Complex Langevin simulations for QFTs

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ACHT workshop, 28.09.2023.

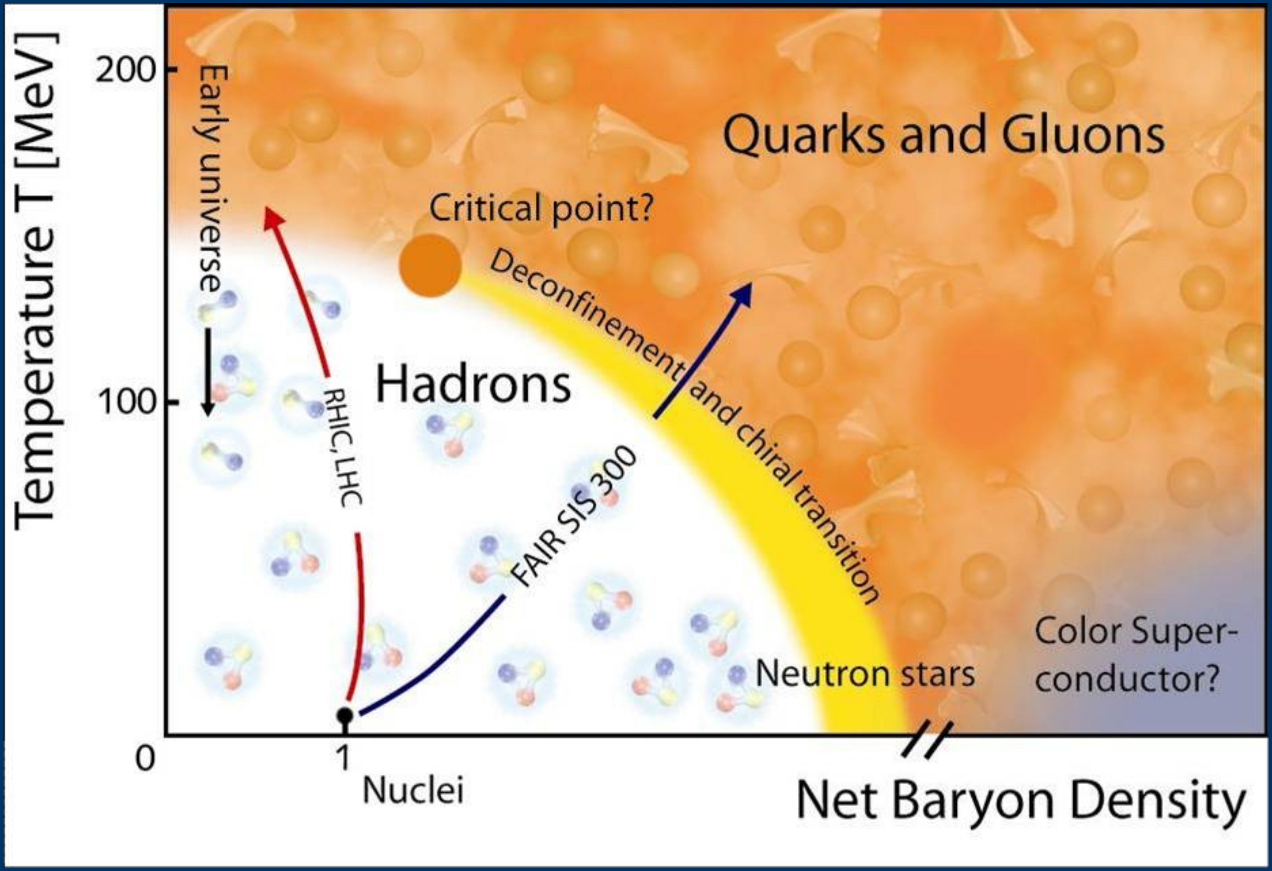
1. Introduction to Complex Langevin
2. Boundary terms; test in full QCD
3. Kernels in the CLE – How to get rid of boundary terms – realtime scalars
4. Results for full QCD: EoS and phase diagram, dynamic stabilization

Phase diagram of QCD

Zero density axis well known

transition temperature

zero temperature:
hadron masses
scattering amplitudes, etc.

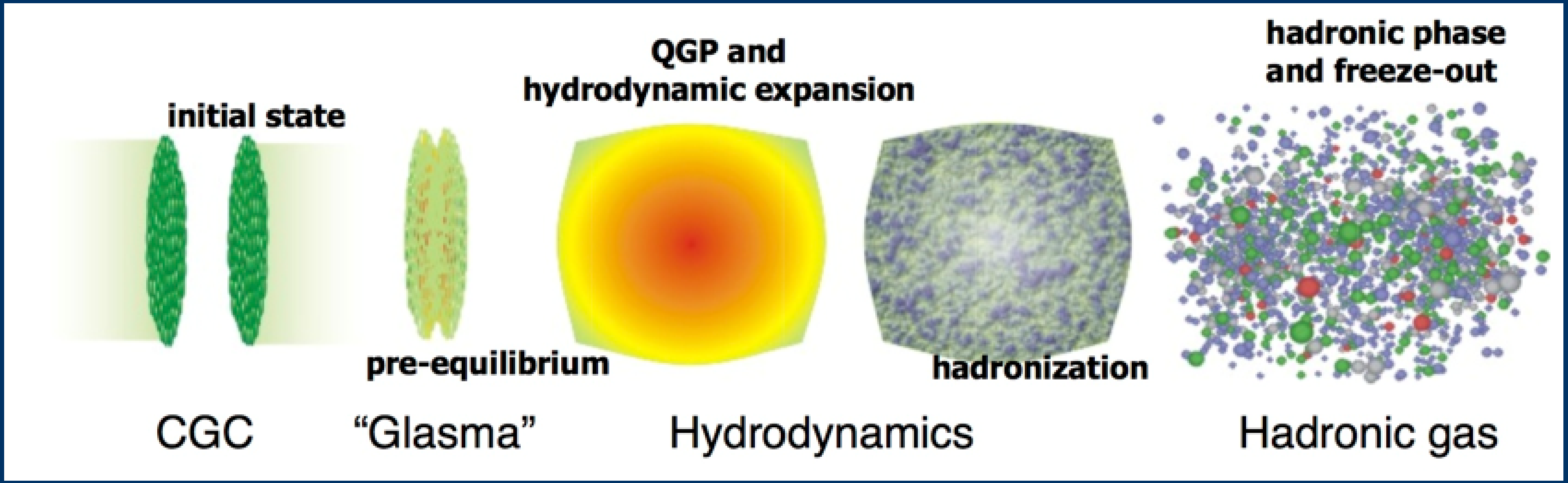


At nonzero density much less solid knowledge

What phases are present?
Is there a critical point?
compressibility of nuclear matter?

Why is non-zero density so hard?

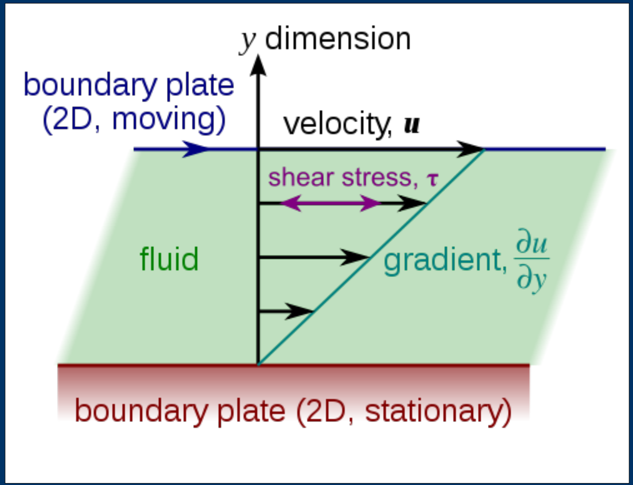
Heavy-Ion collisions



How does the Glasma equilibrate?
Non-equilibrium Quantum Field theory

$$|\Psi(t=0)\rangle \rightarrow |\Psi(t)\rangle$$

For hydrodynamics one needs equilibrium values of:
Equation of State ← “easy” to calculate
Transport coefficients: e.g. viscosity ← Hard problem, Real-time correlator



Hard problem
Real-time correlator

$$\eta = \frac{1}{TV}\int_0^\infty dt\,\langle \sigma_{xy}(0)\sigma_{xy}(t)\rangle$$

Why is real-time QFT so hard?

Importance Sampling

We are interested in a system
Described with the partition sum:

$$Z=\int D\phi\, e^{-S}=\mathrm{Tr}\, e^{-\beta(H-\mu N)}=\sum_C W[C]$$

Typically exponentially many configurations,
no direct summation possible.

If the Weight is positive, build a Markov chain with the Metropolis algorithm

$$\ldots \rightarrow C_{i-1} \rightarrow C_i \rightarrow C_{i+1} \rightarrow \ldots$$

Probability of visiting C $\quad p(C)\sim W[C]$

$$\langle X \rangle=\frac{1}{Z}\mathrm{Tr}\, X e^{-\beta(H-\mu N)}=\frac{1}{Z}\sum_C W[C]X[C]=\frac{1}{N}\sum_i X[C_i]$$

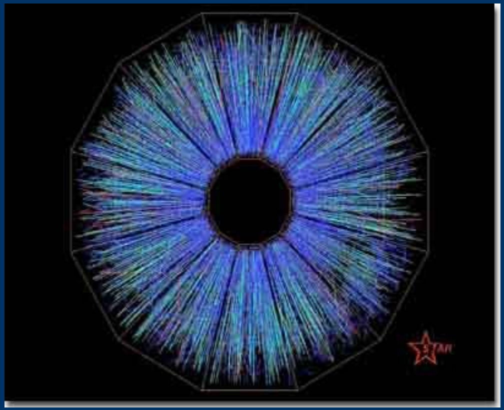
This works if we have $\quad W[C]\geq 0$

Otherwise we have a Sign problem

Sign problems

Real-time evolution in QFT

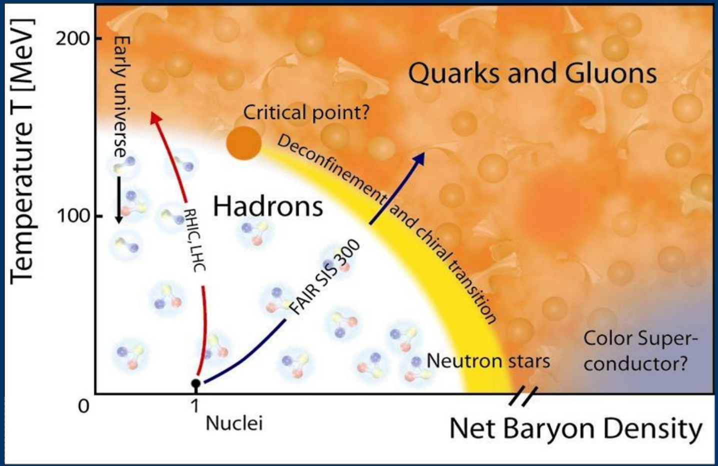
"strongest" sign problem e^{iS}



Non-zero density

$$Z = \mathrm{Tr}\, e^{-\beta(H-\mu N)} = \int DU\, e^{-S[U]} \det(M[U])$$

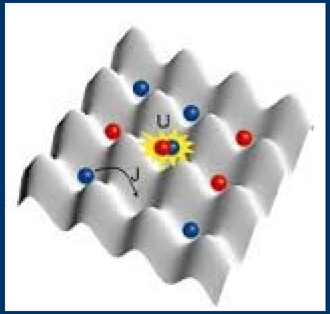
Many systems: Bose gas
XY model
SU(3) spin model
Random matrix theory
QCD



Theta therm

$$S = F_{\mu\nu}F^{\mu\nu} + i\Theta\,\epsilon^{\mu\nu\theta\rho}F_{\mu\nu}F_{\theta\rho}$$

Inbalanced Fermi gas



And everything else with complex action

$w[C] = e^{-S[C]}$ $\quad$ $w[C]$ is positive $\leftrightarrow$ $S[C]$ is real

QCD sign problem

Euclidean SU(3) gauge theory with fermions:

$$Z=\int DU \exp(-S_E[U]) det(M[U])$$

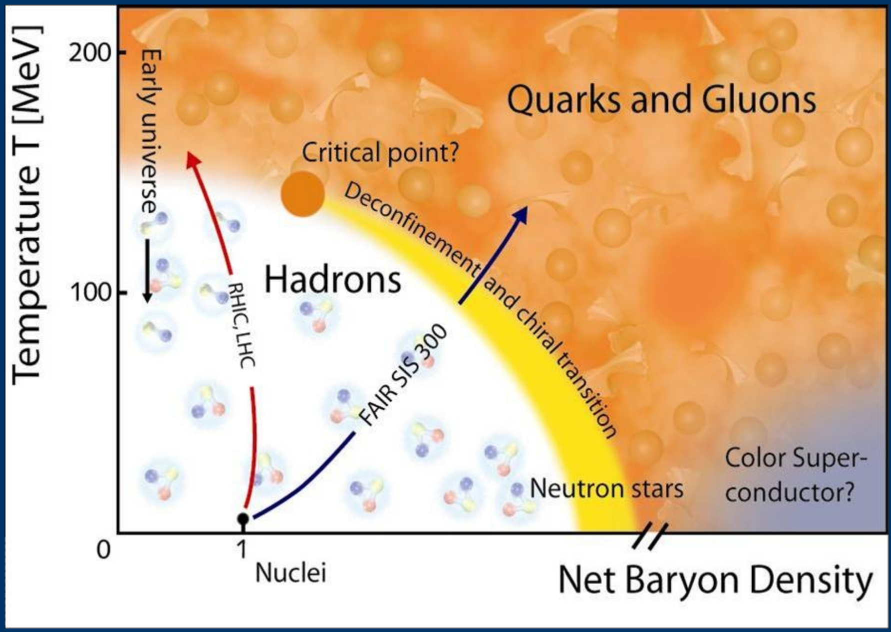
for $\det(M[U])>0$ Importance sampling is possible

Non-zero chemical potential

For nonzero chemical potential, the fermion determinant is complex

$$\det(M(U,-\mu^*))=(\det(M(U),\mu))^*$$

Sign problem $\longrightarrow$ Naive Monte-Carlo breaks down



How to solve the sign problem (of QCD)?

