
- …

$\rightarrow$ Truncate infinite hierarchy of equations via GSA

Introduction to the GSA

Approximate the density matrix of the system to be Gaussian, characterized by:

Gaussian-state Wigner function

$$W(x,p) = \mathcal{N} \exp\left\{ -\frac{1}{2} \begin{pmatrix} x - X \\ p - P \end{pmatrix}^{\top} \begin{pmatrix} \sigma_{xx} & \sigma_{xp} \\ \sigma_{xp} & \sigma_{pp} \end{pmatrix}^{-1} \begin{pmatrix} x - X \\ p - P \end{pmatrix} \right\} \quad (3)$$

with $X \equiv \langle \hat{x} \rangle$, $P \equiv \langle \hat{p} \rangle$ and $\sigma_{ab} \equiv \langle\langle \hat{a}\hat{b} \rangle\rangle \equiv \langle \hat{a}\hat{b} + \hat{b}\hat{a} \rangle / 2 - \langle \hat{a} \rangle \langle \hat{b} \rangle$

- Write down e.o.m. for $\hat{x}$, $\hat{p}$, $\hat{x}^2$, $(\hat{x}\hat{p} + \hat{p}\hat{x})/2$ and $\hat{p}^2$
- Take expectation values of the equations using the Gaussian Wigner function

Introduction to the GSA

$\Rightarrow$ Arrive at a *closed* system of equations!

$$\frac{\mathrm{d}}{\mathrm{d}t} X = P, \quad \frac{\mathrm{d}}{\mathrm{d}t} P = -m^2 X - \frac{\lambda}{6}\left(X^3 + 3X\sigma_{xx}\right), \tag{4}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma_{xx} = 2\sigma_{xp}, \quad \frac{\mathrm{d}}{\mathrm{d}t}\sigma_{xp} = \sigma_{pp} - \sigma_{xx}\,\mathcal{C}(t), \quad \frac{\mathrm{d}}{\mathrm{d}t}\sigma_{pp} = -2\sigma_{xp}\,\mathcal{C}(t),$$

with $\mathcal{C}(t) = m^2 + \frac{\lambda}{2}\left(X^2 + \sigma_{xx}\right)$.

$\rightarrow$ Gaussian (quantum) corrections to the classical equations of motion

$\rightarrow$ GSA is not limited to the anharmonic oscillator; same procedure can also be applied to field theories (e.g. ϕ^4-theory)

Coupling to a heat bath

- We want to study dynamics of thermal equilibrium states
  - $\rightarrow$ Introduce coupling to an environment of harmonic oscillators (Caldeira-Leggett model)

Full system under consideration:

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{H}_I, \tag{5a}$$

$$\hat{H}_S = \frac{\hat{p}^2}{2} + \frac{m^2}{2}\hat{x}^2 + \frac{\lambda}{4!}\hat{x}^4, \tag{5b}$$

$$\hat{H}_B = \sum_s \frac{\hat{\pi}_s^2}{2} + \frac{\omega_s^2}{2}\hat{\varphi}_s^2, \tag{5c}$$

$$\hat{H}_I = -\hat{x}\sum_s g_s \hat{\varphi}_s + \hat{x}^2 \sum_s \frac{g_s^2}{\omega_s^2}. \tag{5d}$$

GSA in the Caldeira-Leggett model

Equations of motion:

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\hat{x}(t) = \hat{p}(t), \tag{6a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\hat{p}(t) = -V'(\hat{x}(t)) - \int_0^t \mathrm{d}t'\,\gamma(t-t')\hat{p}(t') + \hat{\xi}(t), \tag{6b}$$

- Dissipation of energy to the environment
- For the simplest model of an Ohmic bath: $\gamma(t) \to 2\gamma\delta(t)$
- Stochastic noise responsible fluctuations

$\hat{\xi}(t) = \sum_s g_s \left[\left(\hat{\varphi}_s(0) - \frac{g_s}{\omega_s^2}\hat{x}(0) \right) \cos(\omega_s t) + \frac{\hat{\pi}_s(0)}{\omega_s} \sin(\omega_s t) \right]$

- Again truncate e.o.m. by averaging over Gaussian Wigner function

GSA in the Caldeira-Leggett model

Gaussian Wigner function describing the *whole* system:

$$W(\vec{x},t) = \mathcal{N} \exp\left\{ -\tfrac{1}{2}(\vec{x} - \vec{X}(t))^\top \Sigma^{-1}(t)(\vec{x} - \vec{X}(t)) \right\}, \tag{7}$$

where $\vec{x} = (x, p, ..., \varphi_s, \pi_s, ...)$ and $\vec{X}(t) = (X(t), P(t), ..., \Phi_s(t), \Pi_s(t), ...)$.

