Novel lattice simulations for transport coefficients in gauge theories

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Pawlowski, Rothkopf, arXiv:1610.09531 [hep-lat]
Pawlowski, Rothkopf, Ziegler, in preparation

Seminar – Theory of Hadronic Matter under Extreme Conditions
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UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386

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Overview

- Introduction
  - Physics motivation of real-time dynamics from lattice QCD
  - Challenges in the reconstruction of spectral functions
- Novel simulation approach for thermal fields on the lattice with non-compact Euclidean time
  - Setup and scalar fields
  - Gauge fields
  - Convergence to the Matsubara results
  - Energy-momentum tensor correlation functions
  - Spectral reconstructions
- Summary and outlook

Introduction

Physics motivation

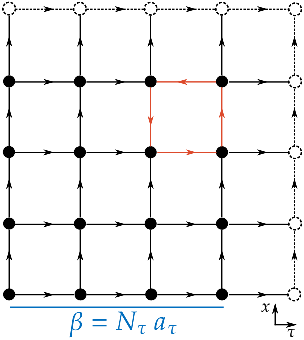
- Thermal physics of hot strongly interacting matter produced in heavy ion collisions
  - Transport phenomena
  - In-medium modification of heavy bound states
- Transport coefficients are real-time quantities related to the energy-momentum tensor (EMT) correlation function
- Example: shear viscosity

$$\eta = \lim_{\omega \to 0} \frac{1}{20} \frac{\rho(\omega, 0)}{\omega}, \quad \rho(\omega, \vec{p}) = \int \frac{d^4x}{(2\pi)^4} e^{-i\omega x_0 + i\vec{p}\cdot\vec{x}} \langle [T_{12}(x), T_{12}(0)] \rangle .$$

$\Rightarrow$ need spectral function $\rho(\omega, \vec{p})$

Lattice QCD at finite temperature

- Gauge fields on links
  $U_\mu(x) = \exp(i g a_\mu A_\mu^a(x) T^a)$
- Dynamical fermions with realistic masses
- finite extent in imaginary time
  $1/T = \beta = N_\tau a_\tau$



$$\langle O(U) \rangle = \frac{1}{Z} \int \mathcal{D}U\, O(U) \exp(-S_E^{\mathrm{QCD}}[U])$$

$$P(U_k) = e^{-S_E^{\mathrm{QCD}}[U_k]} \Rightarrow \langle O(U) \rangle \approx \frac{1}{N_{\mathrm{cf}}} \sum_{k=1}^{N_{\mathrm{cf}}} O(U_k)$$

Reconstruction of spectral functions and its challenges

- Back to real-time EMT-correlator:

$$\rho(\omega,\vec{p}) = \int \frac{d^4x}{(2\pi)^4} e^{-i\omega x_0 + i\vec{p}\cdot\vec{x}} \langle [T_{12}(x), T_{12}(0)] \rangle$$

- Spectral function connects physical real-time observable with Euclidean time simulation

$$D(\tau) \propto \int \mathrm{d}^3x \, \langle T_{12}(\tau,\vec{x}) T_{12}(0,0) \rangle = \int \mathrm{d}\mu \, \frac{\cosh[\mu(\tau-\beta/2)]}{\sinh[\mu\,\beta/2]} \rho(\mu)$$

For the reconstruction technique used in the following see

Y.Burnier, Alexander Rothkopf, Phys.Rev.Lett. 111 (2013) 182003

Reconstruction of spectral functions and its challenges

Two main conceptual problems of standard spectral reconstructions

- Problem 1:

$$D(\tau) = \int_0^\infty \mathrm{d}\mu \, \frac{\cosh[\mu(\tau - \beta/2)]}{\sinh[\mu\,\beta/2]} \rho(\mu)$$

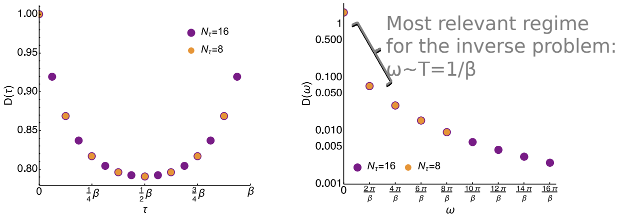
Extraction from imaginary time correlator ill-posed exponentially hard inversion problem.
→ Go to imaginary frequencies and use Källén-Lehman spectral representation

$$D(\omega_n) = \int_0^\infty \mathrm{d}\mu \, \frac{2\,\mu}{\omega_n^2 + \mu^2} \, \rho(\mu)$$

Reconstruction of spectral functions and its challenges

Two main conceptual problems of standard spectral reconstructions

- Problem 2: Increasing the number of points along Euclidean time axis does not help!



