Stochastic Real–Time Methods for Spectral functions

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Based on:
LS, *Stochastic Real–Time Methods for Spectral functions*, Master's Thesis (2022)
J. Roth, D. Schweitzer, LS, L. von Smekal, *Phys. Rev. D* **105** (2022) 116017

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CRC-TR 211 Strong-interaction matter under extreme conditions

HGS-HIRe for FAIR Helmholtz Graduate School for Hadron and Ion Research

QCD phase diagram:

- Lattice: Cross-over for $\mu_B \approx 0$, $T \approx 155$ MeV
- Effective theories: 1st order transition at high μ_B
  $\Rightarrow$ 2nd order transition (CEP) at finite T, μ_B?
- Search for CEP signatures in heavy-ion collisions

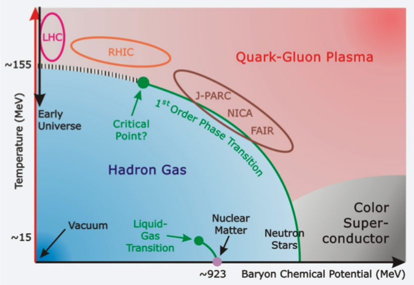

Figure: Semi quantitative phase diagram of QCD, by A. Steidl.

Critical phenomena:

- Strong fluctuations $\Rightarrow$ correlation length diverges

$$\langle \phi(x)\phi(x')\rangle \propto \mathrm{e}^{-|x-x'|/\xi}$$

- Observables $\rightarrow$ Power laws with universal exponents

$$\langle A(T)\rangle \propto (T - T_c)^{\alpha}$$

$\hookrightarrow$ Study simpler systems of the same universality class

- At finite 'distance' from CEP quantum corrections may become important
  $\Rightarrow$ Consider quantum corrections of Gaussian type to classical dynamics

Need an understanding of open quantum-mechanical systems

Stochastic Real-time methods

- Open systems interact with an environment
  $\hookrightarrow$ e.g. pollen grain suspended in water
- The many-body interactions cannot be solved by accounting for every involved particle
  $\hookrightarrow$ need stochastic models
- e.g. Langevin equation $\rightarrow$ Brownian motion

$$m\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = -\gamma\boldsymbol{v} + \boldsymbol{\xi}(t)$$

- a noise term $\boldsymbol{\xi}(t)$ represents the effects of collisions with molecules of the environment

$$\langle \xi_i(t)\xi_j(t')\rangle = 2\gamma T\delta_{i,j}\delta(t-t')$$

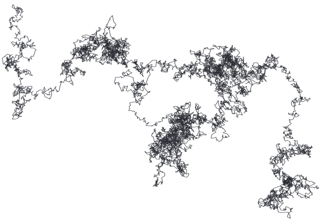

Figure: An example of 2d Brownian motion (P. Mörters)

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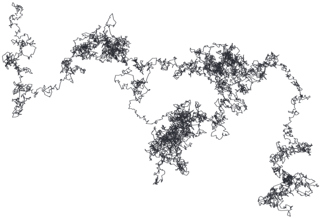

Figure: An example of 2d Brownian motion (P. Mörters)

What about quantum mechanical systems?

- Open systems interact with an environment
  ↪ e.g. atom trapped in a cavity
- The many-body interactions cannot be solved by accounting for every involved particle
  ↪ need stochastic models
- e.g. *Quantum* Langevin equation?
- How can classical behaviour emerge from a quantum-mechanical system?

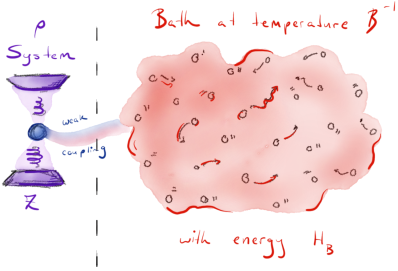

Figure: Visualization of an open quantum system (J. Xuereb, *The Thermodynamics of some Quantum Information Processes*, Masters's Thesis, 2022)

General objective

Obtain a reduced description considering the system's dynamics explicitly and the environment implicitly, e.g. temperature T

⇒ **Generalized Langevin Equations**

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Consider the **system** to be a quantum-mechanical particle moving in a potential:

$$H_S = \frac{p^2}{2} + V(x)$$

...linearly **coupled** to an **environment** modeled as an assembly of harmonic oscillators[1]:

$$H_B + H_I = \sum_s \left(\frac{\pi_s^2}{2} + \frac{\omega_s^2}{2} \left(\varphi_s - \frac{g_s}{\omega_s^2} x \right)^2 \right),$$

Combined Hamiltonian: $H = H_S + H_B + H_I$

- Heisenberg equation of motion for an arbitrary system operator O:

$$\dot{O} = \mathrm{i}[H, O] = \mathrm{i}[H_S, O] + \frac{\mathrm{i}}{2} \sum_s \left[[O, g_s x], \pi_s - g_s x \right]_+$$

need to eliminate explicity dependence on bath variables!

[1] A. Caldeira, A. Leggett, *Physica A* **121**, 3 (1983)

Road to generalized Langevin equations

- Heisenberg equations for the evironment operators

$$\dot{\varphi}_s = \mathrm{i}[H, \varphi_s] = \pi_s - g_s x$$
$$\dot{\pi}_s = \mathrm{i}[H, \pi_s] = -\omega_s^2 \varphi_s$$

↪ write these in terms of ladder operators

$$a_s = \frac{\omega_s \phi_s + \mathrm{i}\,\pi_s}{\sqrt{2\omega_s}}, \quad a_s^\dagger = \frac{\omega_s \phi_s - \mathrm{i}\,\pi_s}{\sqrt{2\omega_s}}$$

- Heisenberg equations become

$$\dot{a}_s = -\mathrm{i}\,\omega_s a_s - g_s \sqrt{\frac{\omega_s}{2}} x$$

↪ can be easily solved

$$a_s(t) = \mathrm{e}^{-\mathrm{i}\,\omega_s (t - t_0)}\, a_s(t_0) - g_s \sqrt{\frac{\omega_s}{2}} \int_{t_0}^{t} \mathrm{e}^{-\mathrm{i}\,\omega_s (t - t')}\, x(t') \mathrm{d}t'$$

(...analogous for $a_s^\dagger$)

Road to generalized Langevin equations

Recall:

$$\dot{O} = \mathrm{i}[H, O] = \mathrm{i}[H_S, O] + \frac{\mathrm{i}}{2}\sum_s \left[[O, g_s x], \pi_s - g_s x\right]_+$$

Now substitute for $\pi_s(t)$ using the solutions $a_s(t)$, $a_s^\dagger(t)$. Then after a bit of algebra[2]...

Generalized Langevin equation

$$\dot{O} = \mathrm{i}[H_S, O] - \frac{\mathrm{i}}{2}\left[[x, O], -\int_{t_0}^{t} f(t-t')\dot{x}(t')\mathrm{d}t' - f(t-t_0)x(t_0) + \xi(t)\right]_+$$

with

$$\xi(t) = \mathrm{i}\sum_s g_s\sqrt{\frac{\omega_s}{2}}\left[-a_s(t_0)\,\mathrm{e}^{-\mathrm{i}\,\omega_s(t-t_0)} + a_s^\dagger(t_0)\,\mathrm{e}^{\omega_s(t-t_0)}\right] \quad \text{“Noise operator”}$$

$$f(t) = \sum_s g_s^2 \cos(\omega_s t) \quad \text{“Memory function”}$$

Let's try to understand these equations...

[2] C. W. Gardiner, P. Zoller, *Quantum noise*. Springer Berlin, 2000

Generalized Langevin equations

Example: Substitute for O, the system's canonical coordinate and momentum operators x, p and see what we get out. . .

$$\dot{x}(t) = p(t)$$
$$\dot{p}(t) = -V'\big(x(t)\big) - \int_{t_0}^{t} f(t-t')\dot{x}(t')\mathrm{d}t' - f(t-t_0)x(t_0) + \xi(t)$$

- Conservative dynamics of the system!