- with covariance matrix:

$$\Sigma = \left(\begin{array}{cc|cccc} \sigma_{xx} & \sigma_{xp} & \cdots & \sigma_{x\varphi_s} & \sigma_{x\pi_s} & \cdots \\ \sigma_{xp} & \sigma_{pp} & \cdots & \sigma_{p\varphi_s} & \sigma_{p\pi_s} & \cdots \\ \hline \vdots & \vdots & \ddots & & & \\ \sigma_{\varphi_s x} & \sigma_{\varphi_s p} & & \sigma_{\varphi_s\varphi_s} & \sigma_{\varphi_s\pi_s} & \\ \sigma_{\pi_s x} & \sigma_{\pi_s p} & & \sigma_{\varphi_s\pi_s} & \sigma_{\pi_s\pi_s} & \\ \vdots & \vdots & & & & \ddots \end{array}\right)$$

GSA in the Caldeira-Leggett model

Equations of motion after averaging over Gaussian Wigner function:

$$\frac{\mathrm{d}}{\mathrm{d}t} X = P, \quad \frac{\mathrm{d}}{\mathrm{d}t} P = -\left(m^2 + \tfrac{\lambda}{2}\sigma_{xx}\right) X - \tfrac{\lambda}{6} X^3 - \gamma P + \xi(t), \tag{8a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \sigma_{xp} = \sigma_{pp} - \sigma_{xx}\, \mathcal{C}(t) - \gamma\sigma_{xp} + \langle\!\langle \hat{x}(t)\hat{\xi}(t)\rangle\!\rangle, \quad \frac{\mathrm{d}}{\mathrm{d}t} \sigma_{xx} = 2\sigma_{xp}, \tag{8b}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \sigma_{pp} = -2\sigma_{xp}\, \mathcal{C}(t) - 2\gamma\sigma_{pp} + \langle\!\langle \hat{p}(t)\hat{\xi}(t)\rangle\!\rangle. \tag{8c}$$

- Dissipation and fluctuations on the level of first- *and* second-order moments
- But... What can we do about $\langle\!\langle \hat{x}(t)\hat{\xi}(t)\rangle\!\rangle$ and $\langle\!\langle \hat{p}(t)\hat{\xi}(t)\rangle\!\rangle$?

Evaluating system-bath correlations

- Remember: $\hat{\xi}(t)$ depends on the initial conditions $\hat{\varphi}_s(0)$ and $\hat{\pi}_s(0)$
  $\rightarrow$ Need to evaluate connected correlations between the particle and the heat bath oscillators, i.e.:

$$G_{x\varphi_s}(t) \equiv \langle\langle \hat{x}(t)\hat{\varphi}_s(0)\rangle\rangle, \; G_{x\pi_s}(t) \equiv \langle\langle \hat{x}(t)\hat{\pi}_s(0)\rangle\rangle \tag{9a}$$
$$G_{p\varphi_s}(t) \equiv \langle\langle \hat{p}(t)\hat{\varphi}_s(0)\rangle\rangle, \; G_{p\pi_s}(t) \equiv \langle\langle \hat{p}(t)\hat{\pi}_s(0)\rangle\rangle \tag{9b}$$

- Considering their respective equations of motion leads to

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} G_{x\varphi_s}(t) + \gamma \, \frac{\mathrm{d}}{\mathrm{d}t} G_{x\varphi_s}(t) + \mathcal{C}(t)\, G_{x\varphi_s}(t) = \frac{f_{0,s}g_s}{\omega_s} \cos(\omega_s t) \tag{10a}$$
$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} G_{x\pi_s}(t) + \gamma \, \frac{\mathrm{d}}{\mathrm{d}t} G_{x\pi_s}(t) + \mathcal{C}(t)\, G_{x\pi_s}(t) = f_{0,s}g_s \sin(\omega_s t) \tag{10b}$$

$\rightarrow$ Driven oscillator with damping constant γ and frequency $\sqrt{\mathcal{C}(t)}$

