## Nonzero density on the lattice

## Dénes Sexty

KFU Graz


## 12-13.05.2022. DK-PI Retreat

1. Lattice QCD - nonzero density in lattice QCD - sign problem
2. Reweighting - Taylor expansion - imaginary mu
3. Complex Langevin and Lefschetz thimbles

## From the action to the phenomenology of QCD

Action of QCD, the theory of strong interactions

$$
S=-\frac{1}{4} \operatorname{Tr} F_{\mu \nu} F^{\mu \nu}+\sum_{1}^{6} \bar{\psi}_{f}\left(i \gamma^{\mu} D_{\mu}+m_{f}\right) \psi_{f} \quad \begin{aligned}
& 1 \text { gauge coupling } \\
& 6 \text { quark masses }
\end{aligned}
$$



Confinement mechanism? Mass of hadrons? Scattering cross sections? Phases transition to Quark-gluon plasma? Critical point at nonzero density? Equation of state?
Compressibility of quark matter? (in neutron stars)
Exotic phases:
Color superconducting phases?
Quarkyonic phase?
QCD in magnetic fields?
.... and so on

## How?

Perturbation theory - asymptotic freedom Kinetic theory Effective models (NJL, Polyakov-NJL, SU(3) spin model, ... ) Functional methods (FRG, 2PI,3PI, Dyson-Schwinger eq.) Lattice


## Phase diagram of QCD



For these lectures we focus on thermodynamics at nonzero density

## Phase diagram of QCD



## Phase diagram of QCD



## Phase diagram of QCD



## Phase diagram of QCD



## Phase diagram of QCD



## compare with: Phase diagram of water


much better known....

## 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?

## 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
Transport coefficients: e.g. viscosity


Hard problem
Real-time correlator

$$
\eta=\frac{1}{T V} \int_{0}^{\infty} d t\left\langle\sigma_{x y}(0) \sigma_{x y}(t)\right\rangle
$$

## Path integral formulation of Quantum Mechanics

Quantum Mechanics with $\quad \hat{H}=\frac{\hat{p}^{2}}{2 m}+V(\hat{q})$
Time evolution given by Schrödinger eq.

$$
i \partial_{t} \Psi(x, t)=\hat{H} \Psi(x, t)
$$

$$
|\Psi(x, t)|=e^{-i t \hat{H}}|\Psi(x, 0)\rangle
$$

## Equivalent formulation

Transition amplitude: $\quad\left\langle q_{2}\right| e^{-i t \hat{H}}\left|q_{1}\right\rangle=\int_{q_{1}}^{q_{2}} D q e^{i s[q(t)]}$
Path integral: $\quad \int_{q_{1}}^{q_{2}} D q=$ normalized sum for all functions $\quad q\left(t_{1} \leqslant t \leqslant t_{2}\right)$ with correct bound. cond. $\quad q\left(t_{1}\right)=q_{1} q\left(t_{2}\right)=q_{2}$


Numerically advantegous $q(t)$ instead of $\Psi(x, t)$

## Thermodynamics with Path integral

Thermodynamics

$$
e^{-i t \hat{H}} \rightarrow e^{-\beta \hat{H}}
$$

Imaginary time - Wick rotation
Imaginary time: $t \rightarrow-i \tau \quad 0<\tau<-i \beta$


$$
\left\langle q_{1}\right| e^{-\beta \hat{H}}\left|q_{2}\right\rangle=\int_{q_{1}}^{q_{2}} D q e^{-S_{E}[q(t)]} \quad S_{E}[q(t)]=\int_{t=0}^{t=\beta} d t\left(\frac{1}{2} m \dot{q}(t)^{2}+V(q(t))\right)
$$

We want $\quad \mathrm{Z}=\operatorname{Tr}\left(e^{-\beta H}\right) \quad\langle X\rangle=\operatorname{Tr}\left(X e^{-\beta H}\right)$

- Periodical boundary conditions in temporal directions

System of size $L_{s}^{3,} L_{t} \rightarrow$ Temperature $=1 / L_{t}$
Temperature only appears as the inverse temporal size.

Temporal size infinite (or "large" compared to spatial) - zero temperature


Discretised action:

Discretise action on a cubic-space time lattice

$$
F_{\mu v}^{a}=\partial_{\mu} A_{v}^{a}-\partial_{v} A_{u}^{a}+g f_{a b c} A_{\mu}^{b} A_{v}^{c}
$$

Gluon fields

$$
A_{\mu}^{a}(x) \rightarrow U_{\mu}(x)=\exp \left(i \int d x A_{\mu}^{a}(x) \lambda_{a}\right)
$$

Link variables $\quad U_{\mu}(x) \in \operatorname{SU}(3)$
Fermion fields

$$
\psi(x) \rightarrow \psi(x)
$$

Site variables
gluons: $\quad-\frac{1}{4} F_{\mu \nu} F^{\mu \nu} \rightarrow \sum_{\text {plaqueteres }} \operatorname{Re} \operatorname{Tr}\left(U_{\mu v}\right)$
fermions:

$$
\begin{gathered}
\bar{\psi}\left(i \gamma^{u} D_{\mu}+m\right) \psi \rightarrow \bar{\psi}\left(i \gamma^{\mu} D_{\mu}^{L, F}+m\right) \psi \\
D_{v}^{L, F} \psi(x)=\frac{1}{a}\left(U_{v}(x) \psi(x+\hat{v})-\psi(x)\right)
\end{gathered}
$$

## Lattice QCD



Discretise action on a cubic-space time lattice
Gluon fields Link variables $\quad U_{\mu}(x) \in \operatorname{SU}(3)$
Fermion fields $\psi(x)$
Path integral:

$$
\int D A_{\mu} \rightarrow \int \prod_{x, \mu} d U_{\mu}(x)
$$

finite number of integrals with respect
to the Haar measure of the $\operatorname{SU}(3)$ group
$\int D \psi D \bar{\psi} \rightarrow \int \prod_{x} d \psi(x) d \bar{\psi}(x)$
finite number of Grassman integrals

Lattice = one of the alternatives to regularize QFT

We want continuum and thermodynamical limit $\quad a \rightarrow 0, V \rightarrow \infty$

## Gauge transformations on the lattice

Gauge transformations


$$
\begin{aligned}
& A_{\mu}(x) \rightarrow-\frac{i}{g}\left(\partial_{\mu} \Omega(x)\right) \Omega^{-1}(x)+\Omega(x) A_{\mu}(x) \Omega(x)^{-1} \\
& \psi(x) \rightarrow \Omega(x) \psi(x)
\end{aligned}
$$

on the lattice

$$
\begin{aligned}
& U_{\mu}(x) \rightarrow \Omega(x) U_{\mu}(x) \Omega^{-1}\left(x+a_{\mu}\right) \\
& \psi(x) \rightarrow \Omega(x) \psi(x)
\end{aligned}
$$

Symmetry group: $\quad \mathrm{SU}(3)^{{N_{s}^{3}}^{3} N_{t}}$
Finite volume of gauge orbits

No need for gauge fixing No ghosts

Observables have to be gauge invariant:

$$
\operatorname{Tr}(U(x, x)) \quad \text { or } \quad \psi^{+}(x) U(x, y) \psi(y)
$$

where $U(x, y)$ is a chain of link variables between $x$ and $y$


Plaquette $U_{\mu v}=U_{\mu}(x) U_{v}(x+\mu) U_{\mu}^{-1}(x+v) U_{v}^{-1}(x)$
Related to Field strength tensor $F_{\mu \nu}$
Wilson loops $W_{m, n, \mu \nu} \quad W_{1,1, \mu v}=U_{\mu \nu}$

$$
\log \left\langle W_{R, T}\right\rangle=\text { energy of static quark pair at dist. } \mathrm{R} \rightarrow \text { String tension }
$$

Polyakov loop $P=\prod_{i=0}^{N_{i}-1} U_{i}$
$L=\langle\operatorname{Tr} P\rangle \simeq e^{-F_{q}(T) / T} \quad$ energy of a static quark
$T=0$ confinement $\rightarrow F(q)=\infty \rightarrow L=0$
$T=$ Large deconfinement $\rightarrow L \neq 0$

## Monte Carlo calculations with importance sampling

We have a (discretised) theory with some action

$$
Z=\int D \phi e^{-\beta S(\phi)} \rightarrow \int \prod d \phi_{i} e^{-\beta S[\phi]}
$$

Interested in observables: $\langle X\rangle=\frac{1}{Z} \int \prod d \phi_{i} X[\phi] e^{-\beta S[\phi]}$
still too many integrals

## Importance sampling:

build a Markov chain on field configurations with the Metropolis algorithm

$$
C=\left\{\phi_{i}\right\} \quad\left(\text { or }\left\{U_{v}\right\} \text { for QCD }\right)
$$