Example: Substitute for O, the system's canonical coordinate and momentum operators x, p and see what we get out...

$$\dot{x}(t) = p(t)$$
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- $f(t)$ makes the e.o.m. at time t depend on values of $\dot{x}(t)$ at previous times
  $\hookrightarrow$ *"memory function"*
- Depends on the form of the coupling constants g_s, i.e. spectrum of the bath
- In a continuum limit we can write:

$$f(t) = \sum_s g_s^2 \cos(\omega_s t) \to \int_0^\infty \frac{\mathrm{d}\omega}{\pi} \frac{J(\omega)}{\omega} \cos(\omega t)$$

- The spectral density $J(\omega)$ is model dependent! Consider the simplest model of an *Ohmic bath*: $J(\omega) = 2\gamma\omega$

$$\Rightarrow f(t) = \frac{2\gamma}{\pi} \int_0^\infty \cos(\omega t)\mathrm{d}\omega = 2\gamma\delta(t)$$

Generalized Langevin equations

Looks the same as Langevin's original formulation, but is an operator equation!

$$\dot{x}(t) = p(t)$$
$$\dot{p}(t) = -V'\big(x(t)\big) - \gamma\dot{x}(t) + \xi(t)$$

- $\xi(t)$ is an externally specified operator that depends on the initial state of the bath

$$\xi(t) = \sum_s g_s \left[\varphi_s(t_0)\cos\left(\omega_s(t-t_0)\right) + \frac{\pi_s(t_0)}{\omega_s}\sin\left(\omega_s(t-t_0)\right)\right]$$

- Interpreting the equations as noise equations is only possible if some assumption is made about the statistics of $\xi(t)$ $\hookrightarrow$ assume that the bath is initially thermal

$$\rho_B = Z\exp(-\beta H_B), \quad \langle\xi(t)\xi(t')\rangle_\beta = \mathrm{Tr}\left(\rho_B\xi(t)\xi(t')\right)$$

with

$$\langle\varphi_s\rangle_\beta = \langle\pi_s\rangle_\beta = \langle\varphi_s\pi_{s'}\rangle_\beta = 0$$
$$\langle\varphi_s\varphi_{s'}\rangle_\beta = \delta_{ss'}\frac{1}{\omega_s}\left(n_B(\omega_s) + \tfrac{1}{2}\right),$$
$$\langle\pi_s\pi_{s'}\rangle_\beta = \delta_{ss'}\omega_s\left(n_B(\omega_s) + \tfrac{1}{2}\right)$$

- We get *colored* noise statistics

$$\langle\xi(t)\xi(t')\rangle_\beta = \frac{\gamma}{\pi}\int_0^\infty \mathrm{d}\omega\,\omega\coth\left(\frac{\omega}{2T}\right)\cos\left(\omega(t-t')\right), \quad \langle\xi(t)\rangle_\beta = 0$$

$\hookrightarrow$ Non-Markovian dynamics!

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Heisenberg-Langevin equations

$$\dot{x}(t) = p(t) \qquad \langle \xi(t)\xi(t')\rangle_\beta = \frac{\gamma}{\pi}\int_0^\infty \mathrm{d}\omega\,\omega\coth\left(\frac{\omega}{2T}\right)\cos\left(\omega(t-t')\right)$$

$$\dot{p}(t) = -V'\big(x(t)\big) - \gamma\dot{x}(t) + \xi(t) \qquad \langle \xi(t)\rangle_\beta = 0$$

- Obtained a reduced description considering the system's dynamics explicitly and the environment implicitly, e.g. temperature T ✓
- **But...** dealing with operators is unpractical → consider expectation values instead
- requires truncation of equations because $\langle V'(x)\rangle \neq V'(\langle x\rangle)$
- Classical limit $\hbar \to 0$
  - expectation values factorize $\langle V'(x)\rangle \to V'(\langle x\rangle)$
  - $\hbar\omega\coth\left(\frac{\hbar\omega}{2T}\right) \to 2T$ *white* noise spectrum

Classical approximation

$$\dot{X}(t) = P(t) \qquad \langle \xi(t)\xi(t')\rangle_\beta = 2\gamma T\delta(t-t')$$

$$\dot{P}(t) = -V'\big(X(t)\big) - \gamma\dot{X}(t) + \xi(t) \qquad \langle \xi(t)\rangle_\beta = 0$$

How can we do better, i.e. include quantum corrections?

Idea: Truncate HLEs to include time evolution of two point functions $\langle x(t)x(t)\rangle$, $\langle x(t)p(t)+p(t)x(t)\rangle$ and $\langle p(t)p(t)\rangle \to$ Gaussian states

- Corresponds to a Gaussian Wigner function, e.g.:

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

$$\sigma_{ab} \equiv \langle\langle ab\rangle\rangle \equiv \langle ab+ba\rangle/2 - \langle a\rangle\langle b\rangle$$

- Example: Quartic oscillator / (0+1)-dim "toy" theory for self-interacting scalar fields

$$V(x) = \frac{\omega_0^2}{2}x^2 + \frac{\lambda}{4!}x^4$$

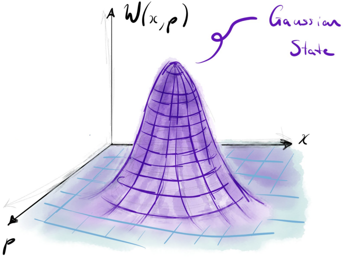

Figure: Illustration of a Gaussian Wigner function (J. Xuereb)

- Expectation values factorize

$$\langle V'(x)\rangle = \int\frac{\mathrm{d}x\mathrm{d}p}{2\pi}\left(\omega_0^2 x + \frac{\lambda}{6}x^3\right)W(x,p) = \omega_0^2 X + \frac{\lambda}{6}\left(X^3 + 3X\sigma_{xx}\right)$$

- Closed system is fully described by five variables and five equations of motion

$$\dot{X} = P,\quad \dot{P} = -\langle V'(x)\rangle,\quad \dot{\sigma}_{xx} = 2\sigma_{xp},\quad \dot{\sigma}_{xp} = \sigma_{pp} - \sigma_{xx}\langle V''(x)\rangle,\quad \dot{\sigma}_{pp} = -2\sigma_{xp}\langle V''(x)\rangle$$

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Idea: Truncate HLEs to include time evolution of two point functions $\langle x(t)x(t)\rangle$, $\langle x(t)p(t)+p(t)x(t)\rangle$ and $\langle p(t)p(t)\rangle$ $\rightarrow$ Gaussian states

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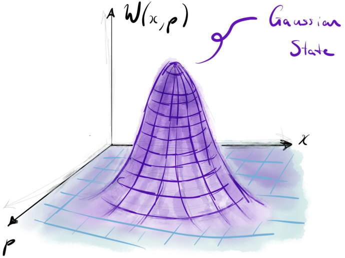

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$$\dot{X}=P,\quad \dot{P}=-\langle V'(x)\rangle,\quad \dot{\sigma}_{xx}=2\sigma_{xp},\quad \dot{\sigma}_{xp}=\sigma_{pp}-\sigma_{xx}\mathcal{C}(t),\quad \dot{\sigma}_{pp}=-2\sigma_{xp}\mathcal{C}(t)$$

Gaussian state approximation

- Introduce heat-bath and interactions
  ↪ Gaussian Wigner function describing combined system

$$W(\boldsymbol{\zeta},t) = \mathcal{N} \exp\left\{-\frac{1}{2}\big(\boldsymbol{\zeta} - \boldsymbol{Z}(t)\big)^{\mathsf{T}} \Sigma^{-1}(t) \big(\boldsymbol{\zeta} - \boldsymbol{Z}(t)\big)\right\}$$

Phase space vector and expectation values

$$\boldsymbol{\zeta} = (x, p, \dots, \varphi_s, \pi_s, \dots)$$
$$\boldsymbol{Z}(t) = \big(X(t), P(t), \dots, \Phi_s(t), \Pi_s(t), \dots\big)$$

Covariance matrix

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

- Equations of motion from averaging HLE's over $W(\boldsymbol{\zeta},t)$

$$\dot{X} = P, \quad \dot{P} = -\left(\omega_0^2 + \frac{\lambda}{2}\sigma_{xx}\right)X - \frac{\lambda}{6}X^3 - \gamma P + \xi(t), \quad \dot{\sigma}_{xx} = 2\sigma_{xp},$$
$$\dot{\sigma}_{xp} = \sigma_{pp} - \sigma_{xx}\mathcal{C}(t) - \gamma\sigma_{xp} + \langle\!\langle x(t)\xi(t)\rangle\!\rangle, \quad \dot{\sigma}_{pp} = -2\sigma_{xp}\mathcal{C}(t) - 2\gamma\sigma_{pp} + \langle\!\langle p(t)\xi(t)\rangle\!\rangle$$

- **Dissipation** and **fluctuations** on the level of first- *and* second-order moments

But... what are $\langle\!\langle x(t)\xi(t)\rangle\!\rangle$ and $\langle\!\langle p(t)\xi(t)\rangle\!\rangle$?