Extrapolation from a positive ensemble

Reweighting $\langle X\rangle_W = \frac{\sum_c W_c X_c}{\sum_c W_c} = \frac{\sum_c W'_c (W_c/W'_c) X_c}{\sum_c W'_c (W_c/W'_c)} = \frac{\langle (W/W') X\rangle_{W'}}{\langle W/W'\rangle_{W'}}$

Taylor expansion $Z(\mu) = Z(\mu=0) + \frac{1}{2}\mu^2 \partial_\mu^2 Z(\mu=0) + \ldots$

Analytic continuation from imaginary sources
(chemical potentials, theta angle,..)

Using analyticity

Complex Langevin
Complexified variables – enlarged manifolds

Other ideas (not yet for QCD)

Lefschetz thimbles , sign improved manifolds,
Dual variables, worldlines,
Density of States, Subsets, Quantum computing, ...

In QCD direct simulation only possible at $\mu = 0$

Taylor extrapolation, Reweighting, continuation from imaginary μ, canonical ens.
all break down around

$$\frac{\mu_q}{T} \approx 1 \qquad \frac{\mu_B}{T} \approx 3$$

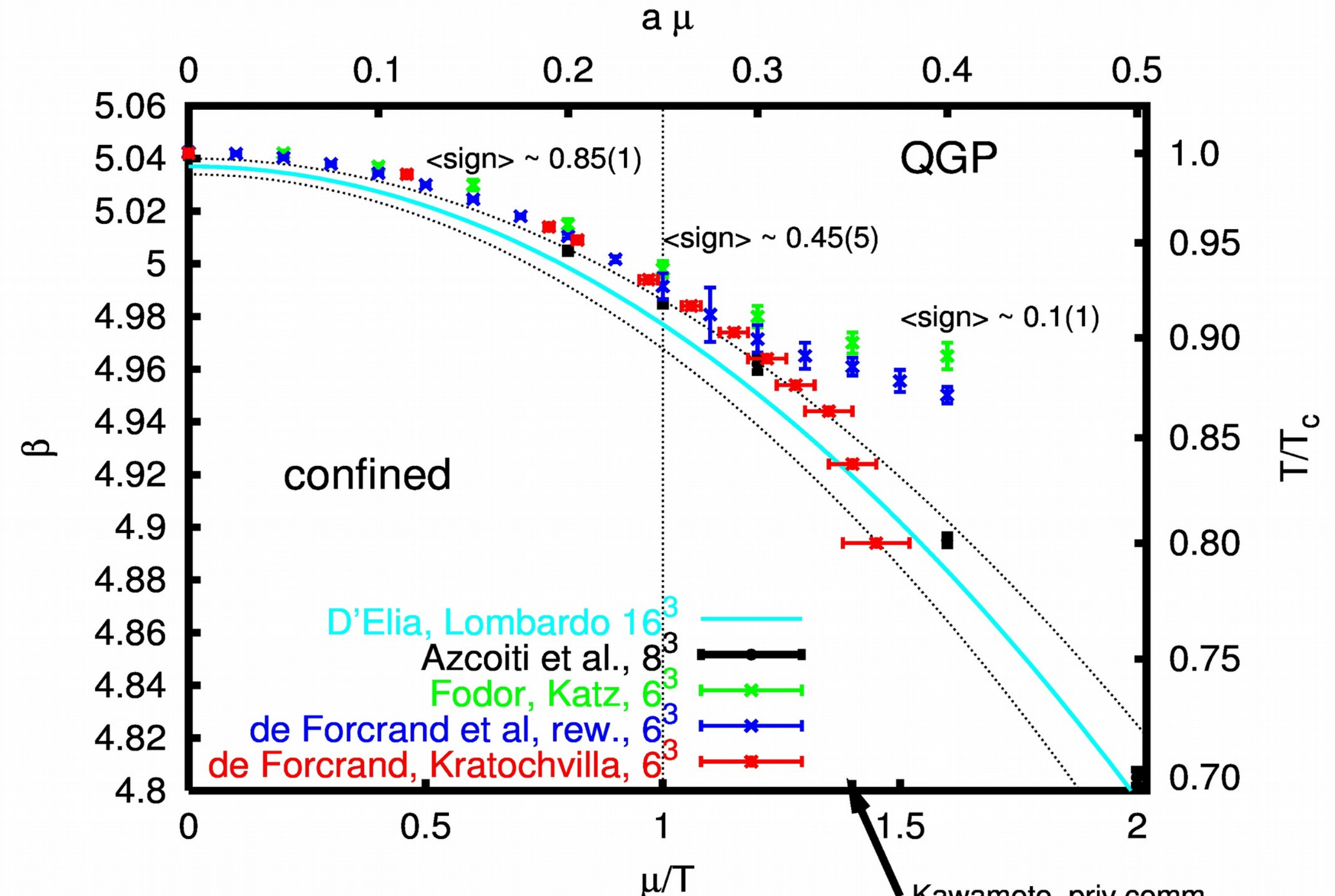
Around the transition temperature
Breakdown at $\mu_q \approx 150 - 200\,\mathrm{MeV}$ $\qquad \mu_B \approx 450 - 600\,\mathrm{MeV}$

Results on

$$N_T = 4, N_F = 4, ma = 0.05$$

using
Imaginary mu,
Reweighting,
Canonical ensemble

Agreement only at $\mu/T < 1$



Langevin Equation (aka. stochastic quantisation)

Given an action $S(x)$

Stochastic process for x: $$\frac{dx}{d\tau} = -\frac{\partial S}{\partial x} + \eta(\tau)$$

Gaussian noise

$$\langle \eta(\tau) \rangle = 0$$
$$\langle \eta(\tau) \eta(\tau') \rangle = \delta(\tau - \tau')$$

Random walk in configuration space

Averages are calculated along the trajectories:

$$\langle O \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T O(x(\tau))\, d\tau = \frac{\int e^{-S(x)} O(x)\, dx}{\int e^{-S(x)}\, dx}$$

Numerically,
results are extrapolated to $\Delta\tau \to 0$

Complex Langevin Equation

Given an action $S(x)$

Stochastic process for x: $\frac{dx}{d\tau} = -\frac{\partial S}{\partial x} + \eta(\tau)$

Gaussian noise
$\langle \eta(\tau) \rangle = 0$
$\langle \eta(\tau)\eta(\tau') \rangle = \delta(\tau - \tau')$

$$\frac{dx}{d\tau} = -\frac{\partial S}{\partial x} + \eta(\tau)$$

The field is complexified

real scalar → complex scalar

link variables: SU(N) → SL(N,C)
compact non-compact

$\det(U) = 1, \quad U^{+} \neq U^{-1}$

Analytically continued observables are calculated along the trajectories:

$$\langle O \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T O(x(\tau) + iy(\tau)) d\tau$$

$$\langle x^2 \rangle_{real} \rightarrow \langle x^2 - y^2 \rangle_{complexified}$$

$$\frac{1}{Z} \int P_{comp}(x) O(x) dx = \frac{1}{Z} \int P_{real}(x, y) O(x + iy) dx\, dy \quad ?$$

Gaussian Example

$$S[x]=\sigma x^2+i\lambda x$$

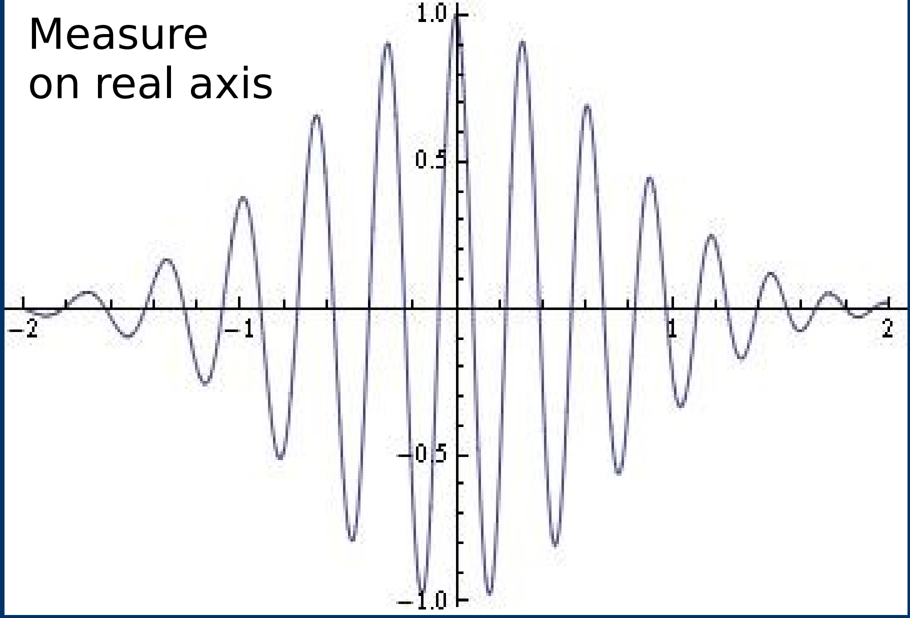
CLE

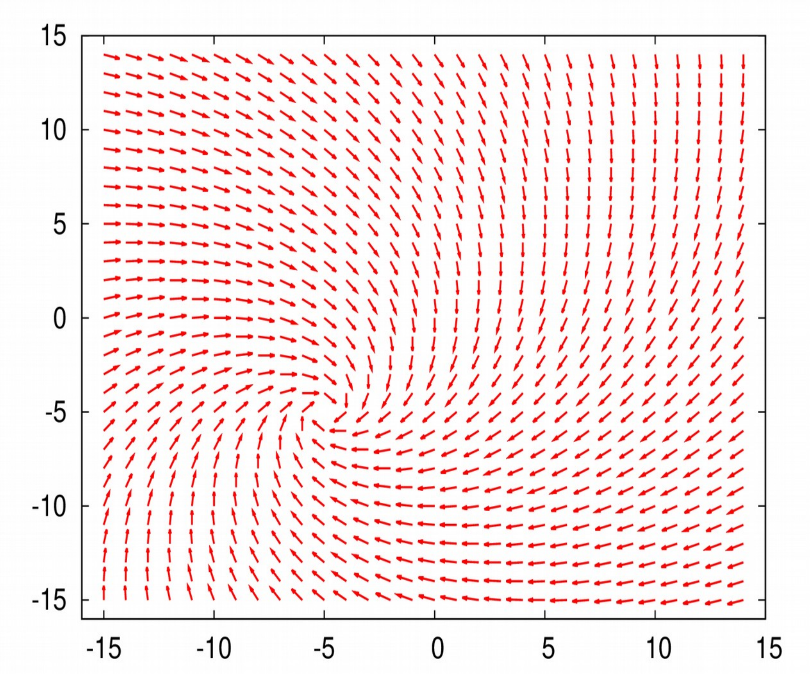
$$\frac{d}{d\tau}(x+iy)=-2\sigma(x+iy)-i\lambda+\eta$$

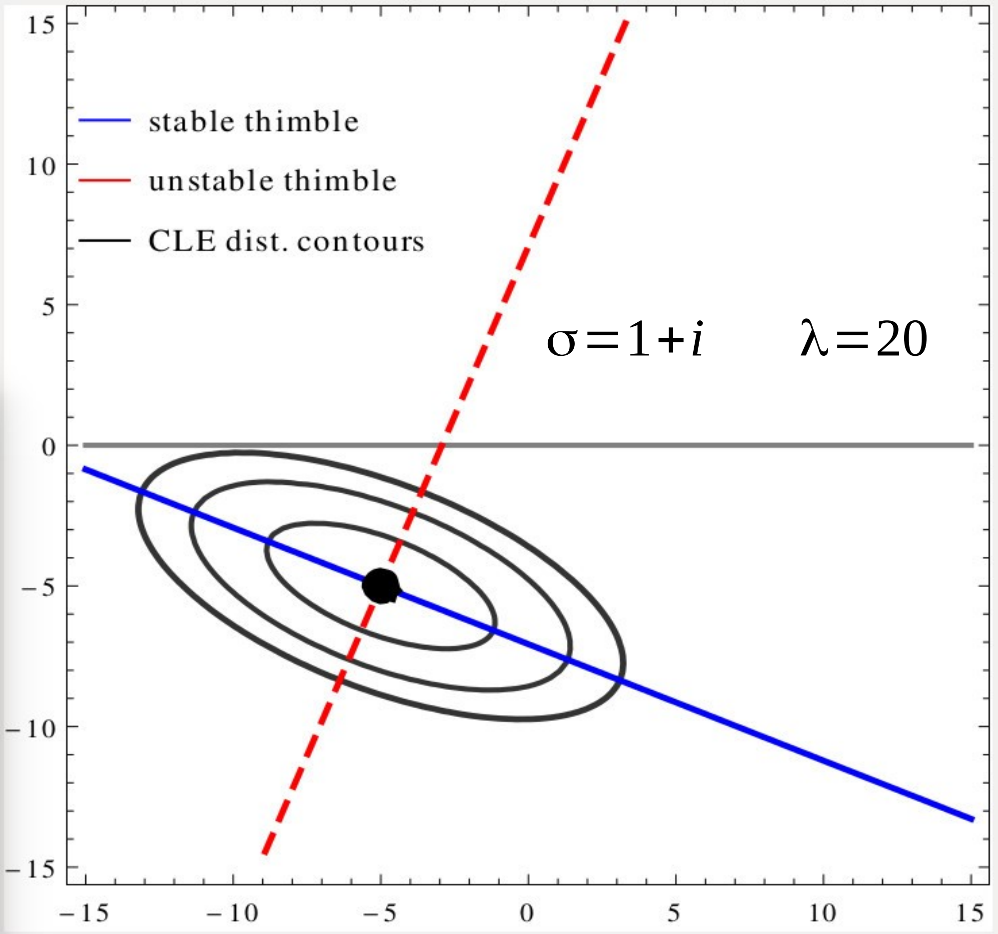
$$P(x,y)=e^{-a(x-x_0)^2-b(y-y_0)^2-c(x-x_0)(y-y_0)}$$