- Standard lattice simulations only access Matsubara frequencies $\omega_n = 2\pi T n, \; n \in \mathbb{Z}$.

Setup of a novel computational approach

Thermal field theory on the Schwinger-Keldysh contour

- Thermal scalar field theory as a real-time initial value problem with $Z = \mathrm{Tr}\left(\rho(0) = e^{-\beta H}\right)$

$$Z = \int \mathrm{d}[\varphi_0^+]\mathrm{d}[\varphi_0^-]\langle\varphi_0^+|\rho(0)|\varphi_0^-\rangle\langle\varphi_0^-|\varphi_0^+\rangle$$

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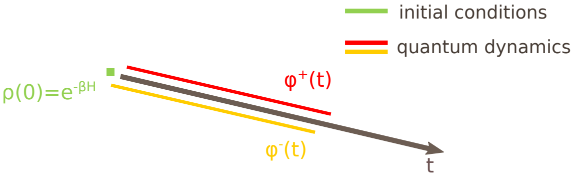

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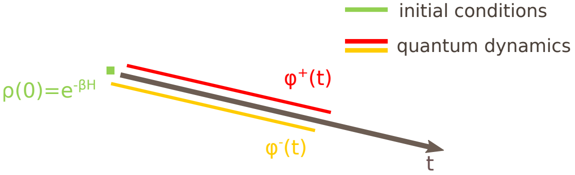
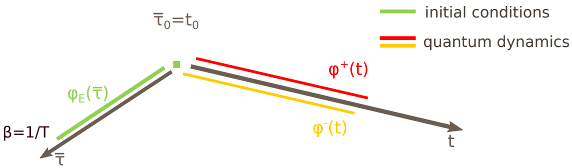


Thermal field theory on the Schwinger-Keldysh contour

- Thermal scalar field theory as a real-time initial value problem with $Z = \mathrm{Tr}\left(\rho(0) = e^{-\beta H}\right)$

$$Z = \int_{\varphi_E(0)=\varphi_E(\beta)} \mathcal{D}\varphi_E e^{-S_E[\varphi_E]} \int_{\varphi^+(t_0)=\varphi_E(0)}^{\varphi^-(t_0)=\varphi_E(\beta)} \mathcal{D}\varphi e^{iS_M[\varphi^+]-iS_M[\varphi^-]}$$

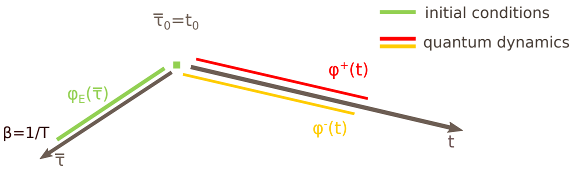


- So far, we have only rewritten the partition function. The imaginary time is a mathematical tool to sample initial conditions $\varphi^+(t_0)$ and $\varphi^-(t_0)$.

Path contribution

- **Thermal equilibrium** $\Rightarrow G^{++} \equiv \langle \varphi^+ \varphi^+ \rangle$ correlator sufficient to compute spectral function ρ, see e.g. Laine and Vuorinen, Basics of Thermal Field Theory, Springer 2016

$$G^{++}(p^0,\vec{p}) = \int \frac{\mathrm{d}q^0}{2\pi} \frac{\rho(q^0,\vec{p})}{q^0 - p^0 + i\varepsilon} - n(p^0)\rho(p^0,\vec{p})$$

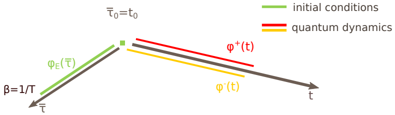


- Using time translation invariance we can set $t_0 \to -\infty$.
- Introducing $\varepsilon > 0$ and $e^{-iHt} \to e^{-iHt(1+i\varepsilon)}$ correlations between any finite t on forward branch and endpoint become exponentially damped.