Gaussian state approximation

Recall: $\xi(t)$ depends on initial conditions $\varphi_s(t_0)$ and $\pi_s(t_0)$
$\hookrightarrow$ need to evaluate correlation functions between the system and bath oscillators

$$G_{x\varphi_s}(t) \equiv \langle\langle x(t)\varphi_s(t_0)\rangle\rangle, \quad G_{x\pi_s}(t) \equiv \langle\langle x(t)\pi_s(t_0)\rangle\rangle$$
$$G_{p\varphi_s}(t) \equiv \langle\langle p(t)\varphi_s(t_0)\rangle\rangle, \quad G_{p\pi_s}(t) \equiv \langle\langle p(t)\pi_s(t_0)\rangle\rangle$$

- Considering their respective Heisenberg equations of motion

$$\ddot{G}_{x\varphi_s}(t) + \gamma\,\dot{G}_{x\varphi_s}(t) + \mathcal{C}(t)\,G_{x\varphi_s}(t) = \tfrac{g_s}{2\omega_s}\cos(\omega_s t)$$
$$\ddot{G}_{x\pi_s}(t) + \gamma\,\dot{G}_{x\pi_s}(t) + \mathcal{C}(t)\,G_{x\pi_s}(t) = \tfrac{g_s}{2}\sin(\omega_s t)$$

- Driven damped oscillator with time dependent eigenfrequency
  $\hookrightarrow$ **no analytic solution...**

Idea: In thermal equilibrium expand $\mathcal{C}(t) \to \langle\mathcal{C}\rangle_\beta + \delta\mathcal{C}(t)$
$\hookrightarrow$ **Eqs. become solvable!** (Only consider static solution in this talk)

Equations of motion:

$$\dot{X} = P, \quad \dot{P} = -\left(\omega_0^2 + \frac{\lambda}{2}\sigma_{xx}\right)X - \frac{\lambda}{6}X^3 - \gamma P + \xi(t), \quad \dot{\sigma}_{xx} = 2\sigma_{xp},$$
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$$\dot{\sigma}_{xp} = \sigma_{pp} + \mathcal{C}_\beta\big(F(\mathcal{C}_\beta) - \sigma_{xx}\big) - \gamma\sigma_{xp}, \quad \dot{\sigma}_{pp} = -2\sigma_{xp}\mathcal{C}_\beta - 2\gamma\sigma_{pp}$$

- No **fluctuations** on the level of second-order moments
  $\hookrightarrow$ **Particular solution:** $\sigma_{xx}(t) \to F(\mathcal{C}_\beta) \approx \frac{1}{2\sqrt{\mathcal{C}_\beta}}$, (for small γ)

Equations of motion:

$$\dot{X} = P$$

$$\dot{P} = -\left(\omega_0^2 + \frac{\lambda}{2}F(\mathcal{C}_\beta)\right)X - \frac{\lambda}{6}X^3 - \gamma P + \xi(t)$$

$\hookrightarrow$ Two corrections to classical Langevin dynamics:

- Frequency shift

$$F(\mathcal{C}_\beta) \approx \frac{1}{2\sqrt{\mathcal{C}_\beta}}$$

$$\mathcal{C}_\beta = \omega_0^2 + \frac{\lambda}{4\sqrt{\mathcal{C}_\beta}} \coth\left(\frac{\sqrt{\mathcal{C}_\beta}}{2T}\right)$$

- Colored noise spectrum

$$\langle \xi(t)\xi(t')\rangle = \frac{2\gamma}{\pi}\int_0^\infty \mathrm{d}\omega\, \omega n_B(\omega)\cos\left(\omega(t-t')\right)$$

We can now calculate real-time observables as functions of $X(t)$ and $P(t)$

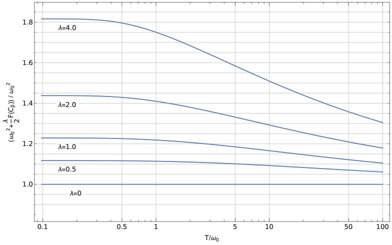

Figure: Temperature dependence of the frequency shift in units of ω_0^2 for different values of λ/ω_0^3

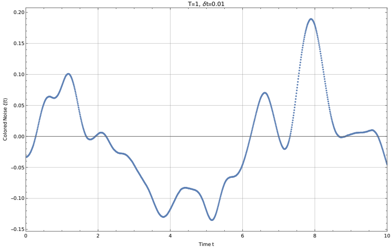

Figure: One typical trajectory of the colored noise as a function of time at temperature $T/\omega_0 = 1$

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Equations of motion:

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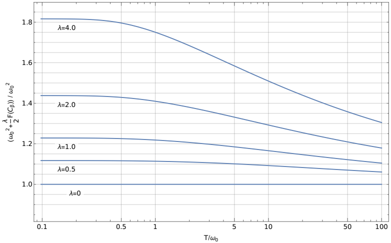

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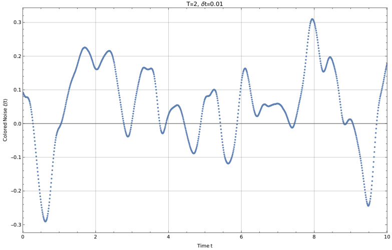

Figure: One typical trajectory of the colored noise as a function of time at temperature $T/\omega_0 = 2$

Equations of motion:

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$$F(\mathcal{C}_\beta) \approx \frac{1}{2\sqrt{\mathcal{C}_\beta}}$$

$$\mathcal{C}_\beta = \omega_0^2 + \frac{\lambda}{4\sqrt{\mathcal{C}_\beta}}\coth\left(\frac{\sqrt{\mathcal{C}_\beta}}{2T}\right)$$

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$$\langle \xi(t)\xi(t')\rangle = \frac{2\gamma}{\pi}\int_0^\infty \mathrm{d}\omega\, \omega n_B(\omega)\cos\left(\omega(t-t')\right)$$

We can now calculate real-time observables as functions of $X(t)$ and $P(t)$

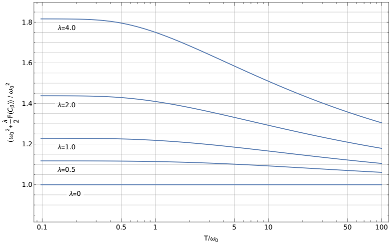


Figure: Temperature dependence of the frequency shift in units of ω_0^2 for different values of λ/ω_0^3

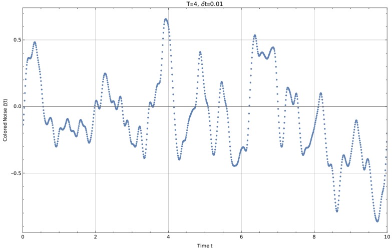


Figure: One typical trajectory of the colored noise as a function of time at temperature $T/\omega_0 = 4$

Gaussian state approximation – Summary

Equations of motion:

$$\dot{X} = P$$

$$\dot{P} = -\left(\omega_0^2 + \frac{\lambda}{2} F(\mathcal{C}_\beta)\right) X - \frac{\lambda}{6} X^3 - \gamma P + \xi(t)$$

$\hookrightarrow$ Two corrections to classical Langevin dynamics:

- Frequency shift

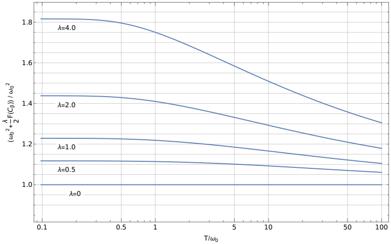
$$F(\mathcal{C}_\beta) \approx \frac{1}{2\sqrt{\mathcal{C}_\beta}}$$

$$\mathcal{C}_\beta = \omega_0^2 + \frac{\lambda}{4\sqrt{\mathcal{C}_\beta}} \coth\left(\frac{\sqrt{\mathcal{C}_\beta}}{2T}\right)$$

- Colored noise spectrum

$$\langle \xi(t)\xi(t') \rangle = \frac{2\gamma}{\pi} \int_0^\infty \mathrm{d}\omega\, \omega n_B(\omega) \cos\left(\omega(t-t')\right)$$

We can now calculate real-time observables as functions of $X(t)$ and $P(t)$



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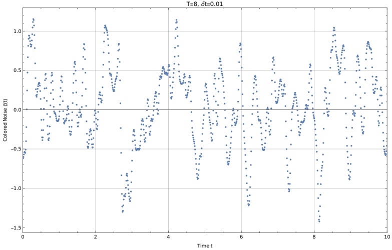

Figure: One typical trajectory of the colored noise as a function of time at temperature $T/\omega_0 = 8$

Spectral function

Spectral function

- Definition:

$$\rho(t-t') = \mathrm{i}\langle[x(t), x(t')]\rangle_\beta$$

- Without dissipation: Sum over energy eigenstates

$$\rho(\omega) = \frac{1}{Z}\sum_{m,n} \mathrm{e}^{-\beta E_n}\big(\delta(\omega - E_m + E_n) - \delta(\omega + E_m - E_n)\big)|\langle n|x|m\rangle|^2$$

- Ohmic bath (valid for small γ):

$$\rho_\gamma(\omega) = \frac{1}{Z}\sum_{m,n} \mathrm{e}^{-\beta E_n}\,|\langle n|x|m\rangle|^2 2\Delta E_{mn} \times \frac{1}{\pi}\frac{\gamma\omega}{(\omega^2 - \Delta E_{mn}^2)^2 + \gamma^2\omega^2}$$

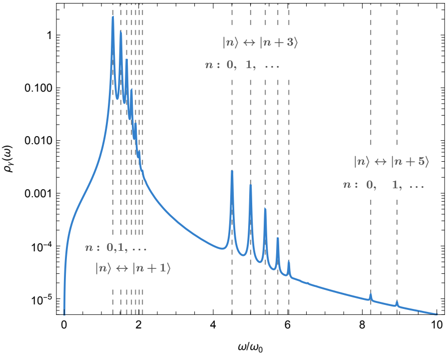

Figure: Exemplary spectral function (in units of ω_0^{-2}) of the anharmonic oscillator from exact diagonalization with damping, for $T/\omega_0 = 1$, $\lambda/\omega_0^3 = 4$, and $\gamma/\omega_0 = 0.03$.

- **Serves as a benchmark for comparing the different approximations**

J. Roth, D. Schweitzer, LS, L. von Smekal, *Phys. Rev. D* **105** (2022) 116017

Fluctuation-dissipation relation

How can we calculate the spectral function from classical observables $X(t)$, $P(t)$?

- *Spectral function* is difficult

$$\rho(t,t') = \mathrm{i}\big\langle\big[x(t),x(t')\big]\big\rangle_\beta \xrightarrow{\text{class.}} \text{Poisson bracket}$$

- *Statistical function* is easy

$$F(t,t') = \tfrac{1}{2}\big\langle\big[x(t),x(t')\big]_+\big\rangle_\beta \xrightarrow{\text{class.}} \text{factor 2}$$

Related via decomposition of time-ordered Green's function:

$$G^{\mathbb{T}}(t,t') = F(t,t') - \frac{\mathrm{i}}{2}\rho(t,t')[\Theta(t-t') - \Theta(t'-t)]$$

1. In thermal equilibrium apply Kubo-Martin-Schwinger condition

$$G^{\mathbb{T}}(t,t') = G^{\mathbb{T}}(t',t+\mathrm{i}\,\beta)$$

2. Obtain a fluctuation-dissipation relation

$$F(\omega) = \coth\left(\frac{\omega}{2T}\right)\pi\rho(\omega)$$

3. Classical limit $\coth\big(\omega/2T\big) \approx 2T/\omega$

$$F_c(\omega) = \frac{T}{\omega}2\pi\rho_c(\omega)$$

4. After Fourier transform

$$\rho_c(t-t') = -\frac{1}{T}\partial_t F_c(t-t')$$
$$= -\frac{1}{2T}\langle P(t)X(t') - X(t)P(t')\rangle_\beta$$

Calculate ρ from classical observables!

- Gaussian state approximation → modified FDR

$$\rho(\omega) = \frac{T}{\omega n_B(\omega)}\rho_c(\omega)$$

...exponentially difficult at small T/ω

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Idea: Compute the retarded propagator G^R directly, then relate to the spectral function via:

$$G^R(t-t') = \Theta(t-t')\rho(t-t')$$

1. Linear response to an external perturbation is given by

$$\delta X(t) = \int \mathrm{d}t' G^R(t-t')h(t')$$

2. Choose the external perturbation to be

$$h(t) = h_0 \delta(t - t_{\text{pert}})$$

3. Then the response becomes

$$\delta X(t) = h_0 G^R(t - t_{\text{pert}})$$

4. Now replace in our Langevin equations

$$X(t) \to X(t) + \delta X(t)$$
$$P(t) \to P(t) + \delta P(t)$$

5. Obtain e.o.m. for the response

$$\delta \dot{X} = \delta P$$

$$\delta \dot{P} = -\left(\omega_0^2 + \frac{\lambda}{2}\left(\sigma_{xx}(t) + X(t)^2\right)\right)\delta X - \gamma \delta P$$

6. Finally insert the relation from step No. 3

$$\ddot{G}^R(t-t_{\text{pert}}) + \gamma \dot{G}^R(t-t_{\text{pert}}) + \left(\omega_0^2 + \frac{\lambda}{2}\left(\sigma_{xx}(t) + X(t)^2\right)\right) G^R(t-t_{\text{pert}}) = 0$$

Inital conditions: $G^R(0) = 0$, and $\dot{G}^R(0) = 1$

Can be numerically integrated using standard techniques!

Results - FDR vs. Linear response

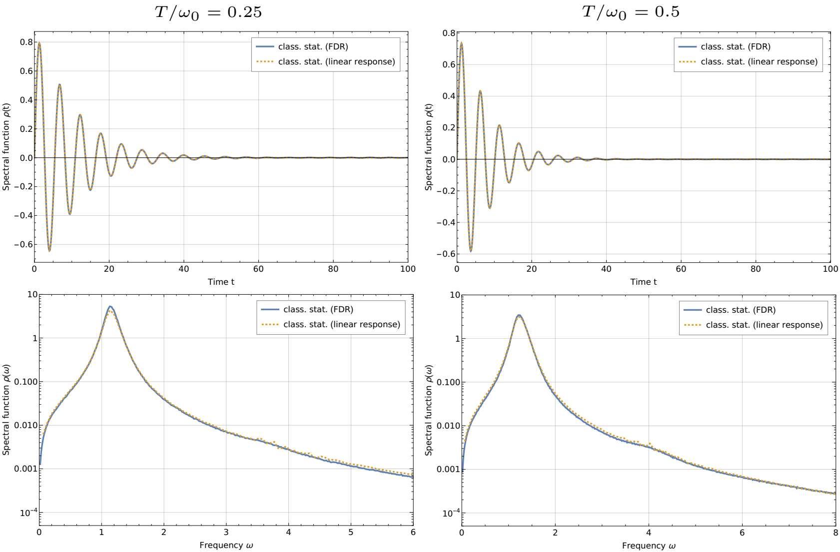


Figure: Classical-statistical spectral functions of the anharmonic oscillator (in units of ω_0^{-2}) for $\lambda/\omega_0^3 = 4$, $\gamma/\omega_0 = 0.12$.

Both methods are valid and produce identical results!