Gaussian distribution
around critical point

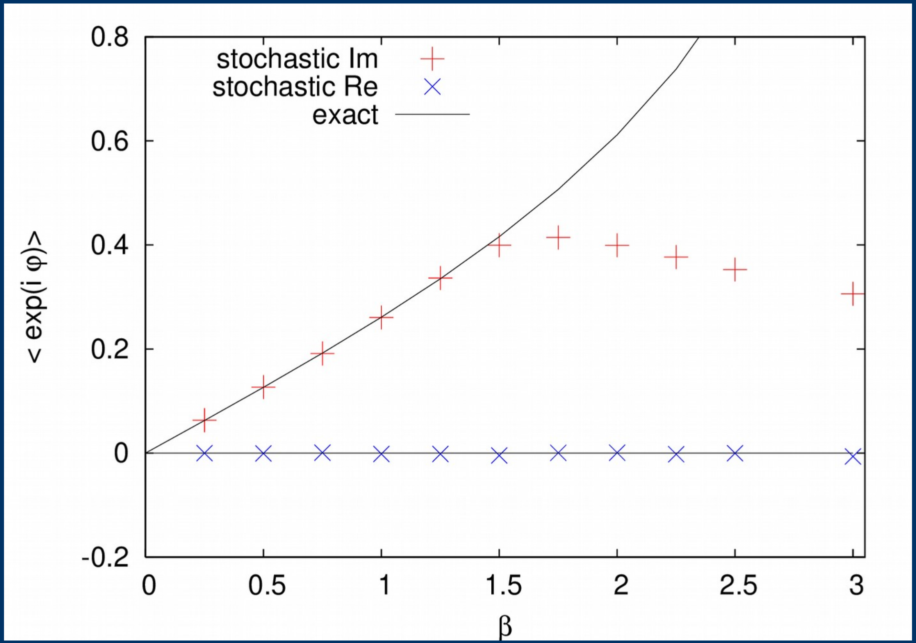
$$\left.\frac{\partial S(z)}{\partial z}\right|_{z_0}=0$$







“troubled past”: Convergence to wrong results
Lack of theoretical understanding
Runaway trajectories



$$S(\varphi) = i\beta\cos\varphi + i\varphi$$

Correct in one parameter region
Incorrect in an other

Convergent in both

Klauder '83, Parisi '83, Hueffel, Rumpf '83, Karsch. Wyld '84, Gausterer, Klauder '86.
Matsui, Nakamura '86, ...
Interest went down as difficulties appeared
Renewed interest in connection of otherwise unsolvable problems
applied to nonequilibrium: Berges, Stamatescu '05, ...
aimed at nonzero density QCD: Aarts, Stamatescu '08 ... many important results since revival

Potential problems of CLE

Requirements for correct results:

fast enough decay $P(x,y) \to 0 \text{ as } x,y \to \infty$

holomorphic action $S(x)$

Ergodicity

Complex Fokker Planck operator with good spectrum $L_c = \sum_i (\partial_i - \partial_i S)\partial_i$

unique null-mode, negative real parts

then CLE converges to the correct result

[Aarts, Seiler, Stamatescu (2009)
Aarts, James, Seiler, Stamatescu (2011)
Aarts. Seiler, Sexty, Stamatescu (2017)
Salcedo, Seiler (2018)
Seiler (2020)
Seiler,Sexty, Stamatescu (2023)]

Problem: decay not fast enough

Using an interpolation function $F(t,\tau)$

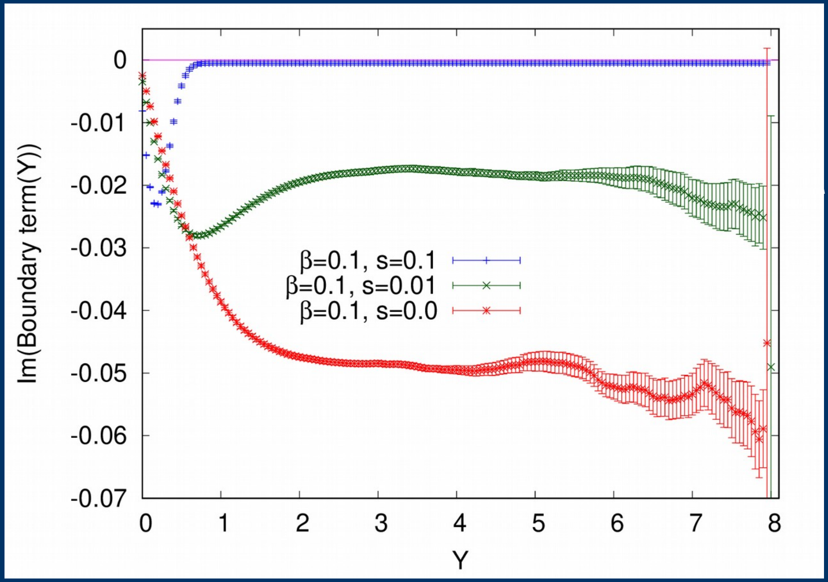
CLE works, if

What we want		What we get with CLE
$\int dx\,\rho(x)O(x)$	$=$	$\int dx\,dy\,P(x,y)O(x+iy)$
$F(t,t)$	$=$	$F(t,0)$

shown with partial integrations

boundary terms can be nonzero
explicit calculation of boundary terms possible

[Scherzer, Seiler, Sexty, Stamatescu (2018)+(2019)]



Unambigous detection of boundary terms
given by plateau as 'cutoff' $Y \to \infty$

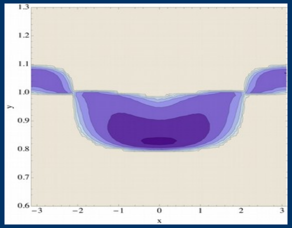
Observable cheap also for lattice systems

Measuring “corrected observable”
in case boundary term nonzero

Problem: Non-holomorphic action for nonzero density

$$S = S_W[U_\mu] + \ln \mathrm{Det}\, M(\mu)$$

measure has zeros $(Det\ M = 0)$
complex logarithm has a branch cut
$\longrightarrow$ meromorphic drift



Already pathologic for real Langevin:

$M = x^2 e^{-x^2}$ zero measure at $x = 0 \rightarrow$ process stays left or right
2 independent stationary states $\rightarrow$ non-ergodic

No problems if poles are not 'touched' by distribution

satisfied for: HDQCD, full QCD at high temperatures

[Aarts, Seiler, Sexty, Stamatescu '17]

Problem: Spectrum on the wrong side

[Seiler, Sexty, Stamatescu (2023)]

Fokker Planck operator

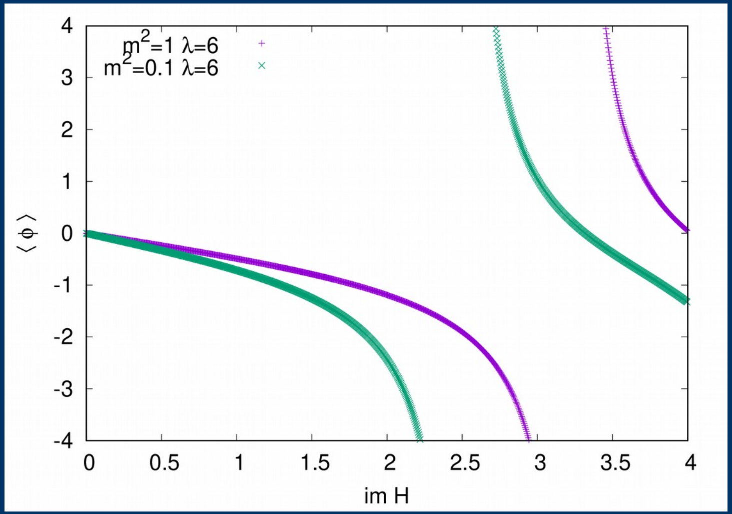
$$L_c = \sum_i \partial_i^2 + K_i \partial_i$$

Determines $\rho(x,t) = e^{t L_c^T} \rho(x,0)$

Toy model:

$$S = \frac{1}{2} m^2 \phi^2 + \frac{\lambda}{24} \phi^4 + H\phi \quad \rightarrow \quad L_c = \partial_z^2 + \left(-m^2 z - \frac{\lambda}{6} z^3 - H \right) \partial_z$$

At imaginary magnetic field
Lee-Yang zeroes appear



At each Lee-Yang zero
an eigenvalue appears with $\mathrm{Re}(\lambda) > 0$

Slow decay is also present: → Boundary terms signal also this problem

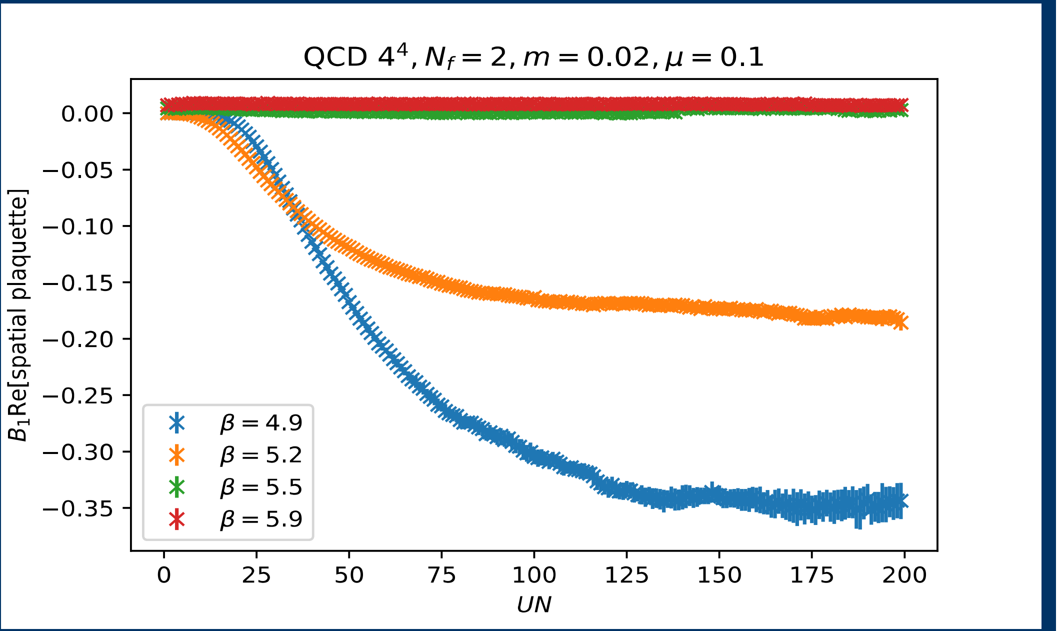
Open question: what happens with spectrum if kernels are used?