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

From $C_{i}$ we propose a random $C_{i+1}$ Accept with some probability

Probability of visiting C $\quad p(C) \sim e^{-\beta S[C]}$

$$
\langle X\rangle=\frac{1}{Z} \operatorname{Tr} \hat{X} e^{-\beta(\hat{H})}=\frac{1}{Z} \int d C e^{-\beta S[C]} X[C]=\frac{1}{N} \sum_{i} X\left[C_{i}\right]
$$

## Scale setting in lattice QCD

How do we set the lattice spacing in QCD? we actually don't prescribe it, but measure it

$$
-\frac{1}{4} F_{\mu \nu} F^{\mu \nu} \rightarrow \sum_{\text {plaquettes }} \operatorname{Re} \operatorname{Tr}\left(U_{\mu \nu}\right)
$$

We can set the inverse coupling in the action: $\quad S_{G}=\frac{1}{g^{2}} \sum_{\text {plaquettes }} \operatorname{Re} \operatorname{Tr}\left(U_{\mu \nu}\right)$
In practice we use $\quad \beta=\frac{2 N_{c}}{g^{2}}$
This sets the gauge coupling on the scale of the lattice spacing
the running coupling grows in the infrared at some length scale confinement appears

Fix lattice spacing such that confinement scale is same as in our world

Historically the string tension is calculated in lattice units and made equal to its experimental value
this yields lattice spacing in MeV

## Scale setting in lattice QCD

Historically the string tension is calculated in lattice units In practice: fitting asymptotic behavior of "Wilson loop" observable
(Nowadays e.g. "Gradient Flow" is used for scale setting.) $W_{R T} \simeq e^{-\alpha R T}$

This process of scale setting is also used in theories not corresponding to our world (e.g. for different masses or even number of fermion flavours)

Typical behavior


So in lattice QCD
$\beta$ increases $\rightarrow$
lattice spacing $a$ decreases $\rightarrow$
Temporal size of lattice decreases $\rightarrow$
Temperature increases

## Lattice QCD - fermions



In continuum: Fermions described with Grassmann variables

$$
\begin{gathered}
Z=\int d \psi d \bar{\psi} e^{\bar{\psi}\left(i \gamma^{\prime \prime} \partial_{u}+m\right) \psi} \\
\int d \eta d v e^{\eta M v}=\operatorname{det} M
\end{gathered}
$$

$M=$ Dirac matrix

In gauge theories: $\partial_{v} \rightarrow \partial_{v}+i g A_{v}=D_{v}$ covariant derivative
quarks: $\quad \bar{\psi}\left(i \gamma^{\mu} D_{\mu}+m\right) \psi \rightarrow \ln \operatorname{det}\left(1+\kappa \sum_{ \pm \mu}\left(1+\gamma_{\mu}\right) U_{\mu}(x) \delta_{y, x+\hat{u}}\right)$
large matrix $\quad N=10^{5}-10^{7}$
source of most of the problems with lattice QCD...

## Fermion doubling

The dispersion relation for a particle should be:

$$
D \psi(x)=\left(i \gamma_{v} p_{v}+m\right) \psi(x) \rightarrow E_{p}^{2}=m^{2}+p^{2}
$$

Is this satisfied for fermions on the lattice? Let's use free fermions: $U_{v}=1$

$$
i \partial_{v} \psi(x) \rightarrow \frac{i}{2 a}(\psi(x+\hat{v})-\psi(x-\hat{v}))
$$

symmetrized derivative as antihermiticity is needed

$$
\partial=\frac{1}{2}\left(\partial_{F}+\partial_{B}\right)
$$

momentum on the lattice $\quad \psi(x) \simeq e^{i k x} \quad k=\frac{2 \pi}{N} i$

$$
\frac{i}{2 a}\left(e^{i k(x+\hat{v})}-e^{i k(x-\hat{v})}\right)=i \sin (k a) e^{i k x}=i k_{L A T} e^{i k x}
$$

If we have bosons in the action with a second derivative term

$$
\Delta e^{i k x}=e^{i k(x+\hat{v})}-2 e^{i k x}+e^{i k(x-\hat{v})}=4 \sin ^{2}\left(\frac{k a}{2}\right) e^{i k x}=k_{L A T}^{2} e^{i k x}
$$



4 dimensional lattice $\rightarrow 2^{4}=16$ fermion modes

$$
k=(0,0,0,0), \quad k=(0,0,0, \pi / a), \ldots
$$

## Fermion doubling - Solutions

## Wilson fermions

Introduce new term in fermion action to suppress unwanted doublers

$$
S=\bar{\psi}(x) \gamma_{\mu}(\psi(x+\mu)-\psi(x-\mu))+m \bar{\psi}(x) \psi(x)
$$

Add a new term to lift energy of edge modes:

$$
S_{W}=\frac{r}{2} \bar{\psi} \Delta \psi \quad \begin{gathered}
\text { Second derivative } \\
\Delta \psi=\psi(x+\hat{\mu})-2 \psi(x)+\psi(x-\hat{\mu})
\end{gathered}
$$

Acts as "momentum dependent mass" $M(p)=m+\frac{2 r}{a} \sum_{v} \sin ^{2}\left(k_{v} a / 2\right)$
As the continuum limit is neared
Edge modes (doublers) become very heavy $m_{\text {doubler }} \simeq O(1 / a)$ Physical modes have $O(a)$ mass contribution

Price to pay:

- Chiral symmetry explicitely broken
- mass parameter needs tuning
- $O(a)$ discretisetion errors (instead of $O\left(a^{2}\right)$ )


## Fermion doubling - Solutions

## Staggered fermions

One notes 4-fold symmetry of the naive fermion action

$$
\psi_{i, a}(x) \rightarrow \psi_{a}(x) \quad \text { throw away } 3 \text { of them }
$$

16 fermion flavours ("tastes") $\rightarrow 4$ fermion tastes

Still needs some rooting:
If we had 2 degenerate fermion flavors in continuum

$$
Z=\int d \psi_{1} d \bar{\psi}_{1} d \psi_{2} d \bar{\psi}_{2} e^{\bar{\psi}_{1}\left(i \gamma^{"} \partial_{\mu}+m\right) \psi_{1}} e^{\bar{\psi}_{2}\left(i y^{u} \partial_{\mu}+m\right) \psi_{2}}=(\operatorname{det} M)^{2}
$$

For staggered we could than use (pretending that it's four degenerate species):

$$
\operatorname{det} M \rightarrow(\operatorname{det} M)^{1 / 4}
$$

In reality taste breaking effects vanish only in the continuum limit

## Improved actions for lattice QCD



Carrying out continuum extrapolation $\quad a \rightarrow 0$

Simulate at multiple lattice spacings
Fitting some observable

$$
O(a)=O_{0}+O_{1} a+O_{2} a^{2}+\ldots
$$

Change action such that $O_{1}$ is eliminated
Gauge improvement
Include larger loops in action
Symanzik action:

$$
S=-\beta \left\lvert\, \frac{5}{3} \sum \operatorname{Re} \operatorname{Tr} \square-\frac{1}{12} \sum \operatorname{Re} \operatorname{Tr} \square \square\right.
$$

Symmetry of discretisation: plaquette action scales with $O\left(a^{2}\right)$
Symanzik sets the coefficient of $O\left(a^{2}\right)$ term in the action to zero at tree level loop effects $\rightarrow O\left(g^{2} a^{2}\right)$
Coefficient of quadratic term much smaller than with plaquette action

## Improved fermion actions

Changeing the Dirac operator
Wilson fermions: clover improvement adds a clover term

Staggered fermions: naik or p4
take into account 3-link terms

Fat links
Smear the gauge fields inside the Dirac operator
APE, HYP

$$
\begin{gathered}
V_{\mu}=(1-\alpha) U_{\mu}+\alpha \sum \text { staples } \\
U_{\mu}^{\prime}=\operatorname{Proj}_{\mathrm{SU}(3)} V_{\mu}
\end{gathered}
$$

Stout

$$
U^{\prime}=e^{i Q_{u}} U_{\mu} \quad Q_{\mu}=\rho \sum \text { staples }
$$


essentially one step of gradient flow with stepsize $\rho$

## Chiral symmetry on the lattice

$$
\psi \rightarrow e^{i \Theta \gamma_{s}} \psi \quad \bar{\psi} \rightarrow \bar{\psi} e^{i \theta \gamma_{s}}
$$

Fermion action $S_{F}=\int \bar{\psi}(x) D(x, y) \psi(y)$ is invariant if $\left\{\gamma_{5}, D\right\}=0$
In continuum the kinetic term respects symmetry mass term gives an explicit breaking

## Nielsen-Ninomiya theorem:

On the lattice a local discretisation that satisfies $\left\{\gamma_{5}, D\right\}=0$ will have doublers
Staggered: Chiral symm exact, still 4 tastes, usually rooted
Wilson: Chiral symmetry broken (only restored in cont. limit.) Eliminates doublers

Overlap fermions: reinvents lattice version of Chiral symmetry Nielsen-Ninomiya does not apply

## Ginsparg Wilson relation and Overlap fermions

$$
\left\{\gamma_{5}, D\right\}=0 \longrightarrow\left\{\gamma_{5}, D\right\}=a D \gamma_{5} D \quad \begin{aligned}
& \text { In the continuum limit } \\
& \text { Reduces to usual chiral symmetry }
\end{aligned}
$$

Corresponding lattice transformations:

$$
\psi \rightarrow e^{i \Theta \gamma_{5}\left(1-\frac{a}{2} D\right)} \psi \quad \bar{\psi} \rightarrow \bar{\psi} e^{i \Theta \gamma_{5}\left(1-\frac{a}{2} D\right)}
$$

A Dirac operator satisfying this can be constructed:

$$
D=\frac{1}{a}\left(1+\gamma_{5} \operatorname{sign}\left(\gamma_{5} A\right)\right)
$$

A is some hermitian, real kernel operator e.g. Wilson fermion operator
sign function makes overlap fermions quite expensive.

