NOVEL LATTICE SIMULATIONS FOR TRANSPORT COEFFICIENTS IN GAUGE THEORIES

Felix Ziegler
in collaboration with Jan M. Pawlowski and Alexander Rothkopf
Heidelberg University

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

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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
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

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

⇒ need spectral function \( \rho(\omega, \vec{p}) \)
Lattice QCD at finite temperature

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

\[
\langle O(U) \rangle = \frac{1}{Z} \int \mathcal{D}U \; O(U) \exp(-S_{QCD}^{E}[U])
\]

\[
P(U_k) = e^{-S_{QCD}^{E}[U_k]} \Rightarrow \langle O(U) \rangle \approx \frac{1}{N_{cf}} \sum_{k=1}^{N_{cf}} O(U_k)
\]
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
  \[ D(\tau) \propto \int d^3x \langle T_{12}(\tau, \vec{x})T_{12}(0, 0) \rangle = \int d\mu \frac{\cosh[\mu(\tau - \beta/2)]}{\sinh[\mu \beta/2]} \rho(\mu) \]

For the reconstruction technique used in the following see
Reconstruction of spectral functions and its challenges

Two main conceptual problems of standard spectral reconstructions

○ Problem 1:

\[ D(\tau) = \int_{0}^{\infty} d\mu \frac{\cosh[\mu(\tau - \beta/2)]}{\sinh[\mu \beta/2]} \rho(\mu) \]

Extraction from imaginary time correlator ill-posed exponentially hard inversion problem.

→ Go to imaginary frequencies and use Källén-Lehman spectral representation

\[ D(\omega_n) = \int_{0}^{\infty} d\mu \frac{2 \mu}{\omega_n^2 + \mu^2} \rho(\mu) \]
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
  \[ Z = \text{Tr}(\rho(0) = e^{-\beta H}) \]

\[ Z = \int d[\varphi^+] d[\varphi^-] \langle \varphi^+ | \rho(0) | \varphi^- \rangle \langle \varphi^- | \varphi^+ \rangle \]

\( \rho(0) = e^{-\beta H} \)

- Initial conditions
Thermal scalar field theory as a real-time initial value problem with

\[ Z = \text{Tr} \left( \rho(0) = e^{-\beta H} \right) \]

\[ Z = \int d[\varphi^+_0]d[\varphi^-_0]\langle \varphi^+_0 | \rho(0) | \varphi^-_0 \rangle \langle \varphi^-_0 | \varphi^+_0 \rangle \int [d\varphi_t] \langle \varphi^-_0 | e^{iHt} | \varphi_t \rangle \langle \varphi_t | e^{-iHt} | \varphi^+_0 \rangle \]
Thermal scalar field theory as a real-time initial value problem with

\[ Z = \text{Tr} \left( \rho(0) = e^{-\beta H} \right) \]

\[
Z = \int d[\phi^+_o]d[\phi^-_o] \langle \phi^+_o | e^{-\beta H} | \phi^-_o \rangle \langle \phi^-_o | \phi^+_o \rangle \int_{\phi^+_o} \mathcal{D}\phi e^{iS_M[\phi^+] - iS_M[\phi^-]} \]

Initial conditions
Quantum dynamics
Thermal field theory on the Schwinger-Keldysh contour

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

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

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

\[
G^{++}(p^0, \vec{p}) = \int \frac{dq^0}{2\pi} \frac{\rho(q^0, \vec{p})}{q^0 - p^0 + i\epsilon} - n(p^0)\rho(p^0, \vec{p})
\]

- Using time translation invariance we can set \( t_0 \to -\infty \).

- Introducing \( \epsilon > 0 \) and \( e^{-iHt} \to e^{-iHt(1+i\epsilon)} \) correlations between any finite \( t \) on forward branch and endpoint become exponentially damped.
From no on, we focus on the **forward** $\varphi^+$ path.