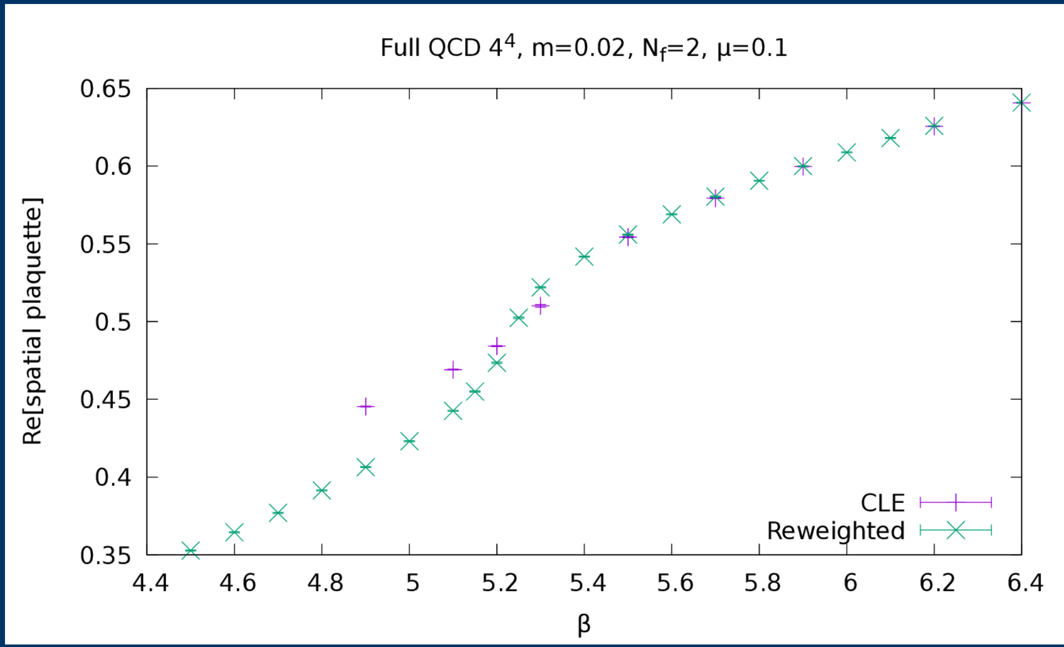
Boundary terms

In full QCD this confirms already known signals
Quantifies error

Faster than exponential decay of histograms of observables
Drift criterion = same for drift term observable

Boundary terms appear at small β = large lattice spacing





[Hansen, Sexty in. prep]

Real-time two point function of quantum oscillator

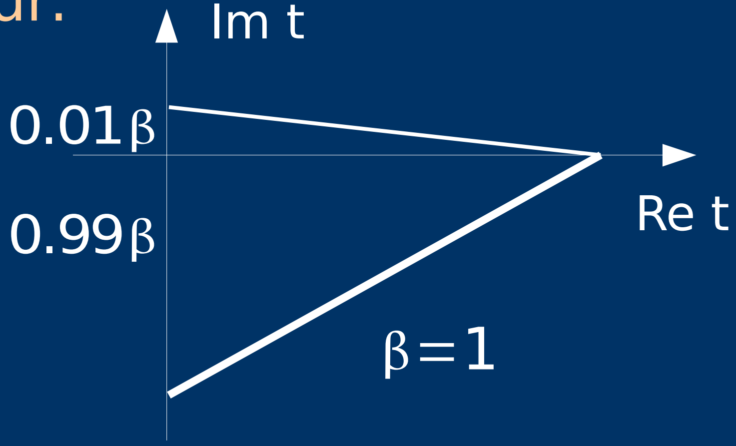
Thermal equilibrium:
periodic boundary cond.

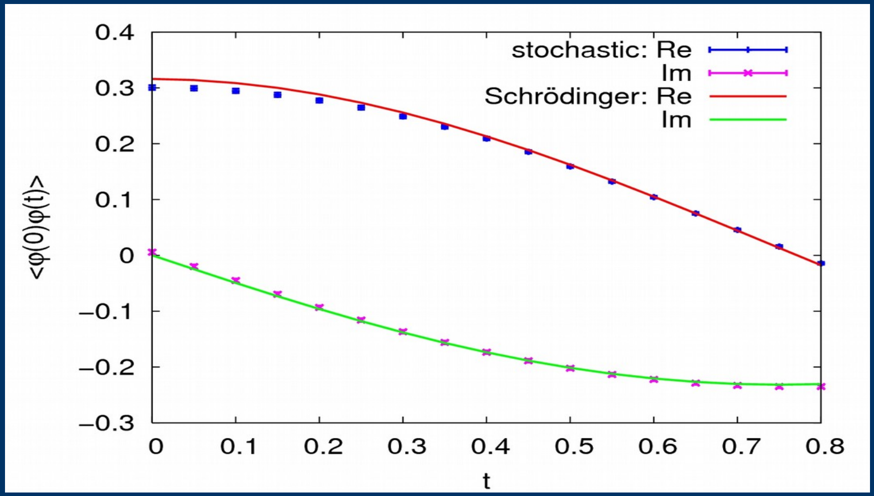
[Berges, Borsanyi, Sexty, Stamatescu (2006)]

Imaginary extent gives $\beta = \frac{1}{T}$

short real-time extent

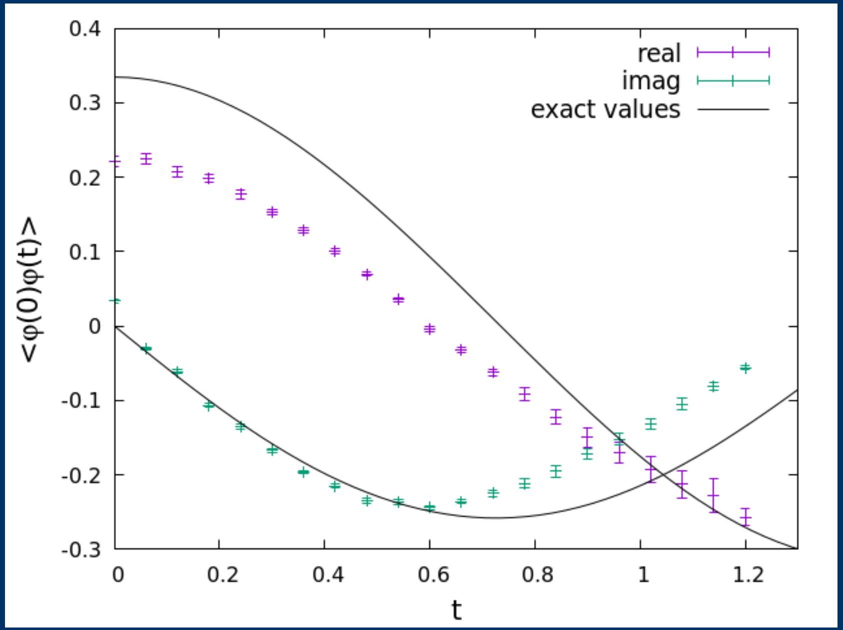
Asymmetric contour:





large real-time extent

Boundary terms appear



Kernels in the Langevin equation

Introducing a Kernel [Soderberg (1987), Okamoto et. al. (1988)]

$$\dot{z} = -\frac{\partial S}{\partial z} + \eta \quad \rightarrow \quad \dot{z} = -K(z)\frac{\partial S}{\partial z} + \frac{\partial K(z)}{\partial z} + \sqrt{K(z)}\,\eta$$

Fokker-Planck: $\partial_\tau P(z,\tau) = \partial_z K(z)(\partial_z + \partial_z S) P(z,\tau)$

Leaves the stationary distribution unchanged

Many variables – matrix Kernel

$$\frac{d\phi_i}{d\tau} = -H_{ij}(\phi) H^T_{jk}(\phi) \frac{\partial S}{\partial \phi_k} + \partial_k (H_{ij}(\phi) H^T_{jk}(\phi)) + H_{ij}(\phi)\eta_j$$

Can one use a Kernel to decrease boundary terms in the CLE?

Yes! search for a kernel using stochastic gradient descent
Loss function: Size of the distribution in imaginary directions

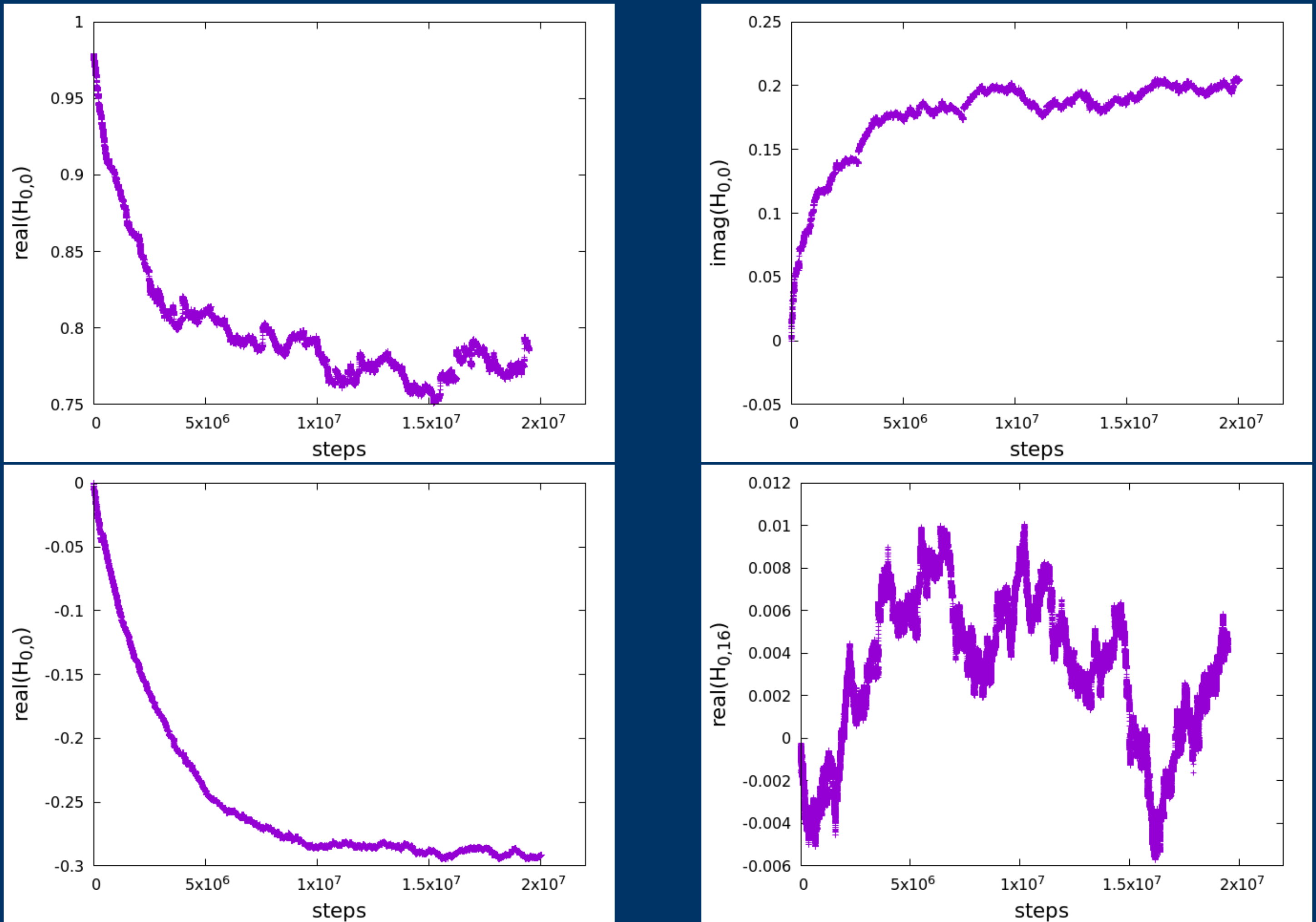
[Lampl, Sexty 2309.06103]

Stochastic gradient descent

Loss function: $$N(\phi) = \sum_t F_1(\mathrm{Re}\,\phi_t)^2 + F_2(\mathrm{Im}\,\phi_t)^2$$

Learning step: $$H_{ij} \rightarrow H_{ij} - \Delta L \frac{\partial N}{\partial H_{ij}}$$ average gradient over many steps