## Fermions in lattice QCD - local updates

In pure gauge theory: $\quad \mathrm{Z}=\int D U e^{-S_{g}}$

Update proposal: change one link variable with a random SU(3) rotation
Action change calculated cheaply considering the 6 plaquettes which contain the link

Easily parallelisable

$$
\text { Cost to update all links: } O\left(N_{s}^{3} N_{t}\right)
$$

With fermions:

$$
Z=\int D U e^{-S_{s}} \operatorname{det} M\left[U_{v}\right]
$$

Determinant depends on all link variables $\longrightarrow$ Nonlocal action
Cost of determinant: $O\left(N^{3}\right)=O\left(N_{s}^{9} N_{t}^{3}\right)$
Cost to update all links: $O\left(N_{s}^{12} N_{t}^{4}\right)$

Action change very expensive, not parallelisable

## Hybrid Monte Carlo with pseudofermions

HMC: introduce momenta for all fields with trivial kinetic terms

$$
\begin{aligned}
& S\left[\phi_{i}\right] \rightarrow H_{H M C}\left[\phi_{i}, p_{i}\right]=S\left[\phi_{i}\right]+\sum \frac{p_{i}^{2}}{2} \\
& e^{-\beta S_{\text {нМС }}} \quad \text { Gaussian distribution for all momenta }
\end{aligned}
$$

To generate a new configuration:
-fill all momenta with gaussian random numbers
-integrate Canonical equations of motion numerically

$$
\dot{\phi}_{i}=\frac{\partial H}{\partial p_{i}}=p_{i} \quad \dot{p}_{i}=-\frac{\partial H}{\partial \phi}=-\frac{\partial S[\phi]}{\partial \phi_{i}}
$$

with stepsize $\Delta t$
from $t=0$ to $t=1$
-forget momenta: new configuration of $\phi$

Discretisation effects change distribution somewhat
An accept-reject step at the end gets rid of this stepsize dependence
$\Delta t$ small $\rightarrow$ energy conserved, $e^{-\Delta S} \approx 1 \rightarrow$ acceptance large
$\Delta t$ large $\rightarrow$ energy conservation imprecise, $e^{-\Delta S}<1 \rightarrow$ acceptance small

## Hybrid Monte Carlo with pseudofermions

Fermions give the determinant

We can do that with bosonic fields If we invert the matrix

$$
\begin{gathered}
\int d \eta d v e^{\eta M v}=\operatorname{det} M \\
\int \prod d \phi_{R, i} d \phi_{I, i} e^{-\phi_{i}^{t} M_{i}^{-1} \phi_{j}}=\operatorname{det} M
\end{gathered}
$$

For given $M, \phi$ has Gaussian distribution
Strategy:

1. Generate pseudofermion fields for given link variables from random generator
2. Update links using HMC
3. goto 1.

$$
\begin{array}{ll}
\text { Force calculation needs } M^{-1} \phi & \begin{array}{l}
\text { Calculated with } \\
\text { Conjugate gradient }
\end{array}
\end{array}
$$

Cost to update all links: $\approx O\left(\left(N_{s}^{3} N_{t}\right)^{5 / 4} m_{q}^{-\alpha}\right)$
Further improvements:
-Rational Hybrid Monte Carlo for rooting the determinant
-imprecise CG solution for HMC force calculation
-different HMC stepsizes for different mass quarks
-higher order discretisations of canonical eqs.
Etc.

## Costs of QCD lattice calculations

Cost to update all links: $\approx O\left(\left(N_{s}^{3} N_{t}\right)^{5 / 4} m_{q}^{-\alpha}\right) \quad \alpha \approx 4-6$
$\left(N_{s}^{3} N_{t}\right)^{5 / 4}$ as HMC stepsize needs to decrease as volume increases.

Fermions are expensive at smaller quark masses


More CG iterations needed
Fermion force larger
Calculate more often
Autocorrelation time increases

## Fermions in lattice QCD

$$
Z=\int D U e^{-S_{g}} \operatorname{det} M\left[U_{v}\right]
$$

Determinant depends on all link variables $\longrightarrow$ Nonlocal action

- Local metropolis update very inefficient

Solution 2: Langevin equation

## Langevin Equation (aka. stochatic quantisation)

Given an action $S(x)$

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

$$
\begin{aligned}
& \text { Gaussian noise } \\
& \langle\eta(\tau)\rangle=0 \\
& \left\langle\eta(\tau) \eta\left(\tau^{\prime}\right)\right\rangle=\delta\left(\tau-\tau^{\prime}\right)
\end{aligned}
$$

Random walk in configuration space

Averages are calculated along the trajectories:

$$
\langle O\rangle=\lim _{T \rightarrow \infty} \frac{1}{T} \int_{0}^{T} O(x(\tau)) d \tau=\frac{\int e^{-S(x)} O(x) d x}{\int e^{-S(x)} d x}
$$

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

## Fermions in lattice QCD

$$
Z=\int D U e^{-s_{0}} \operatorname{det} M\left[U_{v}\right]
$$

Determinant depends on all link variables $\longrightarrow$ Nonlocal action

- Local metropolis update very inefficient

Solution 2: Langevin equation
SU(3) Group manifold: $U(\tau+\Delta \tau)=\exp \left(i \lambda_{a}\left(\Delta \tau K_{a}+\sqrt{\Delta \tau} \eta_{a}\right)\right) U(\tau)$
Drift term $K_{a}=-D_{a} S[U]$ noise: $\left\langle\eta_{a} \eta_{b}\right\rangle=2 \delta_{a b}$
Fermionic Drift from noise vectors: $\left\langle\psi_{a i}^{*}(x) \psi_{b j}(x)\right\rangle=\delta_{a b} \delta_{i j} \delta_{x y}$

$$
K_{a x v, F}=D_{a x v}\left(\ln \operatorname{det} M^{N_{F}}\right)=N_{F} \operatorname{Tr}\left(\left(D_{a x v} M\right) M^{-1}\right)=N_{F}\left\langle\psi^{+}\left(D_{a x v} M\right) M^{-1} \psi\right\rangle
$$

Needs 1 Conjugate gradient inversion per update

## Langevin vs HMC for lattice QCD

## HMC:

- 1 CG per fermion per update
- rooting requires rational Hybrid Monte Carlo
- distance to previous configuration $\simeq \tau$ momenta refreshed after every trajectory
- easy to decrease costs for heavy fermions
- no stepsize dependence


## Langevin:

- 1 CG per fermion per update
- rooting is trivial
- distance to previous configuration $\simeq \sqrt{\tau}$
- Stepsize needs to be extrapolated to zero

Nowadays HMC is used (almost?) exclusively at zero chemical potential

## Chemical potential in the continuum

Fermion action: $\quad S=\int_{0}^{1 / T} \int d^{3} x \bar{\psi}\left(\gamma_{v} \partial_{v}+m\right) \psi$
This action has the symmetry: $\psi \rightarrow e^{i \omega} \psi \quad \bar{\psi} \rightarrow e^{-i \omega} \bar{\psi}$
Corresponding conserved charge: $\quad N=\int d^{3} x \bar{\psi} \gamma_{4} \psi=\int d^{3} x \psi^{+} \psi$
We want grand canonical potential $\quad \mathrm{Z}=e^{-\beta(H-\mu N)}$

$$
\frac{\mu N}{T}=\int_{0}^{\beta} d \tau \int d^{d} x \mu \bar{\psi} \gamma_{4} \psi
$$