Results - FDR vs. Linear response

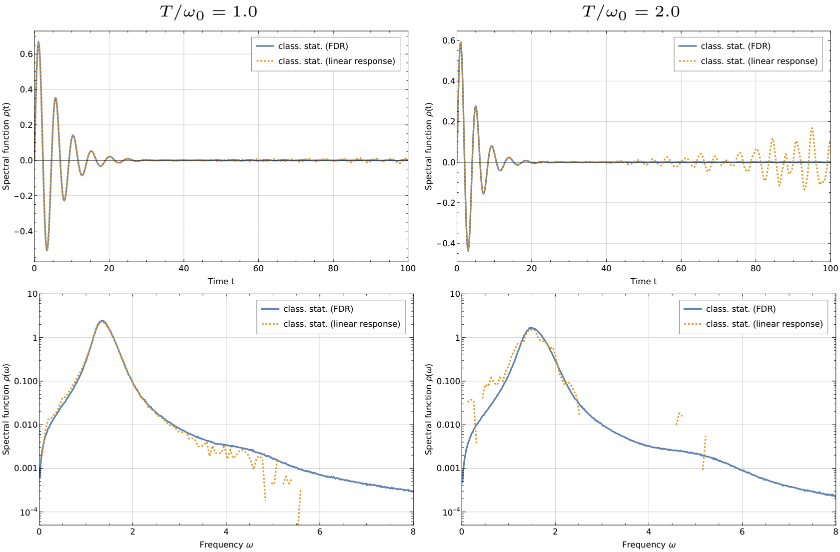


Figure: Classical-statistical spectral functions of the anharmonic oscillator (in units of ω_0^{-2}) for $\lambda/\omega_0^3 = 4$, $\gamma/\omega_0 = 0.12$.

Linear response is computationally more expensive → Solution: Parallel processing on GPUs

Results - FDR vs. Linear response

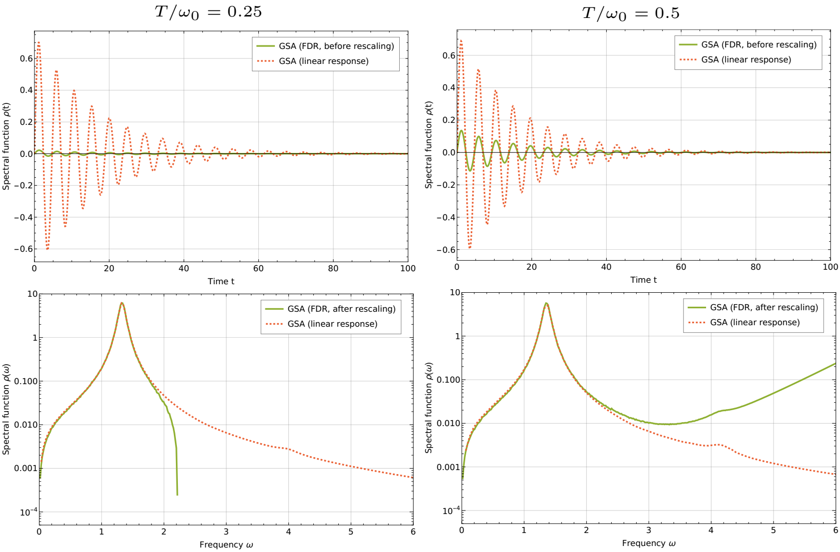


Figure: Spectral functions of the anharmonic oscillator in (static) GSA (in units of ω_0^{-2}) for $\lambda/\omega_0^3 = 4$, $\gamma/\omega_0 = 0.12$.

Linear response is the method of choice to compute spectral functions in the GSA!

Results - FDR vs. Linear response

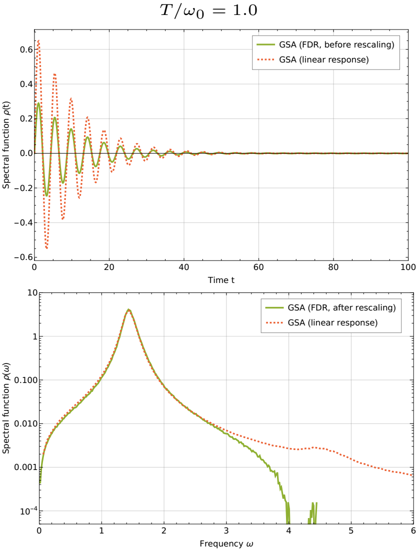


Figure: Spectral functions of the anharmonic oscillator in (static) GSA (in units of ω_0^{-2}) for $\lambda/\omega_0^3 = 4$, $\gamma/\omega_0 = 0.12$.

Near the classical limit (large $\frac{T}{\omega}$), the approximate FDR may be a useful alternative

- Only $|0\rangle \leftrightarrow |1\rangle, |3\rangle$ transitions visible
- Main peak in GSA matches up perfectly!
- Classical peak position too low
- Quasiclassical peak too broad
- $|0\rangle \leftrightarrow |3\rangle$ transition unresolved in approximations

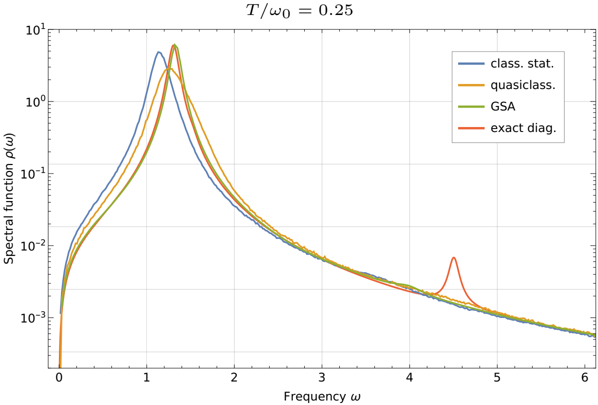


Figure: Spectral function of the anharmonic oscillator (in units of ω_0^{-2}) for $\lambda/\omega_0^3 = 4$, and $\gamma/\omega_0 = 0.12$.

Results - Comparison of stochastic real-time methods

- $|1\rangle \leftrightarrow |2\rangle, |4\rangle$ transitions emerge
- Main peak in GSA interpolates between both
- Classical peak position still too low
- Quasiclassical peak still too broad
- $|0\rangle \leftrightarrow |3\rangle$ transition visible in GSA

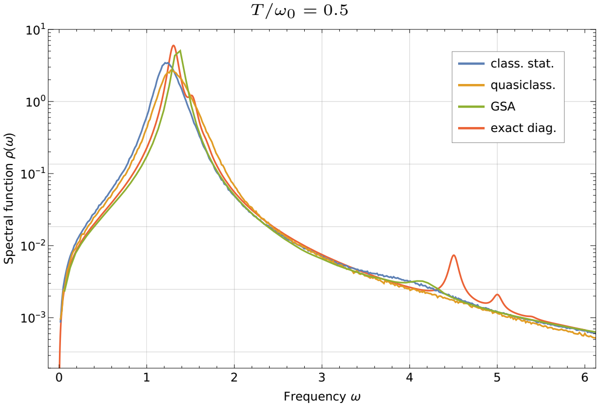


Figure: Spectral function of the anharmonic oscillator (in units of ω_0^{-2}) for $\lambda/\omega_0^3 = 4$, and $\gamma/\omega_0 = 0.12$.

- Increasing number of $|n\rangle \leftrightarrow |n+1\rangle\,, |n+3\rangle$ transitions
- Main peak is approximated reasonably well by all methods
- $|n\rangle \leftrightarrow |n+3\rangle$ transitions best approximated in GSA

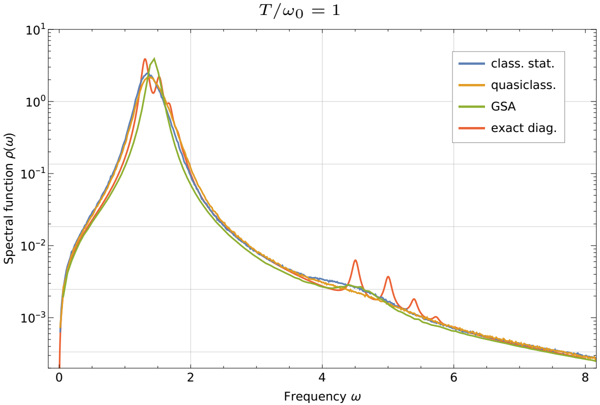


Figure: Spectral function of the anharmonic oscillator (in units of ω_0^{-2}) for $\lambda/\omega_0^3 = 4$, and $\gamma/\omega_0 = 0.12$.