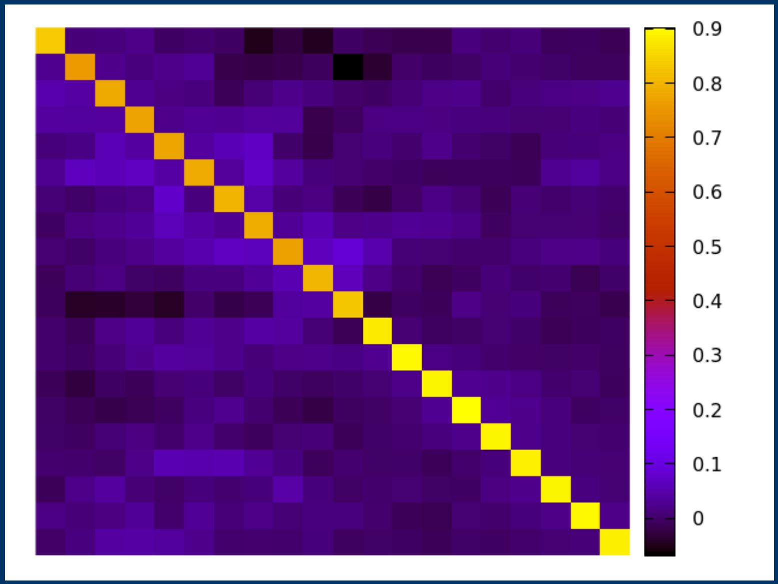
Wait for convergence



First step: Field independent matrix kernel

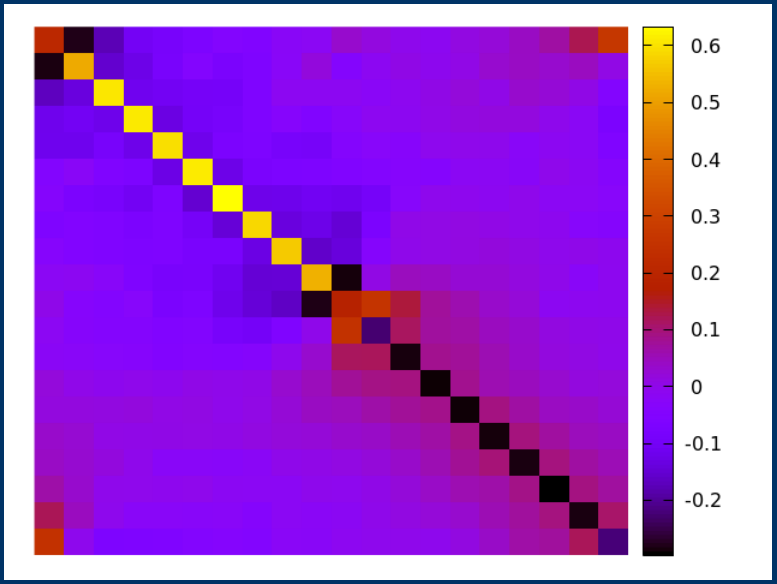
real part

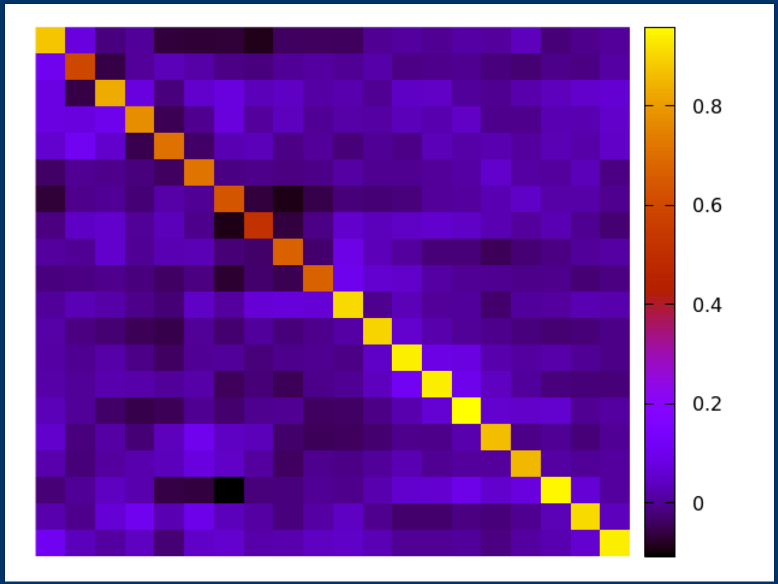
imaginary part



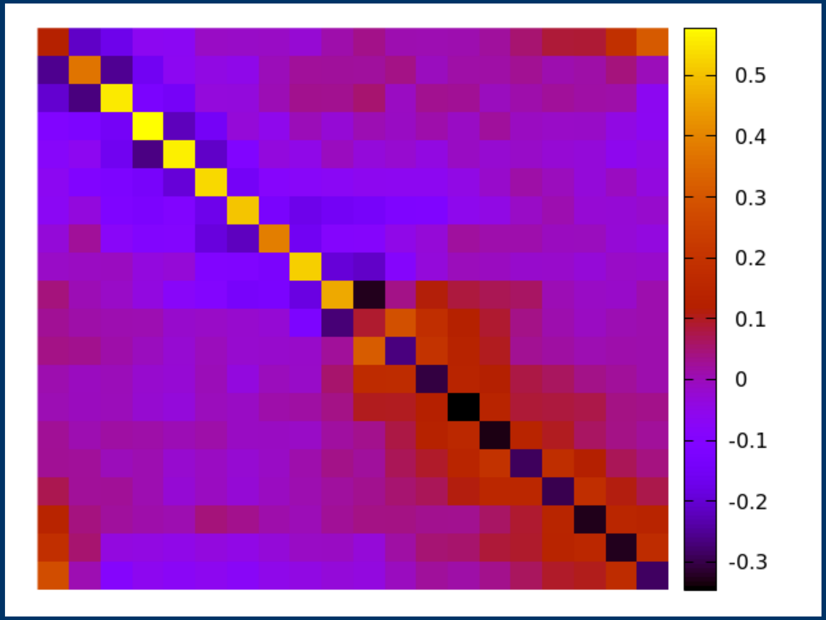
Real-time extent

$t = 1.2$





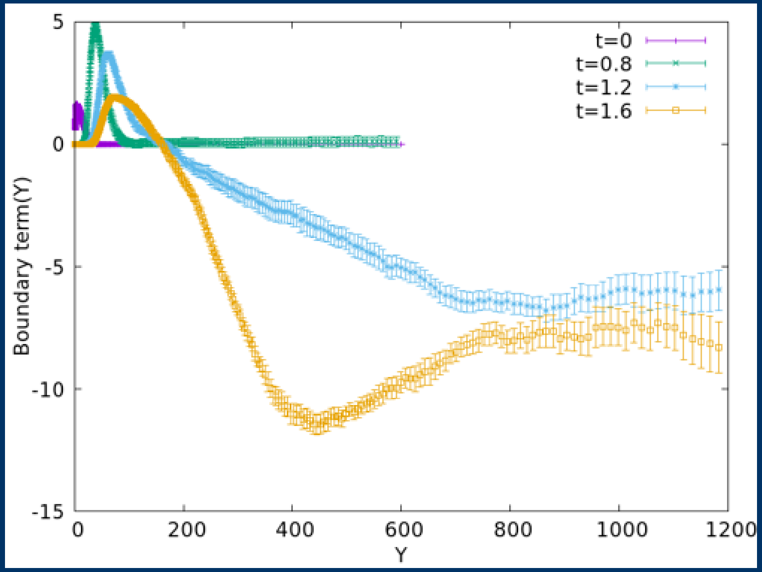
$t = 2.0$



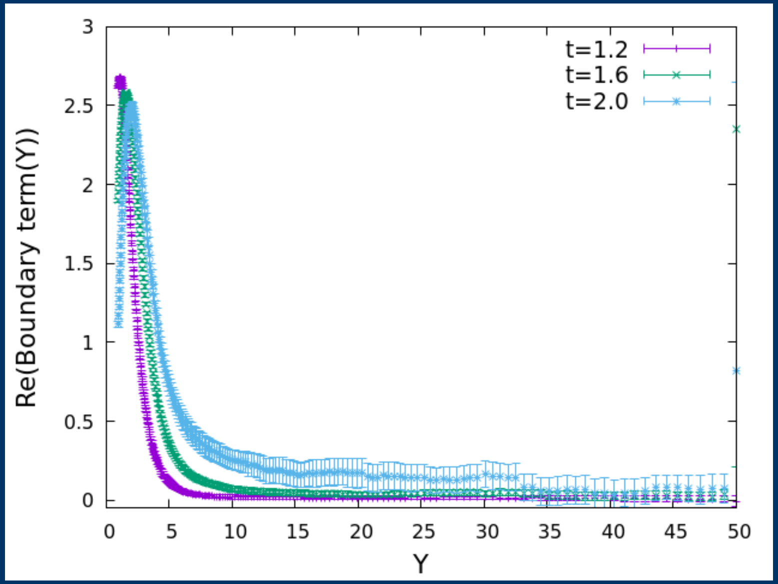
Boundary terms

Boundary terms of $\phi(t)^2$

Without Kernel:



With optimized kernel:

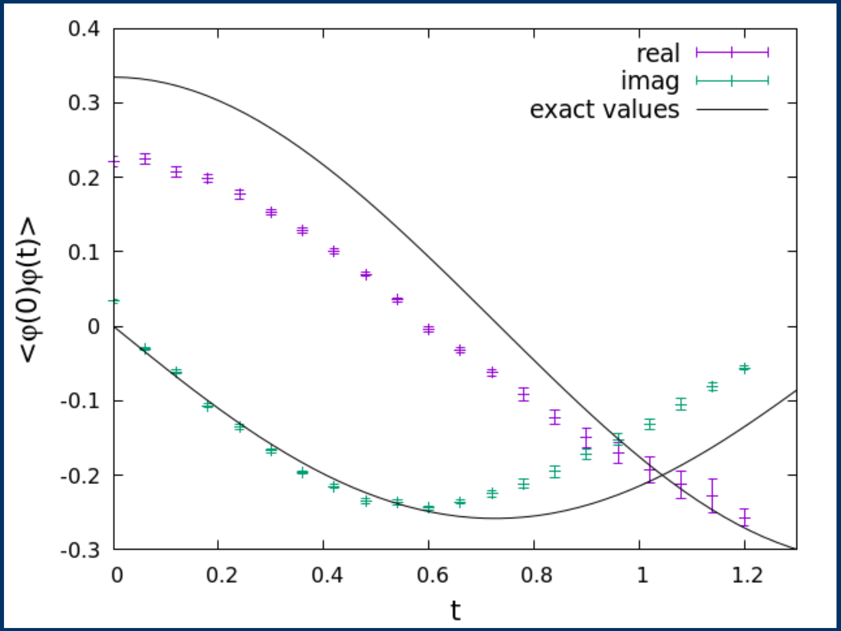


Actually, for an anharmonic quantum oscillator it's also easy to calculate exact results (e.g. diagonalize Hamiltonian)