So the action becomes: $\quad S=\int_{0}^{1 / T} \int d^{3} x \bar{\psi}\left(\gamma_{v}\left(\partial_{v}+i A_{\mu}\right)+\mu \gamma_{4}+m\right) \psi=\int \bar{\psi} M \psi$
At $\mu=0 \quad \gamma_{5}$-Hermiticity: $\left(\gamma_{5} M\right)^{+}=\gamma_{5} M$

$$
(\operatorname{det} M)^{*}=\operatorname{det} M^{+}=\operatorname{det}\left(\gamma_{5} M \gamma_{5}\right)=\operatorname{det} M \rightarrow \operatorname{det} M \text { is real }
$$

At $\mu \neq 0 \quad M^{+}(\mu)=\gamma_{5} M\left(-\mu^{*}\right) \gamma_{5}$

$$
\operatorname{det}\left(M\left(U,-\mu^{*}\right)\right)=(\operatorname{det}(M(U), \mu))^{*} \quad \text { Determinant is complex }
$$

## Chemical potential in the continuum

## Fermions: At zero mu determinant is real

For staggered at zero mu, it can be shown that det is positive
For Wilson at zero mu
sometimes the determinant is negative ("exceptional configs.") in the continuum limit exceptional configs don't appear

## At nonzero mu

the action becomes: $\quad S=\int_{0}^{1 / T} \int d^{4} x \bar{\psi}\left(\gamma_{v}\left(\partial_{v}+i A_{\mu}\right)+\mu \gamma_{4}+m\right) \psi=\int \bar{\psi} M \psi$

$$
\operatorname{det}\left(M\left(U,-\mu^{*}\right)\right)=(\operatorname{det}(M(U), \mu))^{*} \quad \text { Determinant is complex }
$$

Chemical potential appears as imaginary Abelian gauge field in temporal direction

Imaginary chemical potential $\longrightarrow$ Determinant is real again

## Chemical potential in the continuum

$\mathrm{U}(1)$ symmetric bosons

$$
S=\int d^{4} x\left(\left|\partial_{\nu} \phi\right|^{2}+m^{2}|\phi|^{2}\right)+\lambda|\phi|^{4} \quad \text { Symmetry: } \phi \rightarrow e^{i \alpha} \phi
$$

Conserved charge: $\quad N=\int d^{3} x i\left(\phi^{*} \partial_{4} \phi-\left(\partial_{4} \phi^{*}\right) \phi\right)$
$Z=e^{-\beta(H-\mu N)} \quad$ Leads to:

$$
\begin{aligned}
& S=\int d^{4} x\left[\left(\partial_{4}+\mu\right) \phi^{*}\left(\partial_{4}-\mu\right) \phi+\partial_{i} \phi^{*} \partial_{i} \phi+m^{2}\left|\phi^{2}\right|+\lambda\left|\phi^{4}\right|\right] \\
& S=\int d^{4} x\left[\left|\partial_{v} \phi^{2}\right|+\left(m^{2}-\mu^{2}\right)\left|\phi^{2}\right|+\mu\left(\phi^{*} \partial_{4} \phi-\left(\partial_{4} \phi^{*}\right) \phi\right)+\lambda\left|\phi^{4}\right|\right]
\end{aligned}
$$

Bosons also have a quadratic term in the chemical potential
Linear term is imaginary $\quad S(\mu)=S(-\mu)^{*}$
Imaginary $\mu \rightarrow$ Action is real

## Chemical potential on the lattice

How does $\mu$ appear in lattice QCD?
adding $\mu \bar{\phi} \gamma_{4} \psi$ to the action $\rightarrow$ ultraviolet divergences
Instead we add it as an imaginary Abelian vectorfield
Forward hopping terms: $e^{i A_{4}}=e^{a \mu}$
Backward hopping terms: $e^{-i A_{4}}=e^{-a \mu}$
Complex determinant at nonzero $\mu$
$M^{+}(\mu)=\gamma_{5} M\left(-\mu^{*}\right) \gamma_{5}$ remains valid on the lattice
$\mu$ Couples to conserved charge $\longrightarrow$ no divergences appear

[Fig: Aarts]

Closed loops don't change
Forward loops gain factor $e^{a u N t}$
Backward loops gain factor $e^{-q u N t}$

$$
a N_{t}=\frac{1}{T} \rightarrow a \mu N_{t}=\frac{\mu}{T}
$$

## Importance Sampling

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

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

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 $\mathrm{C} \quad p(C) \sim W[C]$

$$
\langle X\rangle=\frac{1}{Z} \operatorname{Tr} X e^{-\beta(H-\mu N)}=\frac{1}{Z} \sum_{C} W[C] X[C]=\frac{1}{N} \sum_{i} X\left[C_{i}\right]
$$

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

Otherwise we have a Sign problem

## Toy model with sign problem

$$
Z=\int_{-\infty}^{\infty} e^{-\left(\sigma x^{2}+i \lambda x\right)} d x \quad\left\langle x^{2}\right\rangle=\frac{1}{Z} \int x^{2} e^{-\left(\sigma x^{2}+i \lambda x\right)} d x=?
$$

Sampling method: draw uniform random

$$
-a \leqslant x_{i} \leqslant a
$$

$$
\int_{-a}^{a} f(x) d(x) \approx \frac{1}{N} \sum_{i} f\left(x_{i}\right)
$$



$$
\sigma=\sqrt{2}, \lambda=0
$$



$$
\sigma=1+i, \quad \lambda=20
$$

100 samples to have $10 \%$ relative error

$$
\Delta \sim \frac{1}{\sqrt{N}}
$$

## Sign problems

## Real-time evolution in QFT

"strongest" sign problem
$e^{i S}$


Non-zero density

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

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

Theta therm

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



And everything else with complex action

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

## Inbalanced Fermi gas



## How to solve the sign problem?

Probably no general solution - There are sign problems which are NP hard

Many solutions for particular models with sign problem exist
Sign problem is representation dependent!
if $Z>0$ probably a real representation exists
need to find the "right" degrees of freedom

## How to solve the sign problem?

Probably no general solution - There are sign problems which are NP hard
[Troyer Wiese (2004)]

Many solutions for particular models with sign problem exist
Sign problem is representation dependent!
if $Z>0$ probably a real representation exists need to find the "right" degrees of freedom

Transforming the problem to one with positive weights

$$
\begin{array}{cc}
Z=\operatorname{Tr} e^{-\beta(H-\mu N)}=\sum_{C} W[C]=\sum_{D} W^{\prime}[D] & \text { Dual variables } \\
Z=\operatorname{Tr} e^{-\beta(H-\mu N)}=\sum_{n} Z_{n} e^{\beta \mu n} & \text { Worldlines } \\
Z=\operatorname{Tr} e^{-\beta(H-\mu N)}=\int d E \rho_{\mu}(E) e^{-\beta E} & \text { Denonical ensemble } \\
Z=\operatorname{Tr} e^{-\beta(H-\mu N)}=\sum_{C} W[C]=\sum_{S}\left(\sum_{C \in S} W[C]\right) & \text { Subsets }
\end{array}
$$

How to solve the sign problem?
Extrapolation from a positive ensemble
Reweighting $\langle X\rangle_{W}=\frac{\sum_{c} W_{c} X_{c}}{\sum_{c} W_{c}}=\frac{\sum_{c} W^{\prime}{ }_{c}\left(W_{c} / W^{\prime}{ }_{c}\right) X_{c}}{\sum_{c} W^{\prime}{ }_{c}\left(W_{c} / W^{\prime}{ }_{c}\right)}=\frac{\left\langle\left(W / W^{\prime}\right) X\right\rangle_{W^{\prime}}}{\left\langle W / W^{\prime}\right\rangle_{W^{\prime}}}$
Taylor expansion $\quad Z(\mu)=Z(\mu=0)+\frac{1}{2} \mu^{2} \partial_{\mu}^{2} Z(\mu=0)+\ldots$

Analytic continuation from imaginary sources
(chemical potentials, theta angle,imaginary time,..)
Using analyticity (for complexified variables)
Complex Langevin
Complexified variables - enlarged manifolds

Lefschetz thimble
Integration path shifted onto complex plane

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

Taylor extrapolation, Reweighting, continuation from imaginary $\mu$, canonical ens. all break down around

$$
\frac{\mu_{q}}{T} \approx 1-1.5 \quad \frac{\mu_{B}}{T} \approx 3-4.5
$$

Around the transition temperature Breakdown at $\quad \mu_{q} \approx 150-200 \mathrm{MeV} \quad \mu_{B} \approx 450-600 \mathrm{MeV}$

Results on
$N_{T}=4, N_{F}=4, m a=0.05$
using
Imaginary mu,
Reweighting,
Canonical ensemble