- Linear response approach in GSA became too slow
- FDR approach was used $\hookrightarrow$ numerically difficult
- Classical and quasiclassical results look the same
- Both interpolate the exact sub-peak structure

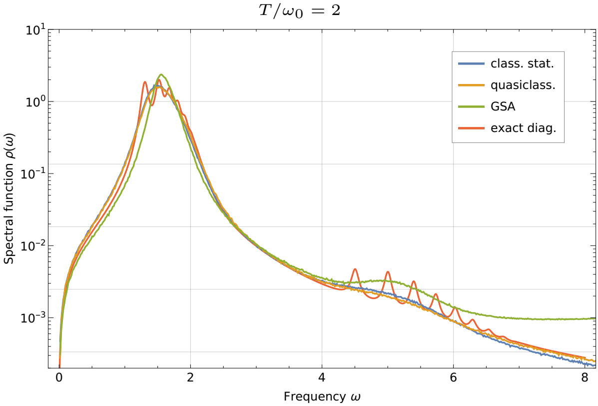
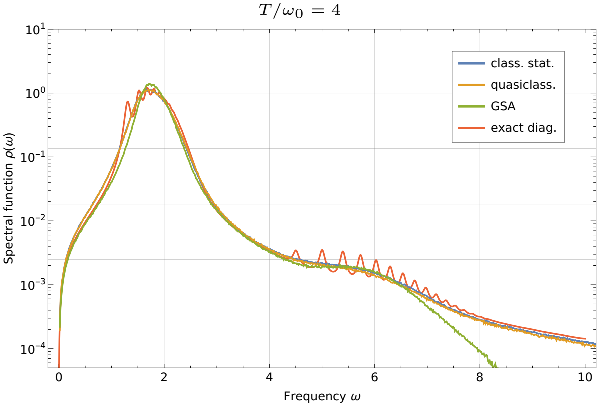


Figure: Spectral function of the anharmonic oscillator (in units of ω_0^{-2}) for $\lambda/\omega_0^3 = 4$, and $\gamma/\omega_0 = 0.12$.

- Finite $\gamma \to$ many individual transitions combine into one broad peak



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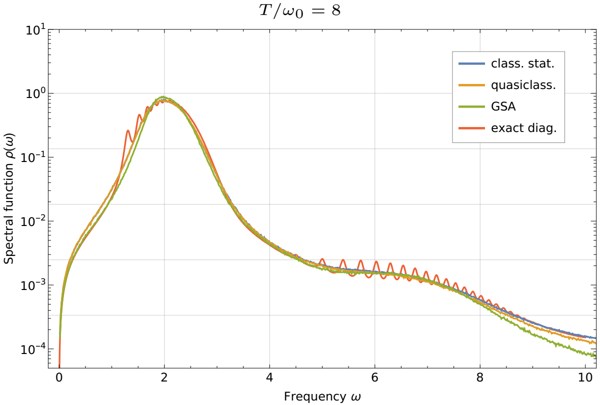
All approximations are consistent with the classical limit!



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Real-time field theory

Summary - Field theory

- Formal description of non-equilibrium QFT via Keldysh[3] formalism
  $\hookrightarrow$ classical Langevin equation naturally emerges for $\hbar \to 0$
- Classical field theory:

$$H_S[\phi,\pi] = \int \mathrm{d}^d x \, \frac{1}{2} \Big(\pi^2(\boldsymbol{x},t) - \big(\nabla\phi(\boldsymbol{x},t)\big)^2 + m^2\phi^2(\boldsymbol{x},t) \Big) + \frac{\lambda}{4!}\phi^4(\boldsymbol{x},t)$$

- Langevin equations:

$$\begin{aligned} \dot{\phi}(\boldsymbol{x},t) &= \pi(\boldsymbol{x},t) \\ \dot{\pi}(\boldsymbol{x},t) &= \nabla^2\phi(\boldsymbol{x},t) - m^2\phi(\boldsymbol{x},t) - \frac{\lambda}{6}\phi^3(\boldsymbol{x},t) - \gamma\pi(\boldsymbol{x},t) + \xi(\boldsymbol{x},t) \end{aligned}$$

- with classical noise spectrum:

$$\langle \xi(\boldsymbol{x},t) \rangle_\beta = 0, \quad \langle \xi(\boldsymbol{x},t)\xi(\boldsymbol{x}',t') \rangle_\beta = 2\gamma T \delta(\boldsymbol{x}-\boldsymbol{x}')\delta(t-t')$$

- analogous expressions in quasiclassical and Gaussian state approximation

[3] L. Keldysh, *Diagram technique for non-equilibrium processes*, Sov. Phys. JETP. **20**, (1965)

- Equations of motion in static Gaussian state approximation:

$$\dot{\phi}(\boldsymbol{x},t) = \pi(\boldsymbol{x},t)$$
$$\dot{\pi}(\boldsymbol{x},t) = \nabla^2\phi(\boldsymbol{x},t) - \left(m^2 + \frac{\lambda}{2}\langle\!\langle\phi\phi\rangle\!\rangle_\beta\right)\phi(\boldsymbol{x},t) - \frac{\lambda}{6}\phi^3(\boldsymbol{x},t) - \gamma\pi(\boldsymbol{x},t) + \xi(\boldsymbol{x},t)$$

- Last problem: **How to compute $\langle\!\langle\phi\phi\rangle\!\rangle_\beta$?**

Recall: $\mathcal{C}_\beta \equiv \langle V''(\phi)\rangle_\beta = m^2 + \frac{\lambda}{2}\left(\langle\phi^2\rangle_\beta + \langle\!\langle\phi\phi\rangle\!\rangle_\beta\right)$

- Can be determined from a Dyson equation

$$\Leftrightarrow \quad \mathcal{C}_\beta = m^2 + \frac{\lambda}{4}\int\frac{\mathrm{d}^dp}{(2\pi)^d}\frac{1}{\sqrt{\mathcal{C}_\beta + \boldsymbol{p}^2}}\coth\left(\frac{\sqrt{\mathcal{C}_\beta + \boldsymbol{p}^2}}{2T}\right)$$

- requiring that thermal fluctuations $\langle\phi^2\rangle_\beta$ vanish for $T \to 0$:

$$\langle\phi^2\rangle_\beta = \int\frac{\mathrm{d}^dp}{(2\pi)^d}\frac{n_B(\omega)}{\sqrt{\mathcal{C}_\beta + \boldsymbol{p}^2}}, \quad \langle\!\langle\phi\phi\rangle\!\rangle_\beta = \frac{1}{2}\int\frac{\mathrm{d}^dp}{(2\pi)^d}\frac{1}{\sqrt{\mathcal{C}_\beta + \boldsymbol{p}^2}}$$

Consistent with the 0-dim. case! (but... needs to be renormalized for $d \geq 2$)

- Regularize divergent $T \to 0$ part with a cutoff Λ:

$$\mathcal{C}_0 = m^2 + \frac{\lambda}{4} \int_0^\Lambda \frac{\mathrm{d}^3 p}{(2\pi)^3} \frac{1}{\sqrt{\mathcal{C}_0 + \boldsymbol{p}^2}}$$
$$= m^2 + \frac{\lambda}{16\pi^2}\Lambda^2 + \frac{\lambda}{32\pi^2}\mathcal{C}_0 \left(1 - \ln 4 - \ln \frac{\Lambda^2}{\mathcal{C}_0}\right)$$

- Define the bare coupling λ to cancel the logarithmic divergence and absorb the quadratic divergence into the relation between bare and renormalized mass

$$\frac{1}{\lambda_R} \equiv \frac{1}{\lambda} + \frac{1}{32\pi^2}\left(\ln \frac{\Lambda^2}{\mathcal{C}_0} - 1 + \ln 4\right), \qquad \frac{m_R^2}{\lambda_R} \equiv \frac{m^2}{\lambda} + \frac{\Lambda^2}{16\pi^2}$$