- Analytic solution is out of reach
  $\rightarrow$ Expand $\mathcal{C}(t)$ around its thermal equilibrium value: $\mathcal{C}(t) = \mathcal{C}_0(\beta) + \delta\mathcal{C}(t)$
  $\rightarrow$ Drop the fluctuations $\delta\mathcal{C}(t)$ ('adiabatic approximation')

GSA in the Caldeira-Leggett model

Final equations of motion:

$$\frac{\mathrm{d}}{\mathrm{d}t} X = P, \quad \frac{\mathrm{d}}{\mathrm{d}t} P = -\left(m^2 + \frac{\lambda}{2}\sigma_{xx}\right) X - \frac{\lambda}{6} X^3 - \gamma P + \xi(t), \tag{11}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma_{xp} = \sigma_{pp} - \sigma_{xx}\,\mathcal{C}_0(\beta) - \gamma\sigma_{xp}, \quad \frac{\mathrm{d}}{\mathrm{d}t}\sigma_{xx} = 2\sigma_{xp},$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma_{pp} = -2\sigma_{xp}\,\mathcal{C}_0(\beta) - 2\gamma\left[\sigma_{pp} - \frac{\omega_R}{4}\left(1+\kappa^2\right)\left(1 + \frac{2}{\pi}\arctan\frac{1-\kappa^2}{2\kappa}\right)\right]$$

- Temperature dependent quantities $\omega_R^2 = \mathcal{C}_0 - \frac{\gamma^2}{4} > 0, \; \kappa = \frac{\gamma}{2\omega_R}$
- σ_{xx}, σ_{xp}, and σ_{pp} approach thermal equilibrium values for $t \to \infty$

$\Rightarrow$ Two corrections of the GSA to the classical time-evolution:

(i) Mass shift $m^2 \to m^2 + \frac{\lambda}{2}\sigma_{xx}(t)|_{t\to\infty}$

(ii) Modified stochastic noise $\xi(t)$:

$\langle|\xi(\omega)|^2\rangle_\beta = 2\frac{\gamma}{\beta}$ (white noise) $\to \gamma\left(\frac{1}{\beta} + \omega\, n_B(\omega)\right)$ (colored noise)

Spectral function

Spectral function defined via decomposition of Green's function:

$$\rho(t,t') = \mathrm{i}\langle[\hat{x}(t),\hat{x}(t')]\rangle_\beta \tag{12a}$$

$$F(t,t') = \frac{1}{2}\langle\{\hat{x}(t),\hat{x}(t')\}\rangle_\beta \tag{12b}$$

- Can be expressed as sum over eigenstates

$$\rho(\omega) = \frac{2\pi\,\mathrm{i}}{Z}\sum_{mn}\mathrm{e}^{-\beta E_n}[\delta(\omega-E_m+E_n)-\delta(\omega+E_m-E_n)]|\langle n|\hat{x}|m\rangle|^2 \tag{13}$$

- Ohmic heat bath is incorporated phenomenologically by replacing

$$\delta(\omega-\Delta E)-\delta(\omega+\Delta E) \to \frac{1}{\pi}\frac{2\gamma\,\Delta E\,\omega}{\gamma^2\omega^2+(\omega^2-\Delta E^2)^2} \tag{14}$$

$\rightarrow$ Valid only for weak coupling (use $\gamma = 0.06$ in all calculations)

Spectral function

'Exact' spectral function for an Ohmic heat bath

$$\rho(\omega) = \frac{2\pi\,\mathrm{i}}{Z} \sum_{mn} \mathrm{e}^{-\beta E_n} \frac{1}{\pi} \frac{2\gamma\,\Delta E\,\omega}{\gamma^2\omega^2 + (\omega^2 - \Delta E^2)^2} |\langle n|\hat{x}|m\rangle|^2 \tag{15}$$

- Numerically determined via discretization of the Schrödinger equation

→ Used as a benchmark result for the other real-time methods

For classical-statistical approach and GSA use fluctuation-dissipation relation to get ρ from F:

$$F(\omega) = -\,\mathrm{i}\left(n_{\mathsf{B}}(\omega) + \tfrac{1}{2}\right)\rho(\omega) \tag{16}$$

- In the classical limit $T \gg \omega$: $n_{\mathsf{B}}(\omega) \approx \frac{T}{\omega} - \frac{1}{2}$

$$F_{\mathsf{cl.}}(\omega) = -\,\mathrm{i}\,\tfrac{T}{\omega}\rho_{\mathsf{cl.}}(\omega) \tag{17}$$