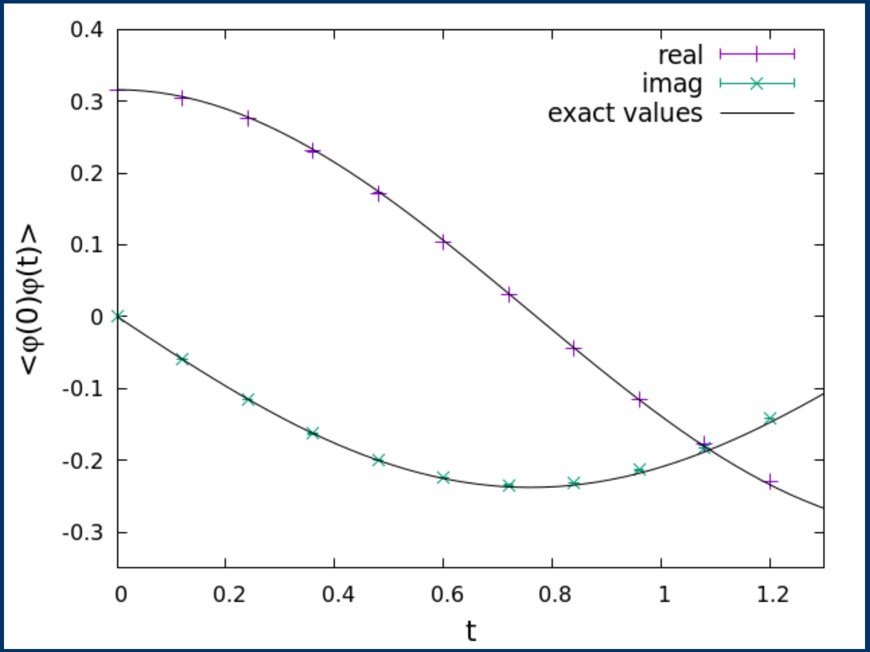
→ Compare to exact

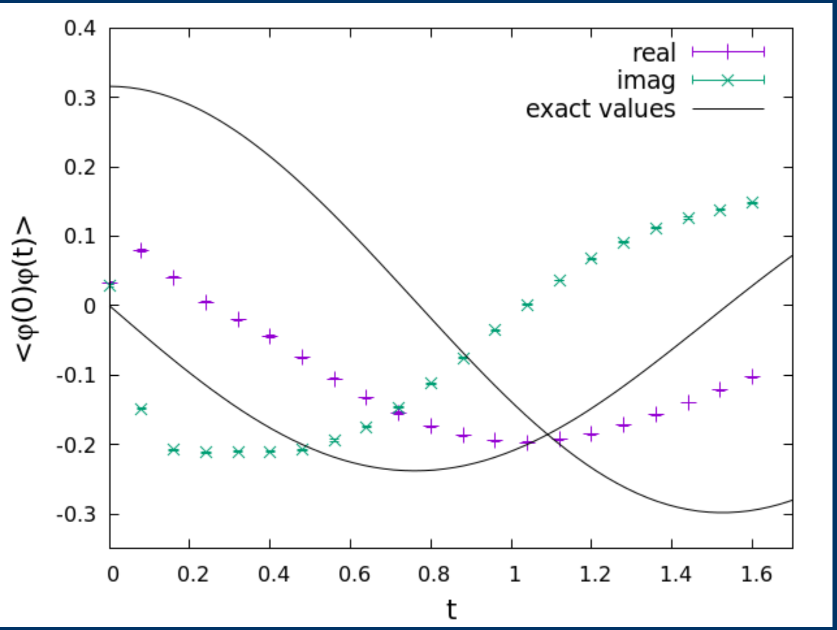
Without kernel

With learned kernel

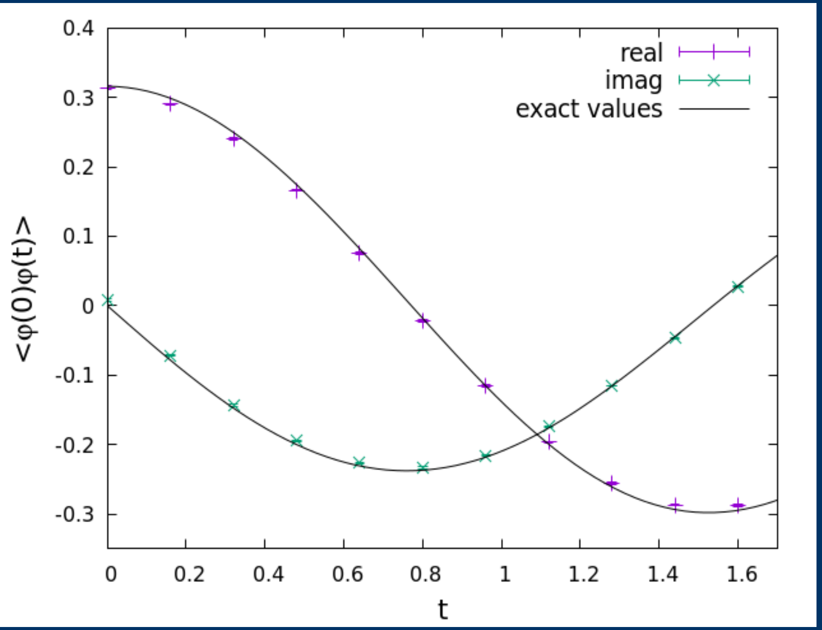


$t = 1.2$



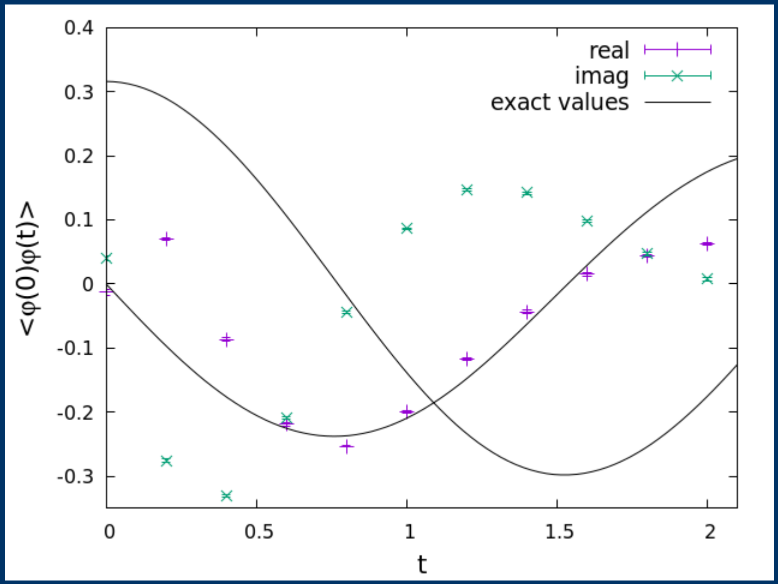


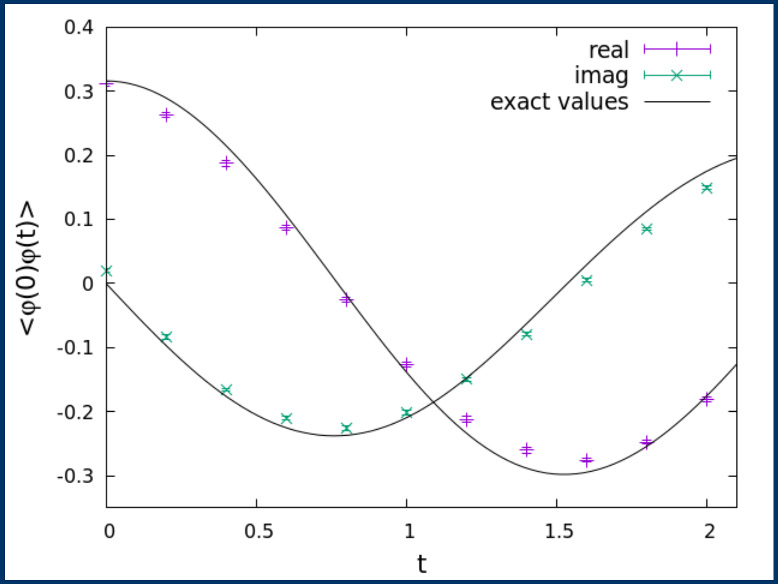
$t = 1.6$



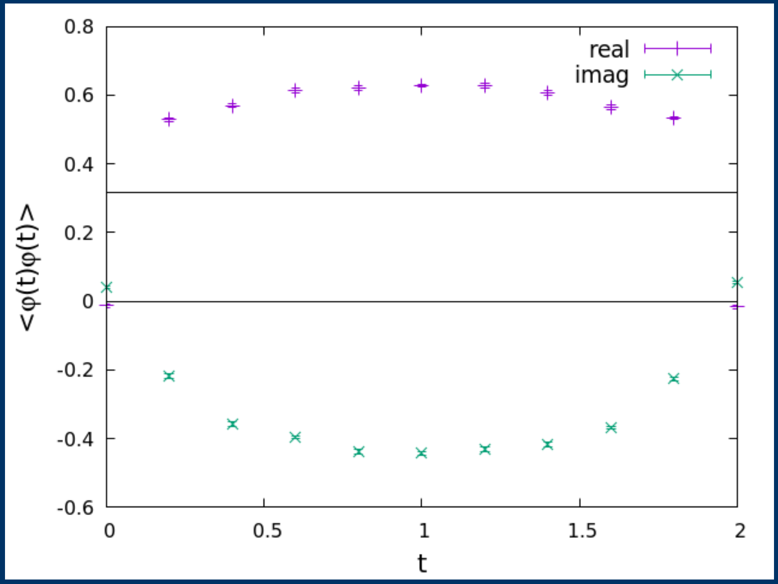
Increasing real time extent, boundary terms appear again

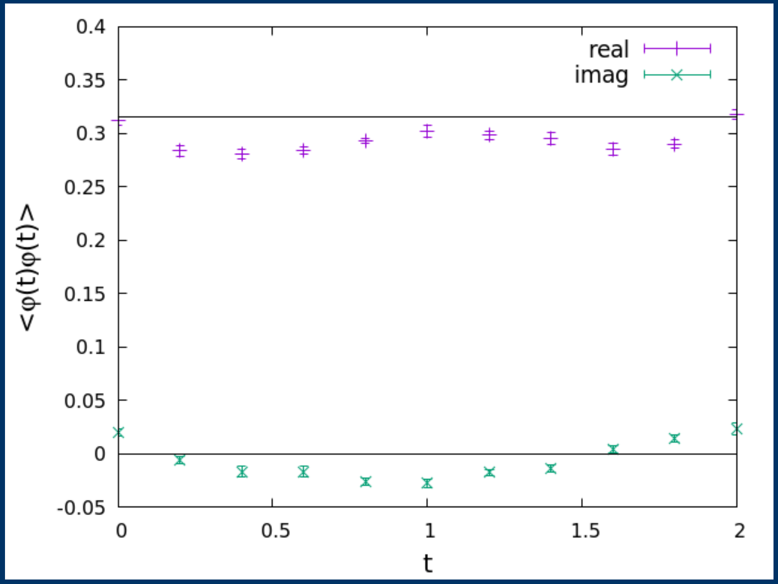
Without kernel | **With learned kernel**





$t = 2.0$





$t = 2.0$

Next step: Field dependent kernels

$H_{ij}=$ simple ansatz

$$S=\frac{1}{2}\sigma z^2+\frac{1}{4}\lambda z^4 \longrightarrow K(z)=C_1 e^{-z^2/a} e^{-i\,1^{\text{¿}}}+C_2\left(1-e^{-z^2/a}\right)e^{-i\theta_2}$$

Small kernel leads to small imaginary parts

→ Loss function needs to punish small $C_{1,} C_2$ values

$$H_{ij}(\phi)=H_{ij}^{(1)}+H_{ij}^{(2)}(\phi)$$

$H_{ij}^{(1)}=$ Optimized constant kernel from before

$H_{ij}^{(2)}(\phi)=$field dependent kernel to be optimized

$H_{ij}^{(2)}=$ neural network

Need to keep holomorphic kernel

→activation function= polynomial, exp or combinations of these

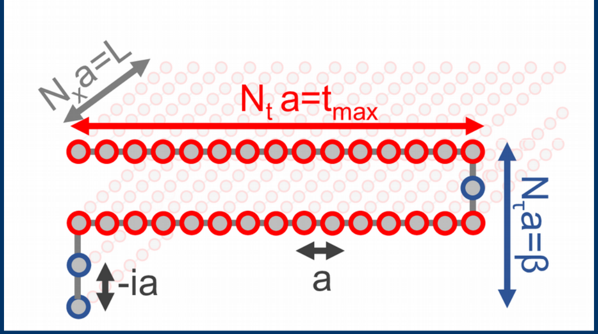
Complex analysis → unbounded activation functions

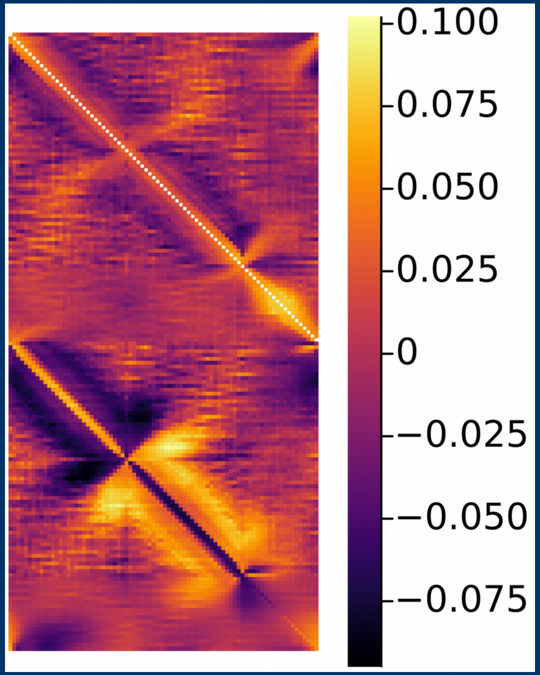
→ Long tailed distributions

More work needed...

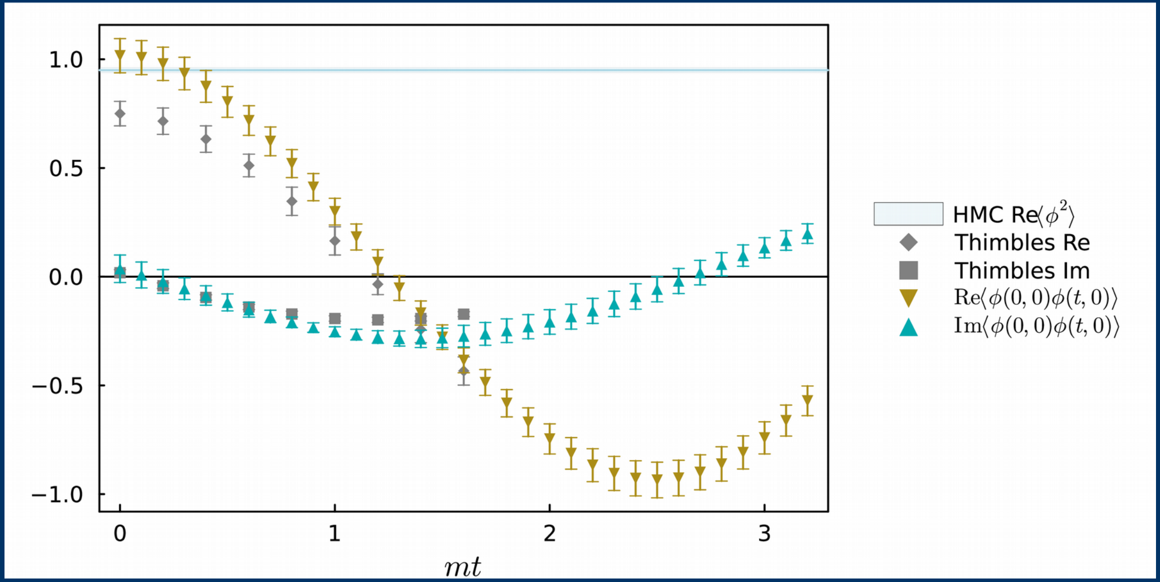
Scalar fields in 1+1 dimension [Alvestad, Rothkopf, Sexty (in prep.)]

Dense constant Kernel
on the Schwinger-Keldysh contour





two point function: $\langle \phi(0)\phi(t)\rangle$



Thimble result till t=1.6 [Alexandru et. al. (2022)]

CLE till t=3.2 (at least)

$N_x=16 \quad N_t=32 \quad N_\tau=4$

Pressure of the QCD Plasma at non-zero density

$$\frac{p}{T^4} = \frac{\ln Z}{V\,T^3}$$ $\longrightarrow$ Derivatives of the pressure are directly measureable

$\longrightarrow$ Integrate from T=0

[Engels et. al. (1990)]

First integrate along the temperature axis, then explore $\mu > 0$

Taylor expansion [Bielefeld-Swansea (2002-)]

Simulating at imaginary μ to calculate susceptibilities

[de Forcrand, Philipsen (2002-)]

Pressure of the QCD Plasma at non-zero density

$$\Delta\left(\frac{p}{T^4}\right)=\frac{p}{T^4}(\mu=\mu_q)-\frac{p}{T^4}(\mu=0)$$

If we want to stay at $\mu=0$

$$\Delta\left(\frac{p}{T^4}\right)=\sum_{n>0,even} c_n(T)\left(\frac{\mu}{T}\right)^n$$

$$c_2=\frac{1}{2}\frac{N_T}{N_s^3}\frac{\partial^2 \ln Z}{\partial\mu^2}$$

$$c_4=\frac{1}{24}\frac{1}{N_s^3 N_T}\frac{\partial^4 \ln Z}{\partial\mu^4}$$

Measuring the coefficients of the Taylor expansion

$$\frac{\partial^2 \ln Z}{\partial\mu^2}=N_F^2\langle T_1^2\rangle+N_F\langle T_2\rangle$$

$$\frac{\partial^4 \ln Z}{\partial\mu^4}=-3\left(\langle T_2\rangle+\langle T_1^2\rangle\right)^2+3\langle T_2^2\rangle+\langle T_4\rangle$$

$$+\langle T_1^4\rangle+4\langle T_3 T_1\rangle+6\langle T_1^2 T_2\rangle$$

$$T_1/N_F=\mathrm{Tr}\left(M^{-1}\partial_\mu M\right)$$

$$T_{i+1}=\partial_\mu T_i$$

$$T_2/N_F=\mathrm{Tr}\left(M^{-1}\partial_\mu^2 M\right)-\mathrm{Tr}\left(\left(M^{-1}\partial_\mu M\right)^2\right)$$

$$T_3/N_F=\mathrm{Tr}\left(M^{-1}\partial_\mu^3 M\right)-3\,\mathrm{Tr}\left(M^{-1}\partial_\mu M\, M^{-1}\partial_\mu^2 M\right)+2\,\mathrm{Tr}\left(\left(M^{-1}\partial_\mu M\right)^3\right)$$

$$T_4/N_F=\mathrm{Tr}\left(M^{-1}\partial_\mu^2 M\right)-4\,\mathrm{Tr}\left(M^{-1}\partial_\mu M\, M^{-1}\partial_\mu^3 M\right)-3\,\mathrm{Tr}\left(M^{-1}\partial_\mu^2 M\, M^{-1}\partial_\mu^2 M\right)-6\,\mathrm{Tr}\left(\left(M^{-1}\partial\mu\, M\right)^4\right)+12\,\mathrm{Tr}\left(\left(M^{-1}\partial_\mu M\right)^2 M^{-1}\partial_\mu^2 M\right)$$