Agreement only at $\mu / T<1$


## Reweighting

$$
\begin{gathered}
\langle F\rangle_{\mu}=\frac{\int D U e^{-S_{E}} \operatorname{det} M(\mu) F}{\int D U e^{-S_{E}} \operatorname{det} M(\mu)}=\frac{\int D U e^{-S_{E}} \operatorname{det} M(\mu=0) \frac{\operatorname{det} M(\mu)}{\operatorname{det} M(\mu=0)} F}{\int D U e^{-S_{E}} \operatorname{det} M(\mu=0) \frac{\operatorname{det} M(\mu)}{\operatorname{det} M(\mu=0)}} \\
=\frac{|F \operatorname{det} M(\mu) / \operatorname{det} M(\mu=0)|_{\mu=0}}{\langle\operatorname{det} M(\mu) / \operatorname{det} M(\mu=0)\rangle_{\mu=0}}
\end{gathered}
$$

$$
\left.\left.\left|\frac{\operatorname{det} M(\mu)}{\operatorname{det} M(\mu=0)}\right|_{\mu=0}=\frac{Z(\mu)}{Z(\mu=0)}=\exp \right\rvert\,-\frac{V}{T} \Delta f(\mu, T)\right)
$$

$\Delta f(\mu, T)=$ free energy density difference

Exponentially small as the volume increases $\langle F\rangle_{\mu} \rightarrow 0 / 0$
Reweighting works for large temperatures and small volumes
Sign problem gets hard at $\quad \mu / T \approx 1$

## Reweighting

Overlap problem
If the two ensembles are far, most configurations are far from the peak of the target distribution

Reweighting factor $\frac{\operatorname{det} M(\mu)}{\operatorname{det} M(0)}$ has long tailed distribution
Most configs have small weight, averages are dominated by a few configs

- even errorbars are untrustworthy

Explicit calculation of determinant Is expensive

$$
O\left(N_{s}^{9} N_{t}^{3}\right)
$$

Sign problem has exponential volume depence
$\longrightarrow$ Volume is limited


## Silver blaze

At low temperature, system is in the ground state

$$
\langle X\rangle=\operatorname{Tr}\left(X e^{-\beta(H-\mu N)}\right) \approx\langle 0| X e^{-\beta(H-\mu N)}|0\rangle
$$

No dependence on the chemical potential

If chemical potential reaches mass of the lightes excitation

- onset transition

Reweighting from phase quanched theory $\int D U e^{-S_{g}}|\operatorname{det} M(\mu)|$
we have $u$ and d quarks: $\quad|\operatorname{det} M(\mu)|^{2}=\operatorname{det} M(\mu) \operatorname{det} M(-\mu)$
$u$ and d has opposite chemical potentials

Phasequenched theory $\longrightarrow$ nonzero isospin chemical potential pions have nonzero isospin charge

## Silver blaze in QCD

Lightest excitation in phasequenched theory:
pion
Onset: $\mu_{c, P Q}=m_{\pi} / 2$

Lightest excitation in baryon chemical pot. theory: proton
Onset: $\mu_{c}=m_{n} / 3$

$$
0<\mu<m_{\pi} / 2
$$

PQ theory in ground state
Full theory in ground state

$$
m_{\pi} / 2<\mu<m_{n} / 3
$$

PQ theory has pion condensate Full theory in ground state

$$
\mu>m_{n} / 3
$$

PQ theory has pion condensate Full theory has nuclear matter
phase average close to 1 mild sign problem
nontrivial cancellations given by phase factors hard sign problem
theories different, hard sign problem

Silver blaze is a good test for methods claiming to solve the sign problem

## Taylor Expansion

$\ln Z(\mu)=\ln Z(0)+\frac{\mu^{2}}{2} \frac{\partial^{2} \ln Z}{\partial \mu^{2}}+\frac{\mu^{4}}{24} \frac{\partial^{4} \ln Z}{\partial \mu^{4}}+\ldots$

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

$Z(\mu)=Z(-\mu) \rightarrow$ only even powers appear

$$
\text { Pressure: } \quad \frac{p}{T^{4}}=\frac{\ln Z}{V T^{3}}
$$

density $=\frac{1}{2} \frac{1}{N_{s}^{3} N_{t}} \frac{\partial \ln Z}{\partial \mu} \quad$ Nonvanishing only at nonzero $\mu$
Charge fluctuations:

$$
c_{2}=\frac{1}{2} \frac{N_{T}}{N_{s}^{3}} \frac{\partial^{2} \ln Z}{\partial \mu^{2}}
$$

Higher order fluctuation related to kurtosis

$$
c_{4}=\frac{1}{24} \frac{1}{N_{s}^{3} N_{T}} \frac{\partial^{4} \ln Z}{\partial \mu^{4}}
$$

$\mu$ dependence of observable: $\partial_{\mu}\left(\frac{1}{Z} \int D U e^{-s} X\right) \simeq\langle X n\rangle$
At higher order again correlators, fluctuations appear

Measuring the coefficients of the Taylor expansion

$$
\begin{aligned}
& \frac{\partial^{2} \ln Z}{\partial \mu^{2}}=N_{F}^{2}\left\langle T_{1}^{2}\right\rangle+N_{F}\left\langle T_{2}\right\rangle \\
& \frac{\partial^{4} \ln Z}{\partial \mu^{4}}=-3\left(\left\langle T_{2}\right\rangle+\left\langle T_{1}^{2}\right\rangle\right)^{2}+3\left\langle T_{2}^{2}\right\rangle+\left\langle T_{4}\right\rangle \\
& +\left\langle T_{1}^{4}\right\rangle+4\left\langle T_{3} T_{1}\right\rangle+6\left\langle T_{1}^{2} T_{2}\right\rangle \\
& T_{1} / N_{F}=\operatorname{Tr}\left(M^{-1} \partial_{u} M\right) \\
& T_{i+1}=\partial_{u} T_{i} \\
& T_{2} / N_{F}=\operatorname{Tr}\left(M^{-1} \partial_{\mu}^{2} M\right)-\operatorname{Tr}\left(\left(M^{-1} \partial_{\mu} M\right)^{2}\right) \\
& T_{3} / N_{F}=\operatorname{Tr}\left(M^{-1} \partial_{\mu}^{3} M\right)-3 \operatorname{Tr}\left(M^{-1} \partial_{\mu} M M^{-1} \partial_{\mu}^{2} M\right) \\
& +2 \operatorname{Tr}\left(\left(M^{-1} \partial_{\mu} M\right)^{3}\right) \\
& T_{4} / N_{F}=\operatorname{Tr}\left(M^{-1} \partial_{\mu}^{2} M\right)-4 \operatorname{Tr}\left(M^{-1} \partial_{\mu} M M^{-1} \partial_{\mu}^{3} M\right) \\
& -3 \operatorname{Tr}\left(M^{-1} \partial_{\mu}^{2} M M^{-1} \partial_{\mu}^{2} M\right)-6 \operatorname{Tr}\left(\left(M^{-1} \partial_{\mu} M\right)^{4}\right) \\
& +12 \operatorname{Tr}\left(\left(M^{-1} \partial_{\mu} M\right)^{2} M^{-1} \partial_{\mu}^{2} M\right)
\end{aligned}
$$

To compare to heavy ion experiments, chemical potentials are needed for conserved charges:

Baryon: $\mu^{B} \quad$ Strangeness: $\mu^{S}$ Electric: $\mu^{Q}$
Higher order fluctuations $\quad \chi_{i, j, k}^{B, Q, S}=\frac{\partial^{i+j+k}\left(p / T^{4}\right)}{\left(\partial \mu^{B}\right)^{i}\left(\partial \mu^{Q}\right)^{j}\left(\partial \mu^{S}\right)^{k}}$
Fluctuations are expected to diverge in the victinity of a critical point
Subject of intense experimental and theoretical work

[Fig: BW collaboration]
Up to $8^{\text {th }}$ order fluctuations calculated on the lattice

## Freezout temperature

To cancel out volume dependce, one looks at ratios, e.g.:

$$
\begin{aligned}
R_{12}^{B}\left(T, \mu_{B}\right)=\frac{M_{B}}{\sigma_{B}^{2}} & =\frac{\chi_{1}^{B}\left(T, \mu_{B}\right)}{\chi_{2}\left(T, \mu_{B}\right)} \quad R_{31}^{B}\left(T, \mu_{B}\right)=\frac{S_{B} \sigma_{B}^{3}}{M_{B}} \frac{\chi_{3}^{B}\left(T, \mu_{B}\right)}{\chi_{1}\left(T, \mu_{B}\right)} \\
R_{31}\left(R_{12}\right) & \rightarrow \text { no need to measure } T, \mu
\end{aligned}
$$

STAR data fits well with lattice data from pseudocritical line

Higher order fluctuations noisy from both sides possible tension

## Imaginary chemical potentials

No sign problem at imaginary chemical potentials

$$
\operatorname{det}\left(M\left(U,-\mu^{*}\right)\right)=(\operatorname{det}(M(U), \mu))^{*}
$$



Fit function unknown $\longrightarrow$ systematic error
Loses predictivity around $\mu_{B} / T \simeq 3 \quad \mu_{q} / T \simeq 1$

Transition Temperature

At zero $\mu$ transition is crossover Ambigous definitions nevertheless converge in cont.lim.