Spectral function

- After Fourier transform:

$$\rho_{\text{cl.}}(t,t') = -\frac{1}{2T}\left(\partial_t - \partial_{t'}\right) F_{\text{cl.}}(t,t') \tag{18}$$

- With the statistical two-point function in the classical limit given by

$$F_{\text{cl.}}(t,t') = \langle \hat{x}(t)\hat{x}(t')\rangle_\beta - \langle \hat{x}(t)\rangle_\beta \langle \hat{x}(t')\rangle_\beta , \tag{19}$$

$$\Rightarrow \rho_{\text{cl.}}(t,t') = -\frac{1}{2T}\langle \hat{p}(t)\hat{x}(t') - \hat{x}(t)\hat{p}(t')\rangle_\beta \tag{20}$$

- Replace operators with expectation values to calculate ρ from (20) in the classical-statistical approach

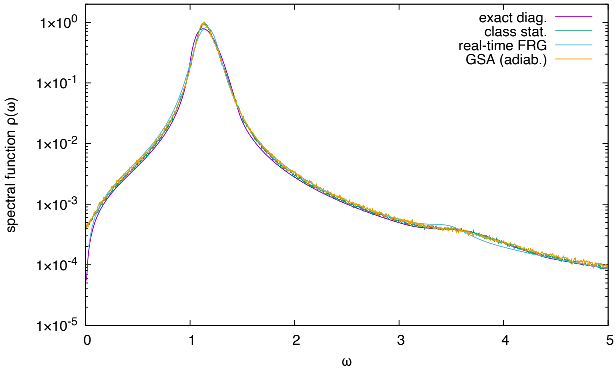
For the GSA, from the general fluctuation dissipation relation, follows:

$$\rho_{\text{GSA}}(\omega) = \frac{2\gamma T}{\langle |\xi(\omega)|^2\rangle_\beta}\rho_{\text{cl.}}(\omega) = \frac{2}{1+\frac{\omega}{T}\,n_B(\omega)}\rho_{\text{cl.}}(\omega) \tag{21}$$

Results

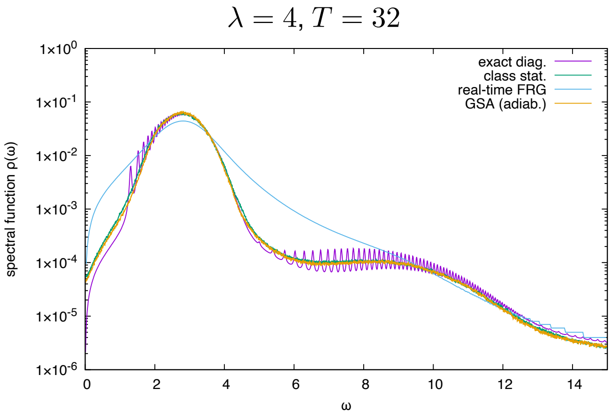
Parameters $m = 1, \gamma = 0.06$ for all results.

$$\lambda = 1/32, T = 32$$



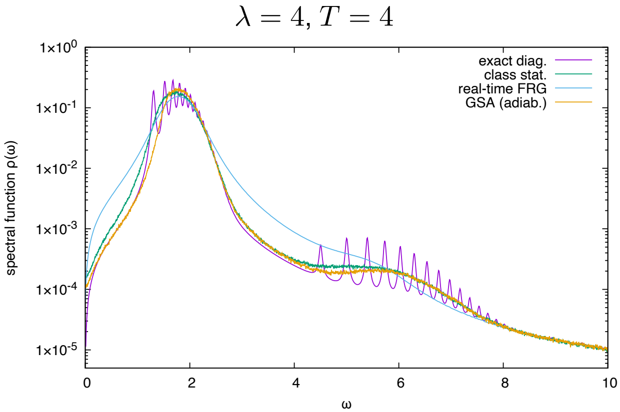
- Dominant Breit-Wigner peak at $\omega_c \gtrsim 1$
- Smaller bump at $\sim 3\,\omega_c$
- All approaches agree with the benchmark solution, only FRG differs slightly

Results



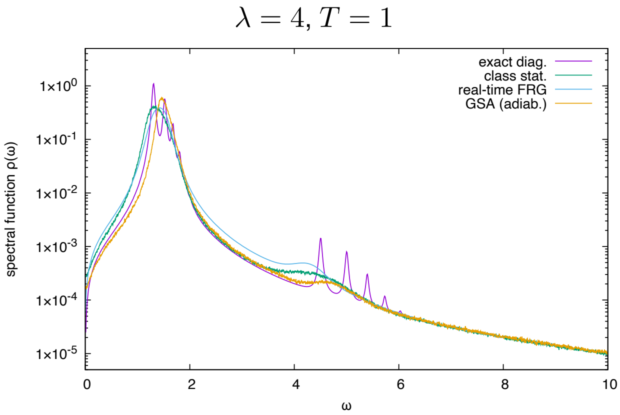
- Emergence of discrete sub-peak structure
- FRG shows notable problems (truncational issue)
- Classical-statistical approach and GSA coincide!