Analytic continuation and general imaginary frequencies

- From no on, we focus on the **forward** φ^+ path.
- **Idea:** Cut open real-time path at $t = \infty$ and rotate path to (additional) non-compact imaginary time axis.

$$Z = \int_{\varphi_E(0)=\varphi_E(\beta)} \mathcal{D}\varphi_E \, e^{-S_E[\varphi_E]} \int_{\varphi^+(t_0,\vec{x})=\varphi_E(0)}^{\varphi^-(t_0,\vec{x})=\varphi_E(\beta)} \mathcal{D}\varphi \, e^{i\,S_M[\varphi^+]-i\,S_M[\varphi^-]}$$



Analytic continuation and general imaginary frequencies

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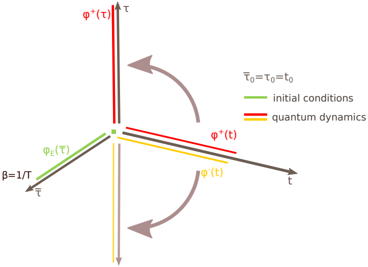
$$Z = \int_{\varphi_E(0)=\varphi_E(\beta)} \mathcal{D}\varphi_E \, e^{-S_E[\varphi_E]} \int_{\varphi^+(\tau_0)=\varphi_E(0)}^{\varphi^+(\infty)} \mathcal{D}\varphi^+ e^{-S_E[\varphi^+]} \int_{\varphi^-(\infty)}^{\varphi^-(\tau_0)=\varphi_E(\beta)} \mathcal{D}\varphi^- e^{-S_E[\varphi^-]}$$

Simulation recipe

- Sample init. conditions $\varphi_E(\bar{\tau}_0) = \varphi^+(\tau_0)$ from $e^{-S_E[\varphi_E]}$ on compact Euclidean time lattice, $\bar{\tau} \in [0, \beta]$.
- Concurrently sample $\varphi^+(\tau)$ from $e^{-S_E[\varphi^+]}$ with $\tau \in [0, \infty)$.



Simulating scalar fields

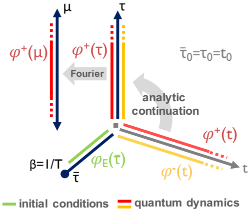
$$S_E = \int d\tau \left[\underbrace{\frac{1}{2}(\partial_\tau \varphi_E)^2 + \frac{1}{2} m^2 \varphi_E^2}_{S_E^0} + \underbrace{\frac{\lambda}{4!}\varphi_E^4}_{S_E^{\text{int}}} \right]$$

$$\partial_{t_5} \varphi_E(\bar{\tau}_k) = -\frac{\delta S_E}{\delta \varphi_E(\bar{\tau}_k)} + \eta(\bar{\tau}_k)$$

$$\partial_{t_5} \varphi^+(\omega_l) = -\frac{\delta S_E^0}{\delta \varphi^+(\omega_l)} - \frac{\delta S_E^{\text{int}}}{\delta \varphi^+(\tau_j)} \frac{\delta \varphi^+(\tau_j)}{\varphi^+(\omega_l)} + \eta(\omega_l)$$

- Use Stochastic Quantization and sample φ_E and φ^+ concurrently from Langevin equations
- Imaginary frequency update in Fourier space
  → kinetic term diagonal and improved convergence

- Temperature in φ_E via compact temporal path
- Temperature in φ^+ via initial condition $\varphi^+(t_0)$



Numerical results for scalar field theories

Two-point correlation function

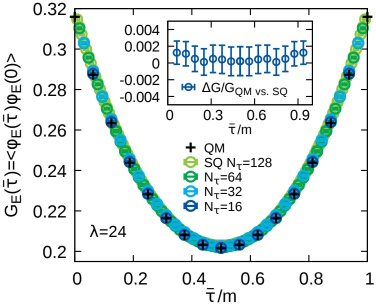


Figure: QM (an-)harmonic oscillator vs. stoch. quantization result on the compact Euclidean time lattice