Pseudocritical line:
$\frac{T_{c}\left(\mu_{B}\right)}{T_{c}(0)}=1-\kappa_{2}\left(\frac{\mu_{B}}{T_{c}}\right)^{2}-\kappa_{4}\left(\frac{\mu_{B}}{T_{c}}\right)^{4}+O\left(\mu_{B}^{6}\right)$

## Critical endpoint?

What seems to be clear so far (for physical quark masses):

No critical point at $\quad \mu_{B} / T<3 \quad \mu_{q} / T<1$
(in the reach of extrapolation methods: Taylor, reweighting, imaginary mu)

Attempts to locate it:
Reweighting
Small lattices Out of the range of expected validity

Convergence radius

[Fodor,Katz(2002)]

Various estimators for Taylor expansions
Could also signal other singularities on complex plane: Lee-Yang zeroes, Roberge-Weiss

$$
r_{2 n}=\sqrt{\frac{\chi_{2 n}}{\chi_{2 n+2}}}
$$

$$
r_{k}=\left|\frac{2}{2 k c_{2 k}+k^{2} c_{k}^{2}}\right|^{\frac{1}{2 k}}
$$

No solid results so far

## Columbia Plot

What would be the phase transition at zero mu be like If we could change the quark masses

Useful tool to understand possible phase transitions

Pure gauge: $Z_{3}$ symmetric change temporal links on a time slice $U_{t} \rightarrow z U_{t} \quad z=e^{i 2 \pi k / N_{c}}$ center of $\operatorname{SU}(\mathrm{N})$

Spontaneously broken in first order transition
quarks give explicit breaking


## Center symmetry and imaginary chemical potential

$$
U_{t} \rightarrow z U_{t} \quad U_{t}^{-1}=z^{-1} U_{t} \quad z=e^{i 2 \pi k / N_{c}}
$$

Chemical potential dependence of Dirac matrix
Can be transformed to a single time-slice
with $\mu_{I}$ temporal links in the Dirac matrix get extra factor:

$$
U_{t} \rightarrow e^{i N_{t} \mu_{t}} U_{t} \quad U_{t}^{-1} \rightarrow e^{-i N_{t} \mu_{t}} U_{N_{t}}^{-1}
$$

equivalent to center transformation if $\frac{\mu_{I}}{T}=\frac{2 \pi k}{N_{c}}$
Roberge-Weiss symmetry: $\quad Z\left(\frac{\mu}{T}\right)=Z\left(\frac{\mu}{T}+\frac{i 2 \pi k}{N_{c}}\right)$
Configurations in the different sectors are center transformed
At large temperatures where Polyakov loop is nonzero phase boundaries thus must exist: Rogerge-Weiss transition

Polyakov loop is order parameter

## Phase diagram in $\mu_{I}-T$ plane



On Temperature axis, there is also a transition

Is it connected with the RW-transition?

## Different scenarios

according to quark masses



Columbia plot extended with $\mu^{2}$ axis


## [Bonati et.al (2012)]

First order region seems to shrink at real $\mu$
Results for heavy quark effective theories for $N_{F}=3$ Tricritical scaling accurately reproduced



## Nonzero density on the lattice

## Dénes Sexty

KFU Graz


12-13.05.2022. DK-PI Retreat

1. Lattice QCD - nonzero density in lattice QCD - sign problem
2. Reweighting - Taylor expansion - imaginary mu
3. Complex Langevin and Lefschetz thimbles

## Importance Sampling

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

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

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 $\mathrm{C} \quad p(C) \sim W[C]$

$$
\langle X\rangle=\frac{1}{Z} \operatorname{Tr} X e^{-\beta(H-\mu N)}=\frac{1}{Z} \sum_{C} W[C] X[C]=\frac{1}{N} \sum_{i} X\left[C_{i}\right]
$$

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

Otherwise we have a Sign problem

## Langevin Equation (aka. stochatic quantisation)

Given an action $S(x)$

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

$$
\begin{aligned}
& \text { Gaussian noise } \\
& \langle\eta(\tau)\rangle=0 \\
& \left\langle\eta(\tau) \eta\left(\tau^{\prime}\right)\right\rangle=\delta\left(\tau-\tau^{\prime}\right)
\end{aligned}
$$

Random walk in configuration space

Averages are calculated along the trajectories:

$$
\langle O\rangle=\lim _{T \rightarrow \infty} \frac{1}{T} \int_{0}^{T} O(x(\tau)) d \tau=\frac{\int e^{-S(x)} O(x) d x}{\int e^{-S(x)} d x}
$$

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

## Complex Langevin Equation

Given an action $S(x)$

$$
\text { Stochastic process for } \mathrm{x}: \quad \frac{d x}{d \tau}=-\frac{\partial S}{\partial x}+\eta(\tau) \quad \begin{aligned}
& \begin{array}{l}
\langle\eta(\tau)\rangle=0 \\
\left\langle\eta(\tau) \eta\left(\tau^{\prime}\right)\right\rangle=\delta\left(\tau-\tau^{\prime}\right)
\end{array}
\end{aligned}
$$

Averages are calculated along the trajectories:

$$
\langle O\rangle=\lim _{T \rightarrow \infty} \frac{1}{T} \int_{0}^{T} O(x(\tau)) d \tau=\frac{\int e^{-S(x)} O(x) d x}{\int e^{-S(x)} d x}
$$

The field is complexified

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

real scalar $\longrightarrow$ complex scalar
link variables: $\underset{\text { compact }}{\operatorname{SU}(N)} \underset{\text { non-compact }}{\text { SL(N,C) }}$

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

Analytically continued observables

$$
\begin{gathered}
\frac{1}{Z} \int P_{\text {comp }}(x) O(x) d x=\frac{1}{Z} \int P_{\text {real }}(x, y) O(x+i y) d x d y \\
\left\langle x^{2}\right\rangle_{\text {real }} \rightarrow\left\langle x^{2}-y^{2}\right\rangle_{\text {complexificed }}
\end{gathered}
$$

## Lefschetz Thimble

Transform integral by shifting contour

$$
\int_{-\infty}^{\infty} d x e^{s(x)} F(x)=\int_{C} d z e^{s(z)} F(z)=\int d t\left(\frac{d z}{d t}\right) e^{s(z(t))} F(z(t))
$$

$\begin{array}{ll}\text { Better than the original contour if } & e^{\operatorname{Re}(S(z(t)))} \text { peak + fast decay } \\ & e^{i \operatorname{Im}(S(z(t)))} \text { milder sign problem than original }\end{array}$

$$
\operatorname{Im}(S(z(t)))=\text { const } \longleftrightarrow \text { steepest descent of } \operatorname{Re}(S(z(t)))
$$

Thanks to Cauchy-Riemann equations

Lefschetz thimble is a contour which starts from saddle points $\partial_{z} S\left(z_{0}\right)=0$

$$
\begin{aligned}
& \frac{\partial z}{\partial t}= \pm \overline{\partial_{z} S(z)} \\
& z \rightarrow z_{0} \text { for } t \rightarrow \infty
\end{aligned}
$$

+ : stable thimble $\downarrow>$ steepest descent
$-:$ unstable thimble $\downarrow$ steepest ascent

$$
Z=\sum_{k} m_{k} e^{-\operatorname{Im} S\left(z_{k}\right)} \int_{T_{k}} d z e^{\operatorname{Re} S(z)}=\sum_{k} m_{k} e^{-\operatorname{Im} S\left(z_{k}\right)} \int_{T_{k}} d t \frac{d z}{d t} e^{\operatorname{Re} S_{k}(t)}
$$

Intersection number (Morse theory)


Residual sign problem from curvature of thimble Is it mild? Is it exponential in the volume?

Global sign problem Easy as long as few thimbles contribute
[Fig: Scorzato]

For large systems: $\quad \sum_{k} m_{k} T_{k} \rightarrow T_{0}$
Choose thimble with the global minimum Regularisation of QFT Resurgence

## Langevin and Lefschetz

Both use analiticity and complexifcation
Direct simulation of complex actions is possible

## Complex Langevin Eq.

Allow complex drift in Langevin eq.