Results



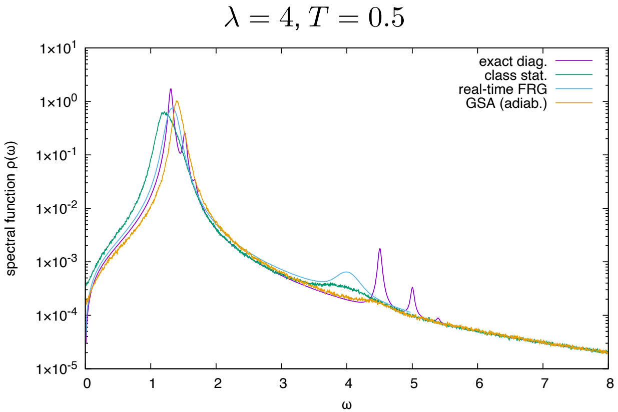
- Reduced temperature leads to fewer peaks
  - $\rightarrow$ Fewer possible transitions
- FRG shows the same truncational issue
- Classical and GSA spectral functions still somewhat similar

Results



- Classical approach underestimates ω_c
- GSA tends to overcorrect ω_c
- GSA is able to describe the second bump better

Results



- FRG describes the main peak best, however second bump is underestimated as in the classical approach
- GSA describes the main peak better than the classical approach and describes the frequency of the second bump best

Summary and Outlook

We saw that

+ adiabatic GSA is consistent with the classical approach in the high temperature limit,
+ GSA includes quantum effects as small corrections to classical simulations at lower temperatures,
– discrete sub-structure remains unresolved.

Opportunities for future studies:

- analyze how the GSA results depend on the precise realization of the heat bath,
- investigate critical dynamics with the GSA,
- try to extend the applicability of the GSA to non-equilibrium dynamics.

BACKUP

Colored noise synthesis

Problem: $\xi(t)$ non-local in time $\rightarrow$ can no longer be generated 'on the fly'

$\rightarrow$ Idea: Before time evolution,sample $\xi(\omega)$ in frequency space and perform a Fourier transform to obtain $\xi(t)$

- Points at which expectation values will be calculated have to be known beforehand

$$t_i \in \{0, h, 2h, \dots, t_{\mathsf{max}} - h, t_{\mathsf{max}}\}$$

- Translate into set of relevant frequencies

$$\omega_i \in \{-\frac{\pi}{h}, -\frac{\pi}{h} + \frac{2\pi}{t_{\mathsf{max}}}, -\frac{\pi}{h} + \frac{4\pi}{t_{\mathsf{max}}}, \dots, \frac{\pi}{h} - \frac{2\pi}{t_{\mathsf{max}}}, \frac{\pi}{h}\}$$

- For all ω_i sample $\xi(\omega_i)$ from a Gaussian distribution with variance $K(\omega_i) = \gamma(\frac{1}{\beta} + \omega_i \, n_{\mathsf{B}}(\omega_i))$
- DFT of $\{\xi(\omega_i)\}$ yields the desired $\{\xi(t_i)\}$

Leapfrog algorithm

- Once before the first step, P and σ_{xp} are staggered backwards half a step according to

$$P(t_0 - h/2) = P(t_0) - \frac{h}{2}\dot{P}(t_0),$$
$$\sigma_{xp}(t_0 - h/2) = \sigma_{xp}(t_0) - \frac{h}{2}\dot{\sigma}_{xp}(t_0).$$

- After that, each step follows the same procedure. First evolve P and σ_{xp} a full step forward in time

$$P(t + h/2) = P(t - h/2) + h\dot{P}(t) + \sqrt{h}\,\xi(t),$$
$$\sigma_{xp}(t + h/2) = \sigma_{xp}(t - h/2) + h\dot{\sigma}_{xp}(t),$$