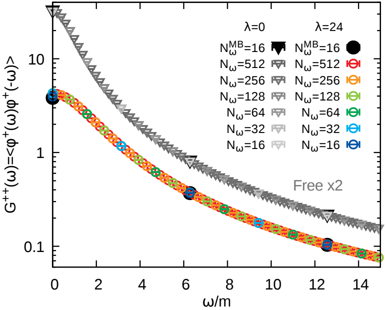
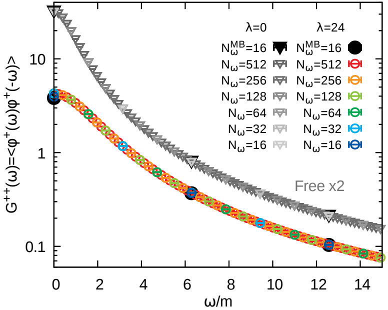


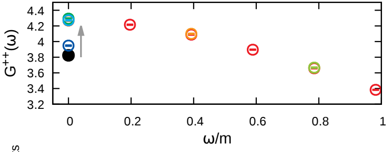
Figure: Free and interacting theory from general frequency simulations

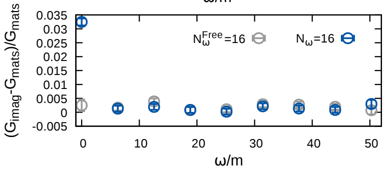
Pawlowski, Rothkopf, arXiv:1610.09531 [hep-lat]

0+1 dimensional real scalar field

Two-point correlation function



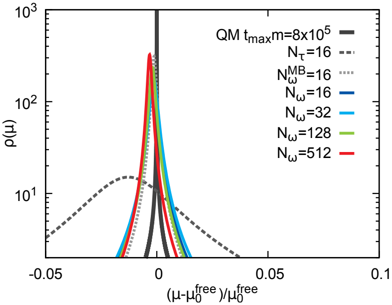


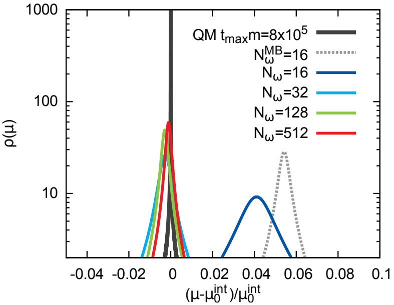


Convergence properties of the correlator

0+1 dimensional real scalar field

Spectral functions

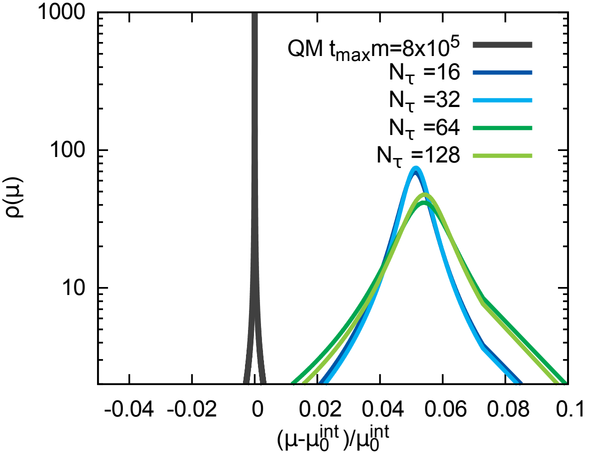




- General imaginary frequencies capture physical properties correctly.
- Information from standard compact Euclidean simulation insufficient.

0+1 dimensional real scalar field

Spectral reconstruction from a **standard** compact Euclidean time correlator $G_E(\bar{\tau})$ does not improve by simply increasing the number of temporal lattice points.



3+1 dimensional complex scalar field

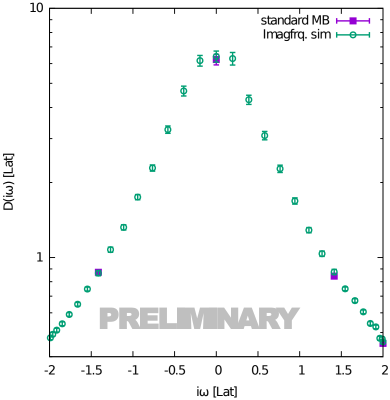


Figure: Field correlator

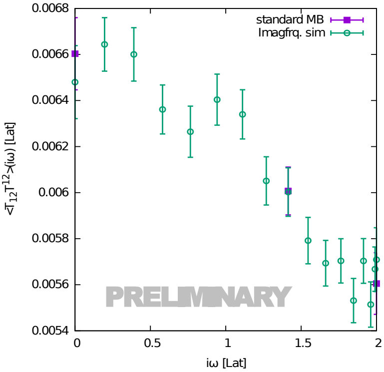


Figure: EMT correlator

Pawlowski, Rothkopf, arXiv:1710.02672 [hep-lat]