Pressure of the QCD Plasma using CLE

[Sexty (2019)]

If we can simulate at $\mu > 0$

$$\Delta\left(\frac{p}{T^4}\right) = \frac{p}{T^4}(\mu = \mu_q) - \frac{p}{T^4}(\mu = 0) = \frac{1}{V T^3}\left(\ln Z(\mu) - \ln Z(0)\right)$$

$$\ln Z(\mu) - \ln Z(0) = \int_0^\mu d\mu \frac{\partial \ln Z(\mu)}{\partial \mu} = \int_0^\mu d\mu \, n(\mu)$$

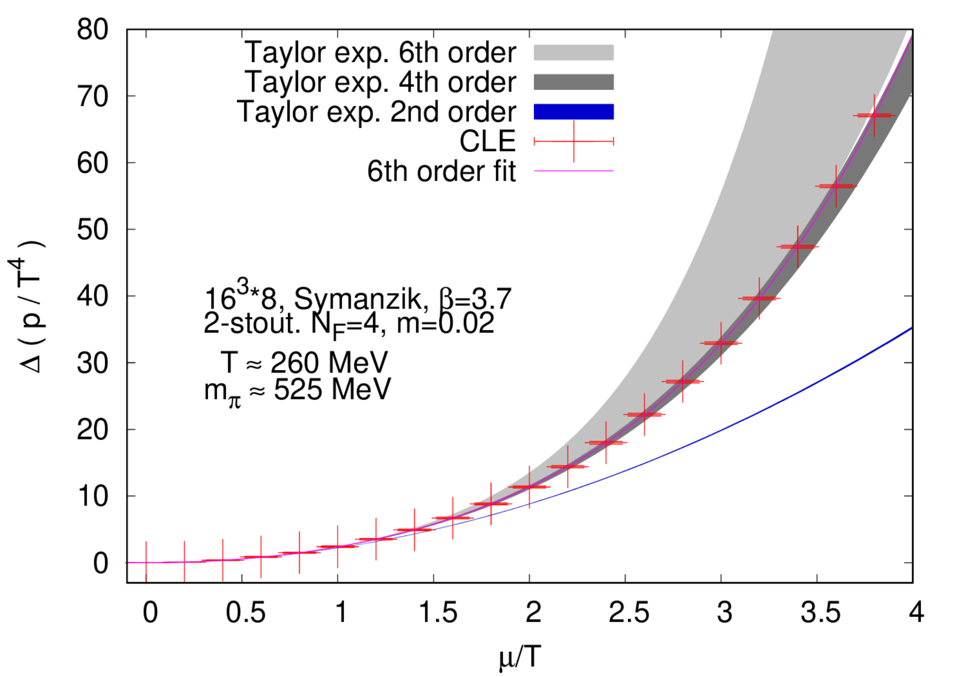
$$n(\mu) = \langle \mathrm{Tr}\left(M^{-1}(\mu) \partial_\mu M(\mu) \right) \rangle$$

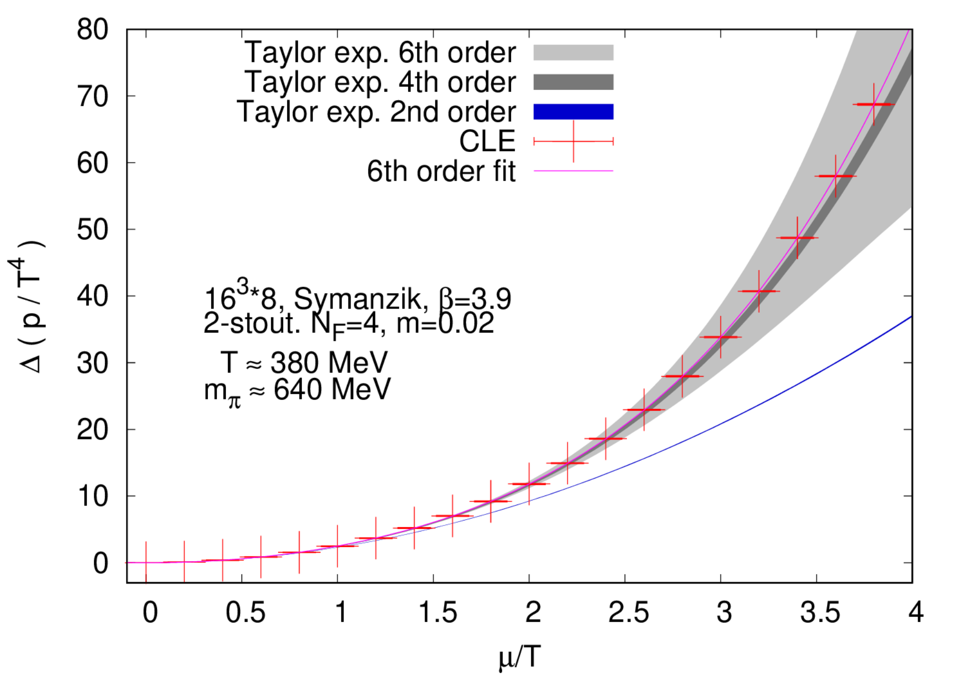
Using CLE it's enough to measure the density – much cheaper

Pressure with improved action

[Sexty (2019)]

In deconfined phase
Symanzik gauge action
stout smeared staggered fermions





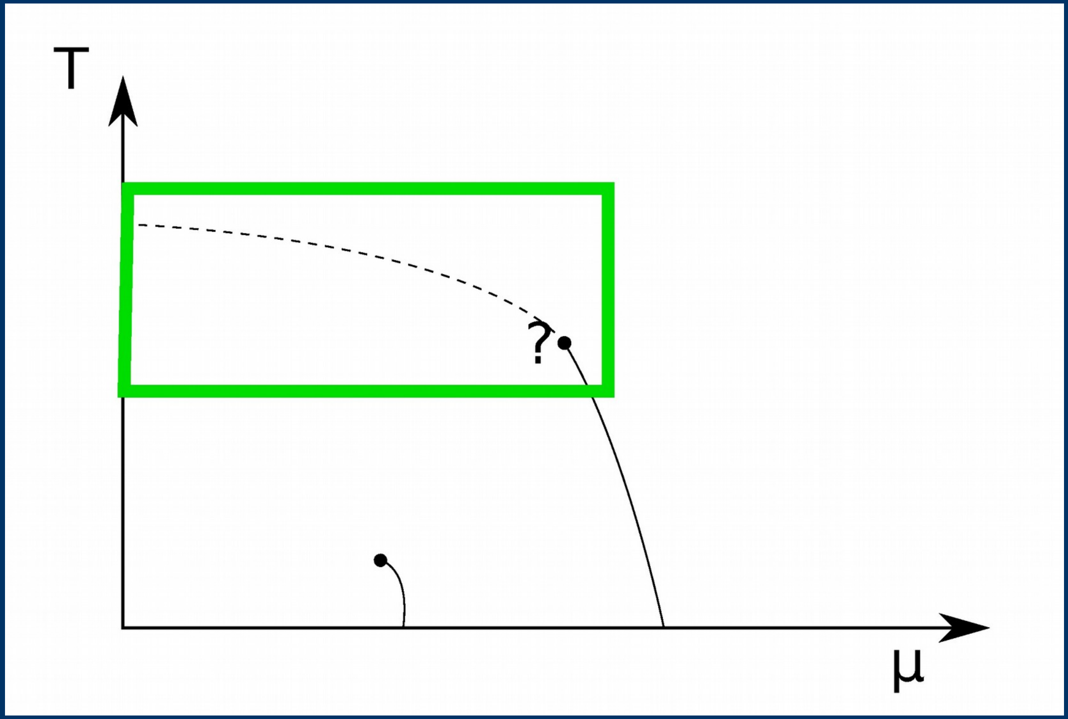
β	c_2 Taylor exp.	c_4 Taylor exp.	c_6 Taylor exp.	c_2 CLE	c_4 CLE	c_6 CLE
3.7	2.206 ± 0.009	0.156 ± 0.016	0.016 ± 0.013	2.33 ± 0.1	0.13 ± 0.02	0.002 ± 0.001
3.9	2.312 ± 0.007	0.150 ± 0.007	0.001 ± 0.005	2.36 ± 0.04	0.14 ± 0.01	0.002 ± 0.001

Good agreement at small μ
CLE calculation is much cheaper

further interesting quantities: Energy density, quark number susceptibility, ...

Mapping out the phase transition line

[Scherzer, Sexty, Stamatescu (2020)]



Follow the phase transition line
starting from $\mu = 0$

Using Wilson fermions

Fixed lattice spacing and spatial vol.
N_t scan

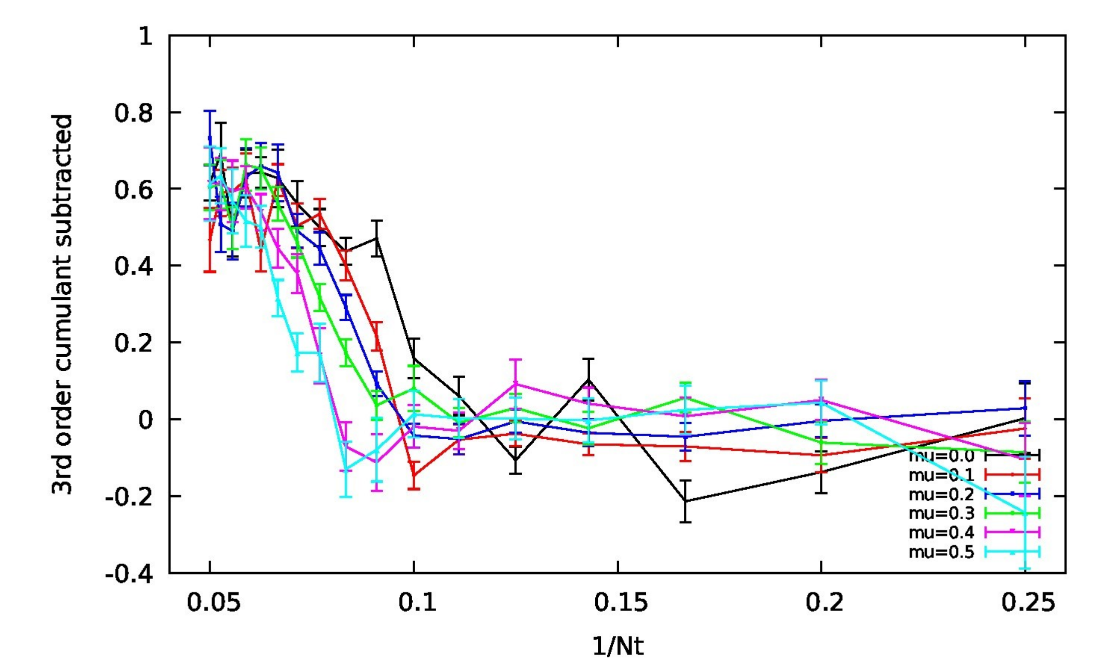
Detection of the phase transition line

Binder cumulant

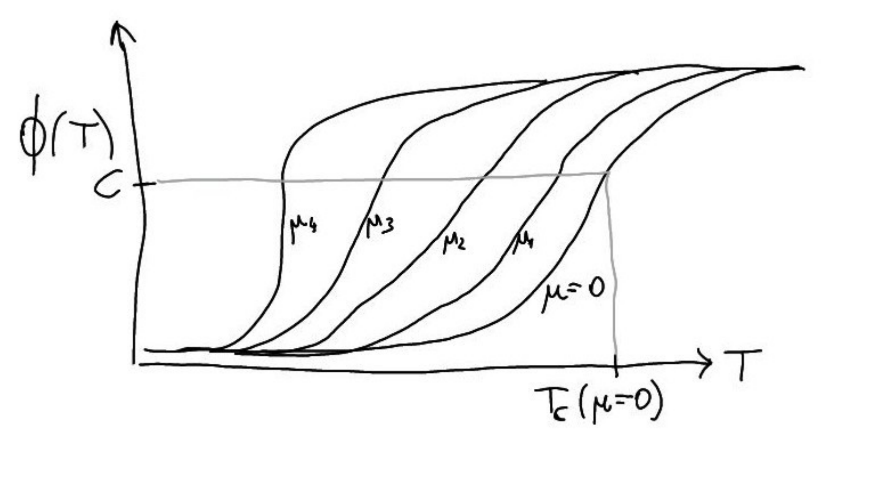
$$B_3 = \frac{\langle O^3 \rangle}{\langle O^2 \rangle^{3/2}}$$

$$O = P - \langle P \rangle \quad \text{with} \quad P = \sqrt{P_{bare} P_{bare}^{-1}}$$