Complexify the field manifold Dimensions are doubled

Check for convergence

$$
\begin{gathered}
\frac{1}{Z} \int P_{\text {comp }}(x) O(x) d x= \\
\frac{1}{Z} \int P_{\text {real }}(x, y) O(x+i y) d x d y
\end{gathered}
$$

## Lefschetz thimble

Shift integration contour into complex plane

Look for critical points, Find contributing thimbles

Reweight the residual sign problem

$$
\begin{gathered}
\frac{1}{Z} \int P_{\text {comp }}(x) O(x) d x= \\
\frac{1}{Z} \int_{T} P_{\text {comp }}(z) O(z) d z
\end{gathered}
$$

## Gaussian Example

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

## CLE

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

$\nabla$

$$
P(x, y)=e^{-a\left(x-x_{0}\right)^{2}-b\left(y-y_{0}\right)^{2}-c\left(x-x_{0}\right)\left(y-y_{0}\right)}
$$

Gaussian distribution around critical point

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



Measure on real axis


## Thimbles in practice

Finding the thimbles is easy in toy models - hard on the lattice
Need to search critical points and zeroes of the measure
Thimble structure changes qualitatively as parameters of the action change Numerically it is costly to parametrize the thimble, calculate Jacobian

Example:

$$
S=-\beta \cos (z)-\ln (1+\kappa \cos (z-i \mu))
$$



$$
\beta=1, \mu=1, \kappa=1 / 2
$$

$$
\beta=1, \mu=1, \kappa=2
$$

## Sign optimized manifolds

Transform integral by shifting contour

$$
\int_{-\infty}^{\infty} d x e^{s(x)} F(x)=\int_{C} d z e^{s(z)} F(z)=\int d t\left(\frac{d z}{d t}\right) e^{s(z(t))} F(z(t))
$$

In some cases it is advantegous to not go to the thimble.

- hard to parametrize numerically
- multiple contributing thimbles

If we have a map of Real manifold $\longrightarrow$ Complexified manifold such that

- Easy to parametrize
- Jacobian is cheap
- Residual sign problem is mild

Cost of simulations is better that both Real manifold and Thimbles
Parametrize using e.g. neural networks Finite flow time Ansatz

$$
\frac{\partial z}{\partial t}= \pm \overline{\partial_{z} S(z)}
$$

Thirring model on sign-optimized manifold
$S=\sum_{x, v} \frac{N_{F}}{g^{2}}\left(1-\cos \left(A_{x v}\right)\right)+\sum_{x, y} \bar{\psi}_{x} D_{x y}(A, \mu) \psi_{y}$
$D_{x y}(A, \mu)=$ staggered fermion matrix, $\quad \operatorname{det}(D) \in \mathbb{C}$

Parametrize new manifold as: $\quad \widetilde{A}_{0}=A_{0}+i\left(\lambda_{0}+\lambda_{1} \cos \left(A_{0}\right)+\lambda_{2} \cos \left(2 A_{0}\right)\right)$

$$
\widetilde{A}_{1}=A_{1} \quad \widetilde{A}_{2}=A_{2}
$$

Search for the minimum of $\left\langle e^{i \varphi}\right\rangle_{P Q}$ numerically, fixing $\lambda_{0}, \lambda_{1}, \lambda_{2}$


## Lefschetz thimbles

Need to find contributing thimbles Or define sign-improved manifold.

How to cheaply parametrize the new manifolds?
How to cheaply simulate on the new manifolds - Jacobian determinant has to be cheap

Is the residual sign problem still exponential in the volume?
If one wants lattice sizes e.g. $16^{4}$ to work,

$$
\text { simulation on } 4^{4} \text { has to have }\left\langle e^{i \varphi}\right\rangle \approx 0.999
$$

Models studied so far:
Toy models, lattice models: fermionic models (Thirring), Bose gas.
First attempts at tackling gauge symmetry

## U(1) One plaquette model with CLE

Using the action $S_{p}=i \beta \cos (\varphi)+i p \varphi$
Langevin equation: $\frac{d \varphi}{d \tau}=-i \beta \sin \varphi+i p+n(\tau)$
Correct results obtained for $\langle\exp (i \varphi)\rangle$ in the region: $\beta \leq p$


## Flowchart: normalized drift vectors

 on the complex plane
## shows fixedpoint (zero drift term)

 structure on the complexp plane

Attractive fixedpoint present
Fast decay correct results

$$
\beta=0.5, p=1
$$



No attractive fixedpoint present (only indifferent) slow decay incorrect results

$$
\beta=1.5, p=1
$$



## Gauge theories and CLE

$$
\begin{array}{ll}
\text { link variables: } \operatorname{SU}(\mathbb{N}) & \text { RL(N,C) } \\
\text { compact } & \text { non-compact } \\
\operatorname{det}(U)=1, \quad U^{+} \neq U^{-1}
\end{array}
$$

Gauge degrees of freedom also complexify

Infinite volume of irrelevant, unphysical configurations
Process leaves the $\operatorname{SU}(\mathrm{N})$ manifold exponentially fast already at $\mu \ll 1$

Unitarity norm:
Distance from SU(N)

$$
\begin{aligned}
& \sum_{i} \operatorname{Tr}\left(U_{i} U_{i}^{+}\right) \\
& \sum_{i j}\left|\left(U U^{+}-1\right)_{i j}\right|^{2} \\
& \operatorname{Tr}\left(U U^{+}\right)+\operatorname{Tr}\left(U^{-1}\left(U^{-1}\right)^{+}\right) \geq 2 N
\end{aligned}
$$

## Gauge cooling

Minimize unitarity norm Distance from SU(N)

$$
\sum_{i} \operatorname{Tr}\left(U_{i} U_{i}^{+}-1\right)
$$

Gauge transformation along
Steepest descent


Gauge cooling
keeps 'skirts' from developing
ensuring correct results


Empirical observation: Cooling is effective for

$$
\begin{aligned}
& \beta>\beta_{\text {min }} \\
& a<a_{\text {max }}
\end{aligned}
$$

but remember, $\beta \rightarrow \infty$ in cont. limit
$a_{\max } \approx 0.1-0.2 \mathrm{fm}$

## Argument for correctness of CLE results

If there is fast decay $\quad P(x, y) \rightarrow 0$ as $x, y \rightarrow \infty$
and a holomorphic action $S(x)$
then CLE converges to the correct result
[Aarts, Seiler, Stamatescu (2009)
Aarts, James, Seiler, Stamatescu (2011)]

Loophole 1: Non-holomorphic action for nonzero density

$$
S=S_{W}\left[U_{\mu}\right]+\ln \operatorname{Det} M(\mu)
$$

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

No problems if poles are not 'touched' by distribution satisfied for: HDQCD, full QCD at high temperatures

[Aarts, Seiler, Sexty, Stamatescu '17]

## Loophole 2: decay not fast enough

## 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' $Y \rightarrow \infty$

Observable cheap also for lattice systems

Measuring "corrected observable" in case boundary term nonzero
$P(x, y, t)$ : probability density on the complex plane at Langevin time $t$ $\rho(x)=\frac{1}{Z} e^{-S(x)}$ : complex measure

CLE works, if

$$
\begin{aligned}
& \text { What we want } \quad \text { What we get with CLE } \\
& \int d x \rho(x) O(x)=\int d x d y P(x, y) O(x+i y)
\end{aligned}
$$

Interpolating function:

$$
\begin{gathered}
F(t, \tau)=\int P(x, y, t-\tau) O(x+i y, \tau) d x d y \\
F(t, 0)=\langle O(x+i y)\rangle_{\rho(t)} \quad F(t, t)=\ldots=\langle O(x)\rangle_{\rho(t)} \\
\partial_{\tau} F(t, \tau)=0 \Rightarrow \text { CLE is correct }
\end{gathered}
$$

## Boundary terms as a volume integral

Calculating an observable defined on a compact boundary in many dimensions can be inconvenient

$$
\begin{aligned}
& \partial_{\tau} F_{o}(Y, t, \tau=0)=B_{O}(Y, t, \tau=0)= \\
& \quad \int_{-Y}^{Y} P(x, y, t) L_{c} O(x+i y)-\int_{-Y}^{Y}\left(L^{T} P\right) O(x+i y, 0)
\end{aligned}
$$

Observable with a cutoff easy to do in many dimensions

$$
L_{c} O(x+i y) \text { consistency conditions } \quad \approx \text { Schwinger-Dyson eqs. }
$$

Order of limits crucial

$$
\lim _{t \rightarrow \infty} \lim _{Y \rightarrow \infty} \int_{-Y}^{Y} P(x, y, t) L_{c} O(x+i y) \text { can be undefined }
$$

One plaquette model

$$
S(x)=i \beta \cos (x)+\frac{s}{2} x^{2}
$$

## Full QCD

Boundary term for spatial plaquettes


last point with no cutoff large fluctuations consistent with zero?