Gauge fields

Simulating gauge fields

- Wilson plaquette action

$$S_E[U] = \frac{2}{g^2} \sum_x \sum_{\mu<\nu} \mathrm{Re}[\mathbb{1} - U_{\mu\nu}(x)]$$

$$= \frac{a^4}{2\,g^2} \sum_x \sum_{\mu,\nu} \mathrm{tr}[F_{\mu\nu}(x)^2] + O(a^2)$$

- Update algorithm

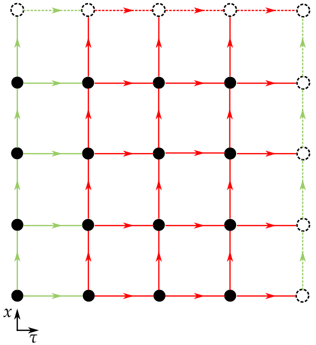
1) Standard heatbath sweep
2) Therm. init. cond. at $\bar{\tau} = \tau = 0$
3) Standard heatbath sweep at $\tau > 0$

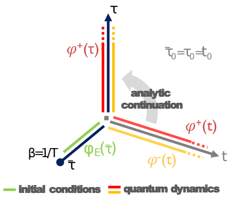
$$U^{(\mathrm{new})}_{x,\mu} = X V^\dagger, \;\; \mathrm{d}P(X) = \mathrm{d}X \exp\left(\frac{1}{2} a\beta \mathrm{Tr}(X)\right),$$

$$X, V = A/a \in SU(2), a = \det(A),$$

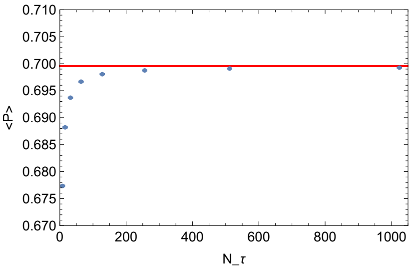
$$A = \sum_{\nu\neq\mu} U_{x+\hat{\mu},\nu} U^\dagger_{x+\hat{\nu},\mu} U^\dagger_{x+\hat{\nu},\nu}$$

$$+ U^\dagger_{x+\hat{\mu}-\hat{\nu},\nu} U^\dagger_{x-\hat{\nu},\mu} U_{x-\hat{\nu},\nu}$$

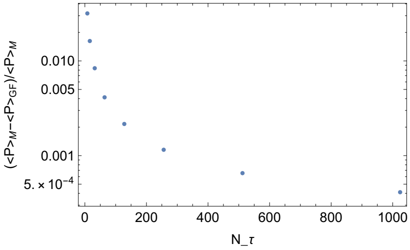




Convergence towards the Matsubara results



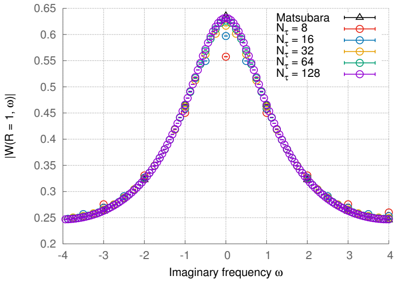
Plaquette expectation value

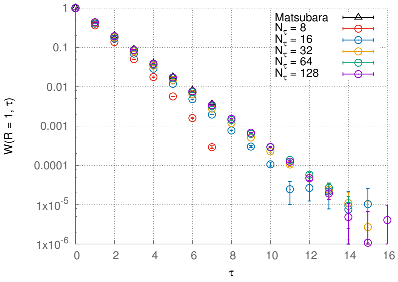


Relative deviation

- Lattice sizes: $8^3 \times 8$ (Matsubara)
  $8^3 \times N_\tau$ (General frequencies)
- $\beta = 2.8$

Wilson loop (confined phase)