- Renormalized equilibrium curvature:

$$\mathcal{C}_0 = m_R^2, \quad \mathcal{C}_\beta = m_R^2 + \frac{\lambda_R}{2} \int \frac{\mathrm{d}^3 p}{(2\pi)^3} \frac{n_B(\sqrt{\mathcal{C}_\beta + \boldsymbol{p}^2})}{\sqrt{\mathcal{C}_\beta + \boldsymbol{p}^2}} + \frac{\lambda_R \mathcal{C}_\beta}{32\pi^2} \ln \frac{\mathcal{C}_\beta}{m_R^2}$$

- Renormalized effective mass:

$$m^2 + \frac{\lambda}{2}\langle\!\langle \phi\phi \rangle\!\rangle_\beta = m_R^2 + \lambda_R \frac{\mathcal{C}_\beta}{32\pi^2} \ln \frac{\mathcal{C}_\beta}{m_R^2} \qquad \checkmark$$

Results - (2+1)d spectral functions

- Class.: Wrong frequency
  $\hookrightarrow$ missing quantum fluctuations
- Quasiclass.: Wrong width
  $\hookrightarrow$ quantum fluctuations are treated as thermal
- GSA: Best of both!

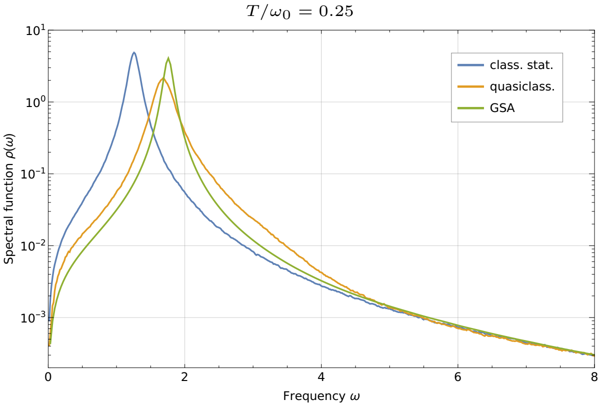

Figure: Zero momentum mode of the spectral function in (2+1) dimensions (in units of ω_0^{-2}) for $\lambda/\omega_0^3 = 24$, and $\gamma/\omega_0 = 0.12$.

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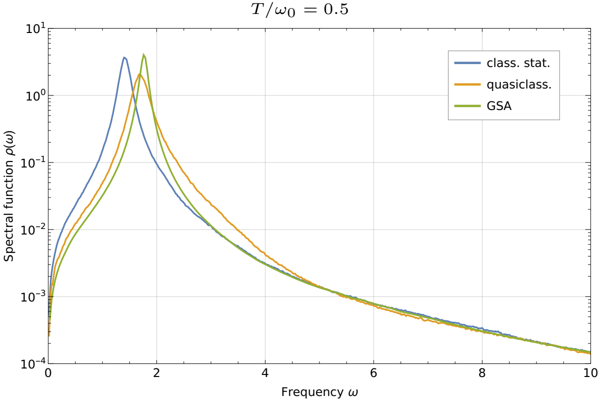

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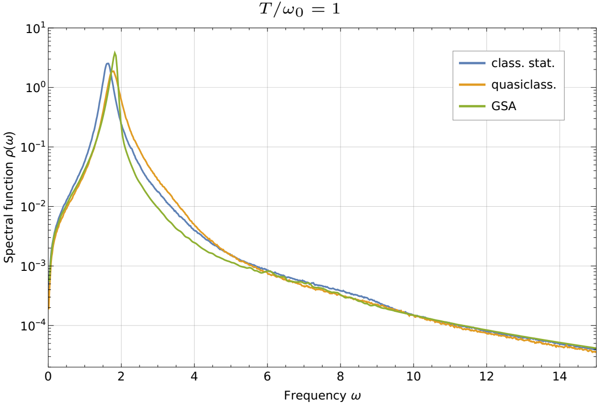

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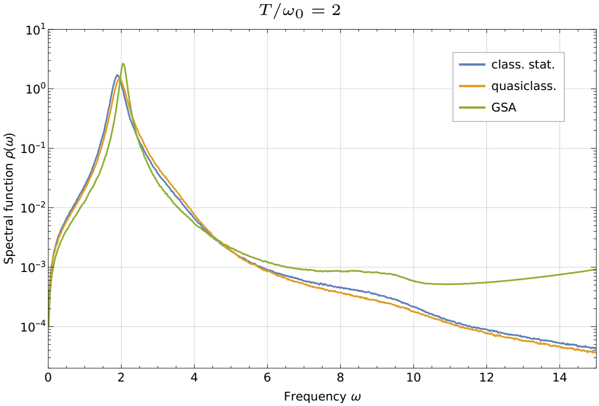

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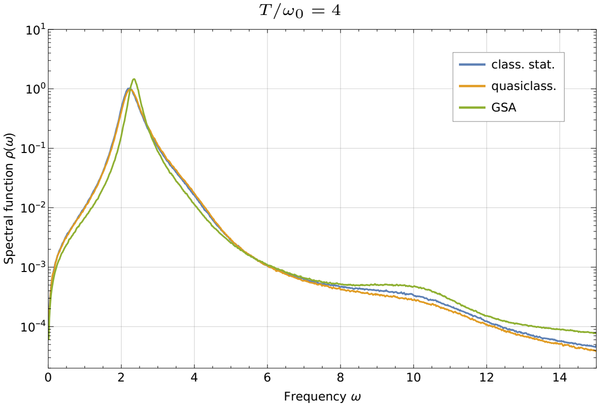

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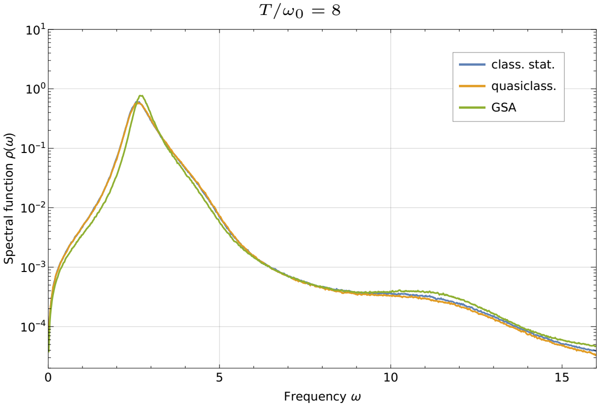

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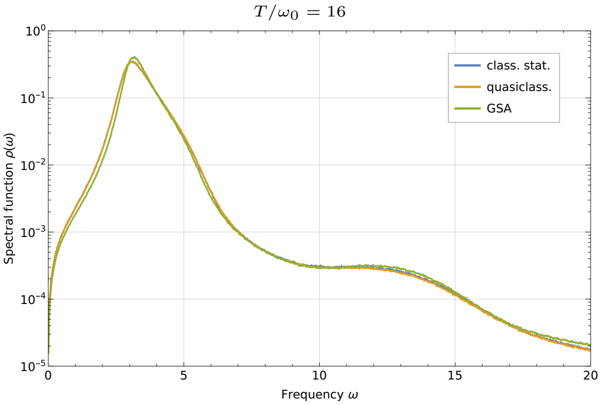

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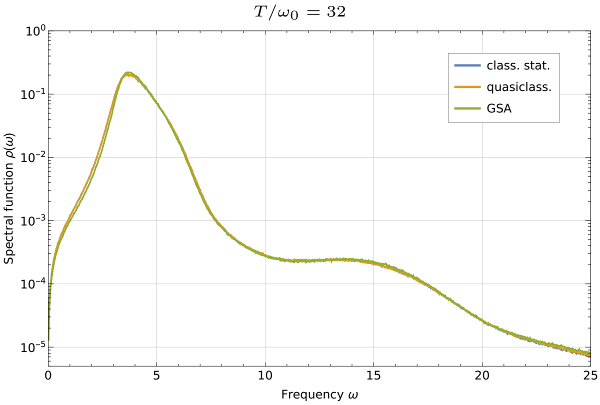