no renormalization
zero crossing defines transition



Shift method



Define $T_c(\mu)$ as $\phi(T_c(\mu),\mu) = C$

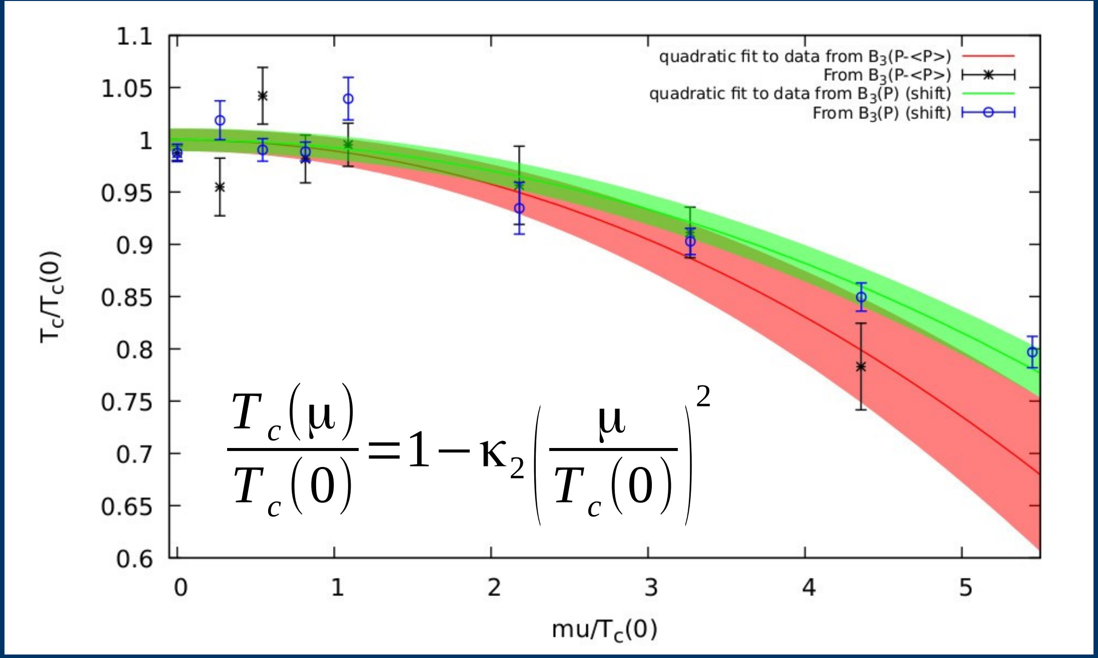
e.g. $B_{3,}$ chiral condensate,
baryon number susceptibility

Works well for small μ
Critial point at μ_4

Lattice spacing: $a = 0.065\ \mathrm{fm}$

Pion mass: $m_\pi = 1.3\ \mathrm{GeV}$

Volumes: $8^3, 12^3, 16^3$



$$\frac{T_c(\mu)}{T_c(0)} = 1 - \kappa_2 \left(\frac{\mu}{T_c(0)} \right)^2$$

Finite size effects large

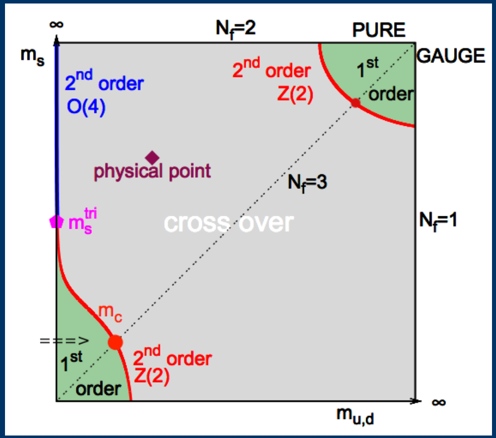
$$\kappa_2 \approx 0.0012$$

Consistent results

In literature
For physical pion mass
$\kappa_2 = 0.015$

Can follow the line to
quite high μ / T

Open questions
Possible for lighter quarks?
Finite size scaling?
Where is the upper right corner of Columbia plot?
Critical point nearby?



Summary

CLE has potential problems with boundary terms and poles

Monitoring of the process is required:
measuring Boundary terms

lattice models with cheap observable
Correction with higher order boundary terms

Kernels help elimnating boundary terms (if they are present)
Real time scalar with learned kernel

Results for the EoS and Phase diag. of QCD

Dynamical stabilization might help at low temperatures of QCD
See next talk by Michael Hansen

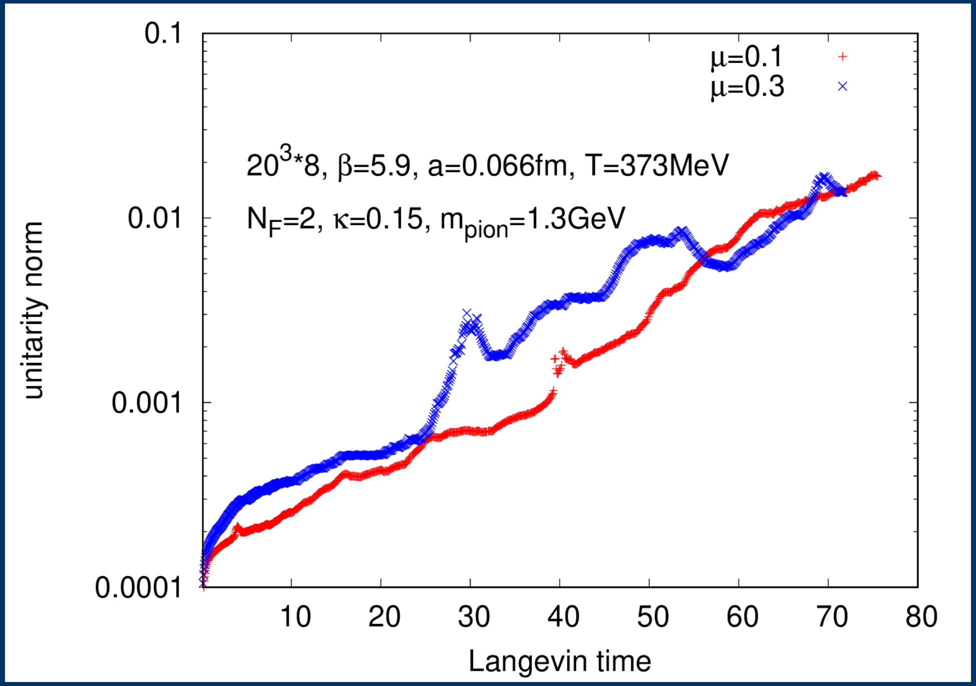
Long runs with CLE

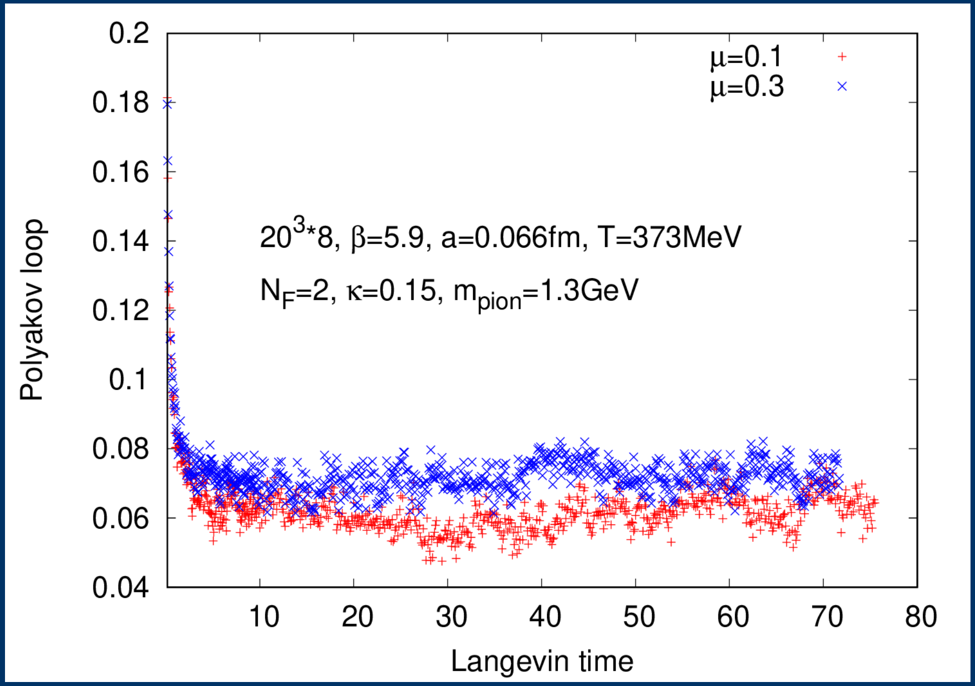
Unitarity norm has a tendency to grow slowly (even with gauge cooling)

$$UN = \sum_{x,\nu} Tr\left(U_{x\nu} U^{+}_{x\nu} - 1\right)$$

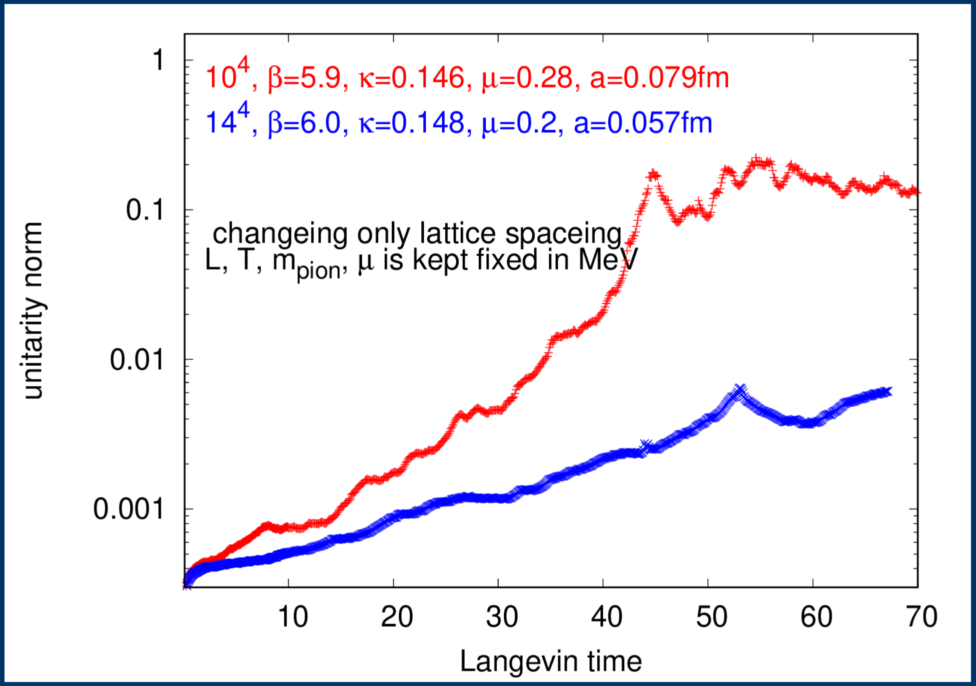
Runs are cut if it reaches ~ 0.1

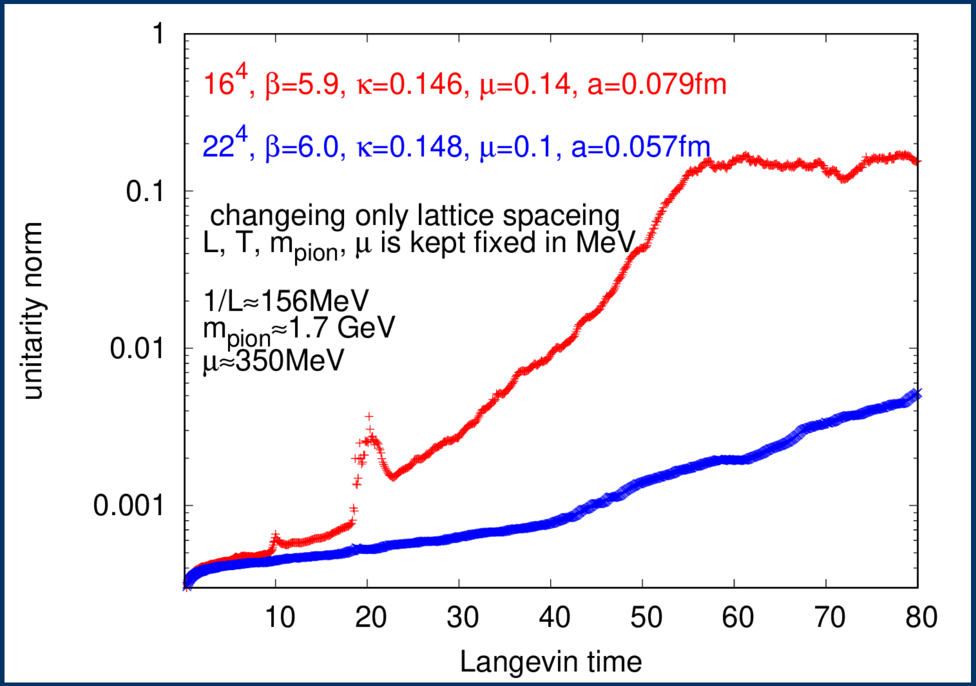
Thermalization usually fast
– might be problematic close to critical point or at low T





Getting closer to continuum limit





Test with Wilson fermions
Increase β by 0.1 – reduces lattice spacing by 30%
change everything else to stay on LCP

behavior of Unitarity norm improves
autocorrelation time decreases as lattice gets finer