- Lattice sizes: $4^3 \times 8$ (Matsubara)
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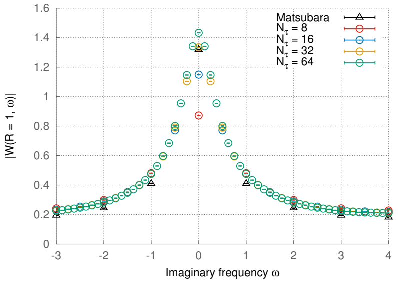
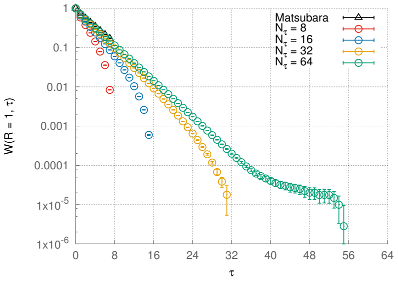
- $\beta = 1.8$
- $N_{\text{cf}} = 8 \times 10^5$ configurations

Wilson loop (deconfined phase)





- Lattice sizes: $4^3 \times 8$ (Matsubara)
  $4^3 \times N_\tau$ (General frequencies)
- $\beta = 3.0$
- $N_{\rm cf} = 1.6 \times 10^6$ configurations

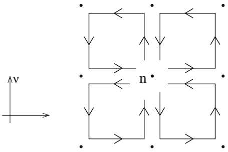
Energy momentum tensor on the lattice

- Continuum formula
  $T_{\mu\nu}(x) = F_{\mu\sigma}(x)F_{\nu\sigma}(x) - \frac{1}{4}\delta_{\mu,\nu}F_{\rho\sigma}(x)F_{\rho\sigma}(x)$
- Discretization of the field strength tensor on the lattice (clover)

$$F_{\mu\nu}(x) = \frac{-i}{8a^2 g}(Q_{\mu\nu}(x) - Q_{\nu\mu}(x))$$

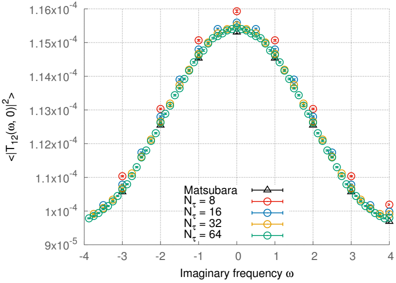
$$Q_{\mu\nu}(x) = U_{\mu,\nu}(x) + U_{\nu,-\mu}(x) + U_{-\mu,-\nu}(x) + U_{-\nu,\mu}(x)$$

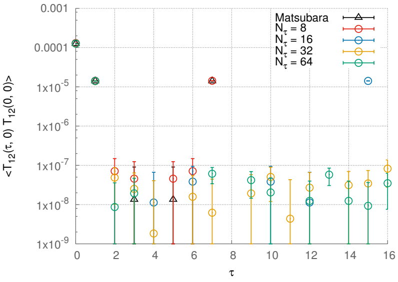
- For the shear viscosity η measure correlation function of time slices $\langle T_{12}(0,0)T_{12}(\tau,0)\rangle$.



see e.g. Gattringer, Lang, Quantum Chromodynamics on the Lattice, Springer 2010

EMT correlator (confined phase)





- Lattice sizes: $4^3 \times 8$ (Matsubara)
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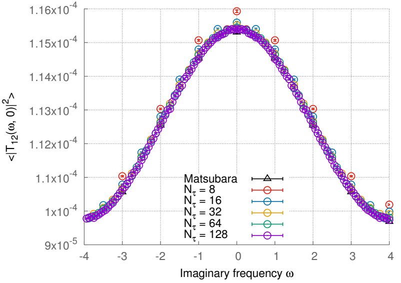

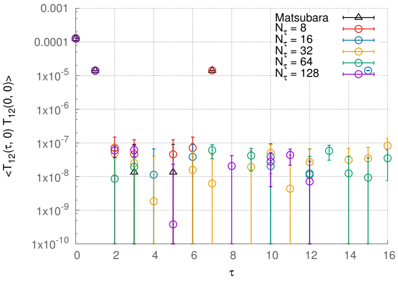

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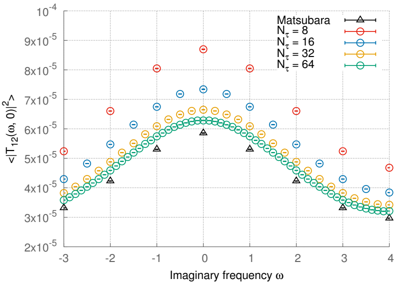
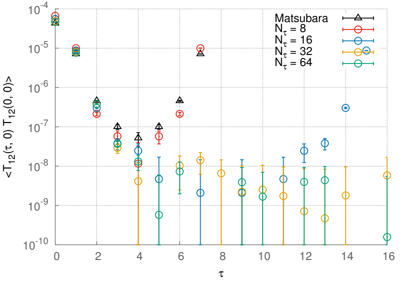
EMT correlator (deconfined phase)