**Idea:** Cut open real-time path at $t = \infty$ and rotate path to (additional) non-compact imaginary time axis.

\[
Z = \int_{\varphi_E(0) = \varphi_E(\beta)} \mathcal{D} \varphi_E e^{-S_E[\varphi_E]} \int_{\varphi^+(t_0, \vec{x}) = \varphi_E(0)} \mathcal{D} \varphi e^{i S_M[\varphi^+] - i S_M[\varphi^-] \int_{\varphi^-(t_0, \vec{x}) = \varphi_E(\beta)}}
\]
Analytic continuation and general imaginary frequencies

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

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

**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 $\tau \in [0, \infty)$. 

Diagram showing quantum dynamics with initial conditions and paths.
Simulating scalar fields

\[ SE = \int d\tau \left[ \frac{1}{2}(\partial_\tau \varphi_E)^2 + \frac{1}{2}m^2\varphi_E^2 + \frac{\lambda}{4!}\varphi_E^4 \right] \]

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

- Use Stochastic Quantization and sample \( \varphi_E \) and \( \varphi^+ \) concurrently from Langevin equations
- Imaginary frequency update in Fourier space
  \( \rightarrow \) kinetic term diagonal and improved convergence

- Temperature in \( \varphi_E \) via compact temporal path
- Temperature in \( \varphi^+ \) via initial condition \( \varphi^+(t_0) \)
Numerical results for scalar field theories
**0+1 dimensional real scalar field**

Two-point correlation function

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**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
○ 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.

![Graph showing spectral reconstruction results with different $N_\tau$ values](image)
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

\[
S_E[U] = \frac{2}{g^2} \sum_x \sum_{\mu < \nu} \text{Re}[1 - U_{\mu \nu}(x)] \\
= \frac{a^4}{2g^2} \sum_x \sum_{\mu, \nu} \text{tr}[F_{\mu \nu}(x)^2] + O(a^2)
\]

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

\[
U_{x, \mu}^{(\text{new})} = XV^+, \quad dP(X) = dX \exp \left( \frac{1}{2} \alpha \beta \text{Tr}(X) \right),
\]

\[
X, V = A/a \in SU(2), \quad a = \det(A),
\]

\[
A = \sum_{\nu \neq \mu} U_{x + \hat{\mu}, \nu} U_{x + \hat{\nu}, \mu} U_{x + \hat{\nu}, \nu}^+ + U_{x + \hat{\mu} - \hat{\nu}, \nu} U_{x - \hat{\nu}, \mu} U_{x - \hat{\nu}, \nu}^+
\]
Convergence towards the Matsubara results

Plaquette expectation value

- 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)
  $4^3 \times N_\tau$ (General frequencies)
- $\beta = 1.8$
- $N_{cf} = 8 \times 10^5$ configurations
Wilson loop (deconfined phase)

- Lattice sizes: $4^3 \times 8$ (Matsubara)
  $4^3 \times N_\tau$ (General frequencies)
- $\beta = 3.0$
- $N_{cf} = 1.6 \times 10^6$ 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)
  \[ F_{\mu\nu}(x) = \frac{-i}{8a^2g}(Q_{\mu\nu}(x) - Q_{\nu\mu}(x)) \]

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

- For the shear viscosity \(\eta\) 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
Lattice sizes: $4^3 \times 8$ (Matsubara)

$4^3 \times N_\tau$ (General frequencies)

$\beta = 1.8$

$N_{cf} = 8 \times 10^5$ configurations
- Lattice sizes: $4^3 \times 8$ (Matsubara)
  $4^3 \times N_{\tau}$ (General frequencies)
- $\beta = 1.8$
- $N_{\text{cf}} = 8 \times 10^5$ configurations
EMT correlator (deconfined phase)

- Lattice sizes: $4^3 \times 8$ (Matsubara) 
  $4^3 \times N_{\tau}$ (General frequencies)
- $\beta = 3.0$
- $N_{cf} = 1.6 \times 10^6$ configurations
EMT correlator (deconfined phase) and spectral function

\[ \langle T_{xy}(\omega, 0) \rangle^2 \]

\[ \omega N_\tau a_\tau / (2\pi) \]

Matsubara \( N_\tau = 8 \)
General freq. \( N_\tau = 64 \)

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
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
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
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
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!
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

- $FBC, N_τ = 8$
- $FBC, N_τ = 16$
- $FBC, N_τ = 32$
- $FBC, N_τ = 64$
- $FBC, N_τ = 128$