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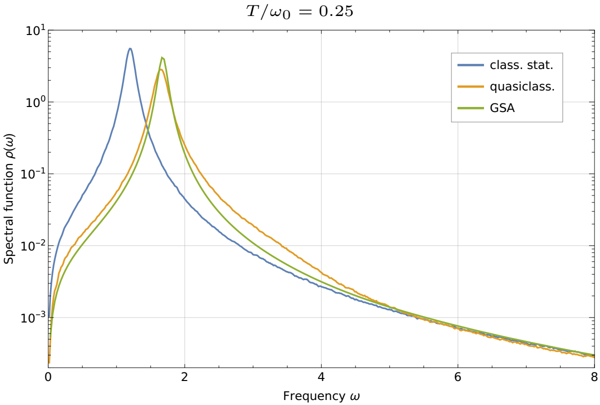
Results - (3+1)d spectral functions

- Qualitatively the same behavior as before
- Quasiclassical and GSA are more similar than in $d = 2$



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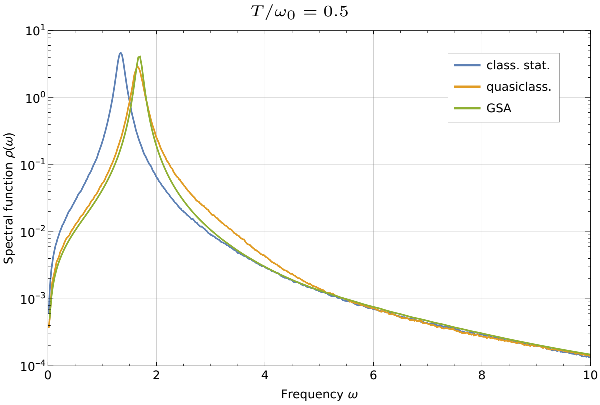

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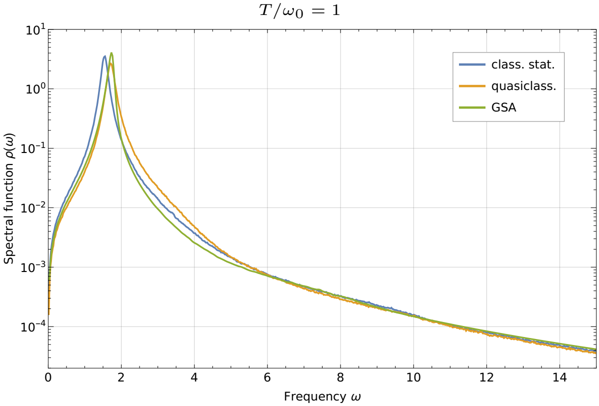

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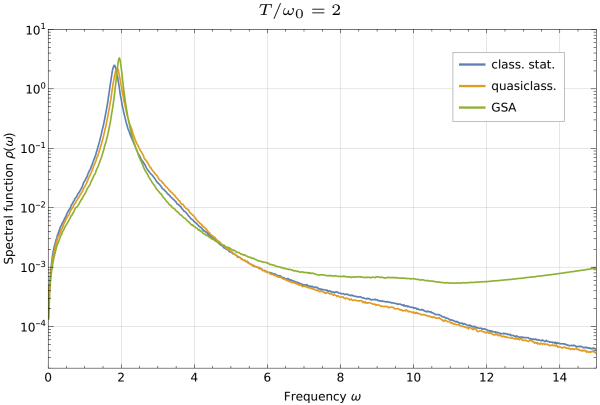

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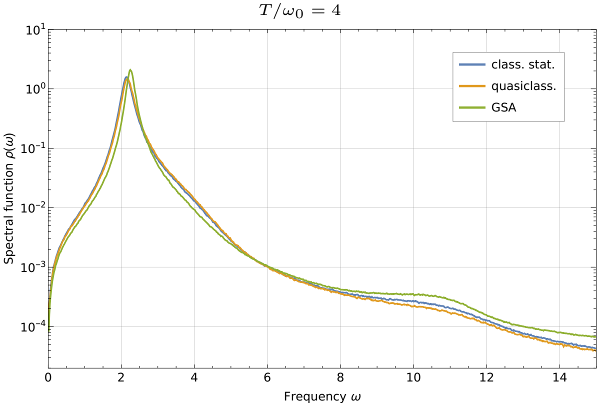

Figure: Zero momentum mode of the spectral function in (3+1) dimensions (in units of ω_0^{-2}) for $\lambda/\omega_0^3 = 24$, and $\gamma/\omega_0 = 0.12$.

Results - (3+1)d spectral functions

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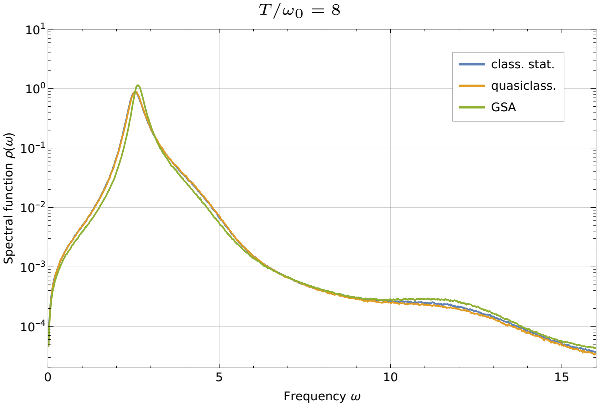

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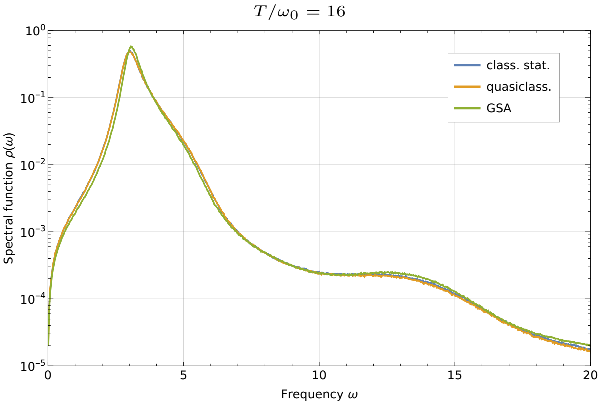

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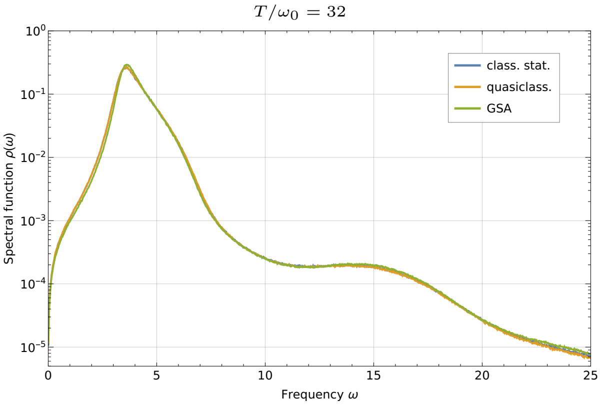

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Conclusion & Outlook

Conclusion

- **Generalized Langevin equations:**
  Effecive description for the behavior of open quantum systems
  $\hookrightarrow$ Classical dynamics emerge naturally for $\hbar \to 0$

- **Gaussian state approximation:**
  Extension of classical simulations by incorporating lowest order quantum corrections
  - Consistent with the classical limit
  - Quasiclassical methods not sufficient
  - Works in (renormalizable) field theory context

- **Linear response:**
  More generally applicable method of computing spectral functions
  - Enables computing spectral functions in GSA
  - Also valid off equilibrium

Outlook

- Parallel processing of Linear response spectral functions on GPUs
- Investigate adiabatic corrections in GSA
- Finite momentum modes of spectral functions
- Static and dynamic critical behavior of Z_2 Ising in GSA
  $\hookrightarrow$ Observe crossover from quantum to classical physics?
- Extend GSA to four-component $O(4)$ model
- Explicit time evolution of $\langle\langle\phi(t,\boldsymbol{x})\phi(t',\boldsymbol{x}')\rangle\rangle$ to study non-equilibrium dynamics
  $\hookrightarrow$ Finite quenching rates (Kibble-Zurek)

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Thank You!

Appendix