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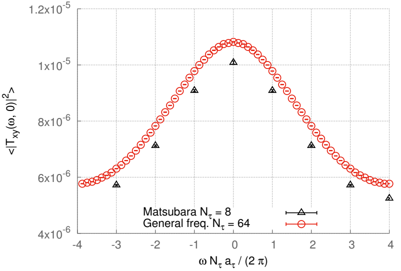
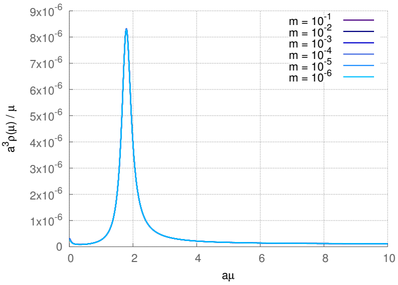
EMT correlator (deconfined phase) and spectral function



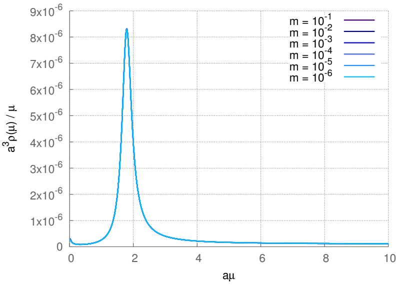


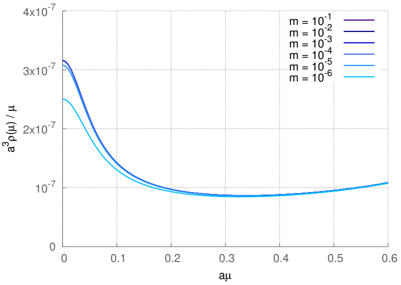
PRELIMINARY

- Lattice sizes: $8^3 \times 8$ (Matsubara)
  $8^3 \times 64$ (General frequencies)
- $\beta = 2.8$
- $N_{cf} \approx 10^6$ configurations

Pawlowski, Rothkopf, Ziegler, work in progress

EMT correlator spectral function





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Pawlowski, Rothkopf, Ziegler, work in progress

Summary

- Thermal fields as initial-value problem formulated in an additional non-compact Euclidean time promising
- Numerical implementation provides significantly improved access to real-time spectral quantities
- Formalism easy to implement for gauge fields

Outlook

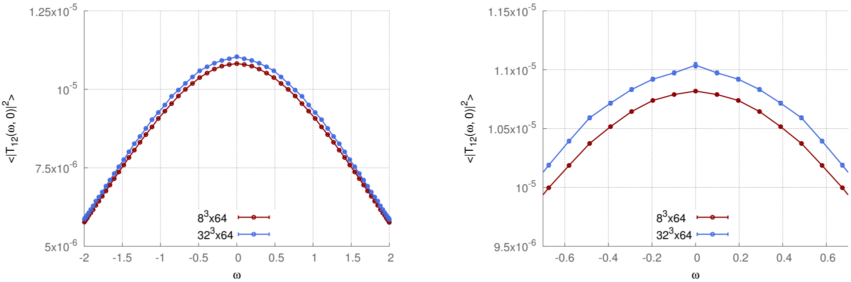
- **Near future:** extract spectral functions and transport coefficients from the energy-momentum tensor correlator
- Extension to $SU(3)$ gauge theory and full QCD (work in progress)
- Formal developments
- Resolving correlators at small momenta

Outlook

- **Near future:** extract spectral functions and transport properties from the energy-momentum tensor correlator
- Extension to $SU(3)$ gauge theory and full QCD (work in progress)
- Formal developments
- Resolving correlators at small momenta

Thank you very much for your attention!

EMT correlator - latest results



PRELIMINARY **PRELIMINARY**

- Matsubara lattice sizes: $8^3 \times 8$ and $32^3 \times 8$
- $\beta = 2.8$
- $N_{\text{cf}} \approx 10^6$ configurations

Pawlowski, Rothkopf, Ziegler, work in progress

Fixed boundary conditions