Leapfrog algorithm

- then evolve X, σ_{xx} and σ_{pp} by a full step using the new values of P and σ_{xp}

$$
\begin{aligned}
X(t+h) &= X(t) + h\dot{X}(t+h/2), \\
\sigma_{xx}(t+h) &= \sigma_{xx}(t) + h\dot{\sigma}_{xx}(t+h/2), \\
\sigma_{pp}(t+h) &= \sigma_{pp}(t) + h\dot{\sigma}_{pp}(t+h/2).
\end{aligned}
$$

- Note that $\dot{\sigma}_{pp}(t+h/2)$ would require the knowledge of $\mathcal{C}(X, \sigma_{xx})|_{t+h/2}$ which is approximated by

$$
\mathcal{C}(t+h/2) = \frac{\mathcal{C}(t) + \mathcal{C}(t+h)}{2}.
$$

Leapfrog algorithm

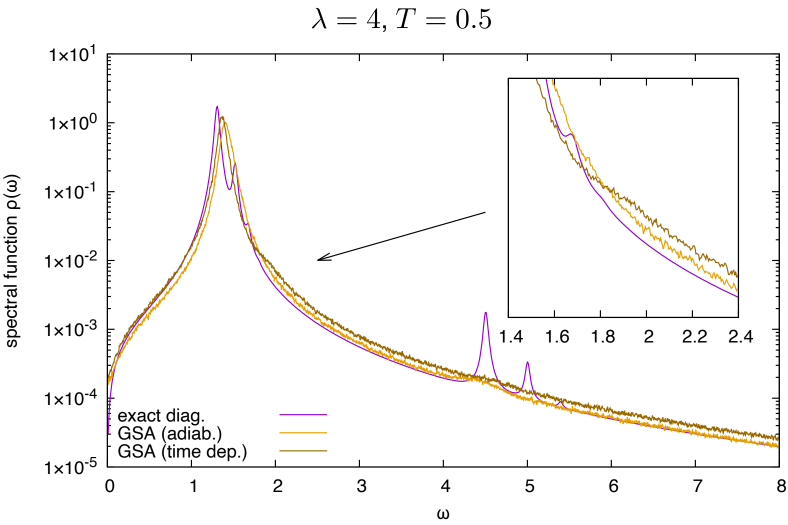
- To obtain all expectation values at the same point in time, P and σ_{xp} can be evolved forward by half a step

$$P(t) = P(t - h/2) - \frac{h}{2}\dot{P}(t),$$
$$\sigma_{xp}(t) = \sigma_{xp}(t - h/2) - \frac{h}{2}\dot{\sigma}_{xp}(t).$$

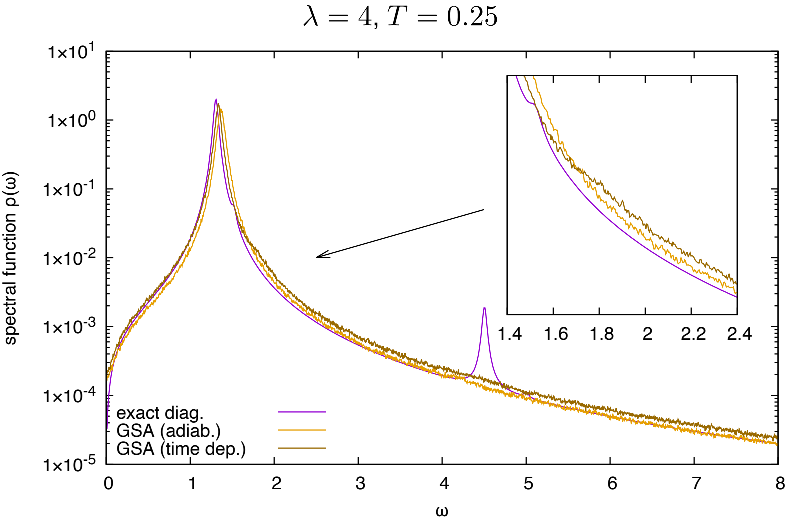
Numerical parameters:

- Integrator step size $h = 0.005$
- Integrate up to $t_{\text{max}} = 800.0$
- Field expectation values for the spectral function are evaluated once every 20 integrator steps
- Spectral functions are averaged over 1000 random instances of the noise
- To ensure thermal equilibrium, before each simulation we let the system thermalize for a time of $t = 10/\gamma \approx 166.67$

(Non-)adiabatic GSA comparison



(Non-)adiabatic GSA comparison



(Non-)adiabatic GSA comparison