## Unambigous detection of boundary terms

Observable cheap also for lattice systems

## Correcting CLE using boundary terms



Interpolation function

$$
F(t, \tau)=\sum A_{n} \exp \left(-\omega_{n} \tau\right)
$$

## Ansatz

$$
F(t, \tau)=A_{0}+A_{1} \exp \left(-\omega_{1} \tau\right)
$$

Higher order boundary terms

$$
\frac{\partial^{n} F(t, \tau)}{\partial \tau^{n}}=B_{n}=\left\langle L_{c}^{n} O\right\rangle
$$

Systematic error of CLE

$$
F(t, 0)-F(t, t)=B_{1}^{2} / B_{2}
$$

Test in $\mathrm{U}(1)$ toy model

$$
S(x)=i \beta \cos (x)+\frac{s}{2} x^{2}
$$

## Measuring $B_{1,} B_{2}$ allows correction of results

 when CLE fails| $\beta, s$ | $B_{1}$ | $B_{2}$ | $B_{1}^{2} / B_{2}$ | CL error | CL | correct | corrected CL |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $0.1,0$ | $-0.04859(45)$ | $0.0493(11)$ | $0.04786(79)$ | $0.04891(45)$ | $-0.00115(45)$ | -0.05006 | $-0.04901(62)$ |
| $0.1,0.01$ | $-0.01795(49)$ | $0.01801(80)$ | $0.01789(60)$ | $0.01689(50)$ | $-0.03318(50)$ | -0.05006 | $-0.05106(40)$ |
| $0.1,0.1$ | $-0.00048(30)$ | $0.00057(35)$ | $0.00039(28)$ | $0.00049(31)$ | $-0.04957(31)$ | -0.05006 | $-0.04997(6)$ |
| $0.5,0$ | $-0.2474(11)$ | $0.237(11)$ | $0.258(11)$ | $0.25818(23)$ | $0.00003(23)$ | -0.25815 | $-0.258(11)$ |
| $0.5,0.3$ | $-0.05309(86)$ | $0.0552(51)$ | $0.0507(41)$ | $0.04183(70)$ | $-0.19658(70)$ | -0.23841 | $-0.2473(37)$ |

## Test in 3d XY model

## $B_{2}$ is very noisy, hard to measure

 Step in the right direction

| $\mathcal{O}$ | $\beta, \mu^{2}$ | $B_{1}$ | $B_{2}$ | $B_{1}^{2} / B_{2}$ | CL error | CL | worldline | corrected CL |
| :---: | :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| S | $0.2,10^{-6}$ | $0.02567(21)$ | $-0.0730(47)$ | $-0.00902(46)$ | $-0.013029(65)$ | $-0.075316(65)$ | $-0.062288(17)$ | $-0.06630(53)$ |
|  | $0.2,0.1$ | $0.03309(25)$ | $-0.0903(79)$ | $-0.01213(89)$ | $-0.0169974(91)$ | $-0.0792922(91)$ | $-0.062295(18)$ | $-0.06716(90)$ |
|  | $0.2,0.2$ | $0.03941(28)$ | $-0.109(13)$ | $-0.0142(17)$ | $-0.0205408(80)$ | $-0.0828399(80)$ | $-0.062299(11)$ | $-0.0686(17)$ |
|  | $0.7,10^{-6}$ | $1.440(15) 10^{-4}$ | $-7.33(17) 10^{-4}$ | $-2.834(46) 10^{-5}$ | $-1.23(33) 10^{-4}$ | $-1.482311(33)$ | $-1.48219(35)$ | $-1.482283(34)$ |
|  | $0.7,0.1$ | $0.004783(50)$ | $-0.0082(23)$ | $-0.00278(69)$ | $-0.002791(31)$ | $-1.526766(31)$ | $-1.52398(35)$ | $-1.52399(72)$ |
|  | $0.7,0.2$ | $0.006013(38)$ | $-0.00873(96)$ | $-0.00414(45)$ | $-0.002488(29)$ | $-1.568899(29)$ | $-1.56641(20)$ | $-1.56476(48)$ |

## XY model in $\mathrm{d}=3$

$$
S=-\beta \sum_{x} \sum_{v=1}^{3} \cos \left(\phi_{x}-\phi_{x+v}-i \mu \delta_{v 0}\right)
$$

Can be solved exactly using dual variables (worldlines)
CLE fails in one of the phases
$\langle S\rangle_{\mathrm{CLE}}-\langle S\rangle_{\text {exact }}$


Test in $\mathrm{U}(1)$ toy model

$$
S(x)=i \beta \cos (x)+\frac{s}{2} x^{2}
$$

## Measuring $B_{1,} B_{2}$ allows correction of results

 when CLE fails| $\beta, s$ | $B_{1}$ | $B_{2}$ | $B_{1}^{2} / B_{2}$ | CL error | CL | correct | corrected CL |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $0.1,0$ | $-0.04859(45)$ | $0.0493(11)$ | $0.04786(79)$ | $0.04891(45)$ | $-0.00115(45)$ | -0.05006 | $-0.04901(62)$ |
| $0.1,0.01$ | $-0.01795(49)$ | $0.01801(80)$ | $0.01789(60)$ | $0.01689(50)$ | $-0.03318(50)$ | -0.05006 | $-0.05106(40)$ |
| $0.1,0.1$ | $-0.00048(30)$ | $0.00057(35)$ | $0.00039(28)$ | $0.00049(31)$ | $-0.04957(31)$ | -0.05006 | $-0.04997(6)$ |
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| $0.5,0.3$ | $-0.05309(86)$ | $0.0552(51)$ | $0.0507(41)$ | $0.04183(70)$ | $-0.19658(70)$ | -0.23841 | $-0.2473(37)$ |

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| :---: | :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
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|  | $0.2,0.2$ | $0.03941(28)$ | $-0.109(13)$ | $-0.0142(17)$ | $-0.0205408(80)$ | $-0.0828399(80)$ | $-0.062299(11)$ | $-0.0686(17)$ |
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|  | $0.7,0.1$ | $0.004783(50)$ | $-0.0082(23)$ | $-0.00278(69)$ | $-0.002791(31)$ | $-1.526766(31)$ | $-1.52398(35)$ | $-1.52399(72)$ |
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## Bose Gas at zero temperature

At zero temperature, nothing happens
until first excited state (=1particle) contributes

No dependence on chemical potential for $\mu<m$

$$
S=\left|\partial_{v} \phi\right|^{2}+\left(m^{2}-\mu^{2}\right)|\phi|^{2}+\mu\left(\phi^{*} \partial_{4} \phi-\partial_{4} \phi^{*} \phi\right)+\lambda|\phi|^{4}
$$

Complexification with Langevin method:
Complex scalar field $\longrightarrow$ Two real fields $\rightarrow$ Two complex fields


## Silver Blaze:

Cancellations should destroy the apparent chemical potential dependence

$$
\langle n\rangle=\frac{1}{\Omega} \frac{\partial \ln Z}{\partial \mu} \quad|\phi|^{2}=\sum_{a=1,2}\left(\left(\phi_{a}^{R}\right)^{2}-\left(\phi_{a}^{I}\right)^{2}+2 i \phi_{a}^{R} \phi_{a}^{I}\right)
$$


$\mu$


## Sign problem

Complex action:

$$
\begin{aligned}
& Z=\int D \phi e^{-s}=\int D \phi\left|e^{-s}\right| e^{i \phi} \\
& Z=\int D \phi\left|e^{-s}\right|
\end{aligned}
$$

Phase quenched theory

Average phase factor

$$
\left\langle e^{i \varphi}\right\rangle_{p q}=\frac{Z_{\text {full }}}{Z_{p q}}=e^{-\Omega \Delta t} \rightarrow 0
$$

Sign problem is exponentially hard in thermodinamic limit


Phase quenched action

$$
V(|\phi|)=\frac{1}{2}\left(m^{2}-\mu^{2}\right)|\phi|^{2}+\lambda|\phi|^{4}
$$

Also shows dependence on chemical potential

Phase factor is crucial for cancellation


## Heavy Quark QCD at nonzero chemical potential (HDQCD)

Hopping parameter expansion of the fermion determinant Spatial hoppings are dropped $\longrightarrow$ unmovable quarks

$$
\begin{aligned}
& \operatorname{Det} M(\mu)=\prod_{x} \operatorname{det}\left(1+C P_{x}\right)^{2} \operatorname{det}\left(1+C^{\prime} P_{x}^{-1}\right)^{2} \\
& P_{x}=\prod_{\tau} U_{0}\left(x+\tau a_{0}\right) \quad C=[2 \kappa \exp (\mu)]^{N_{\tau}} \quad C^{\prime}=[2 \kappa \exp (-\mu)]^{N_{\tau}} \\
& S=S_{W}\left[U_{\mu}\right]+\ln \operatorname{Det} M(\mu)
\end{aligned}
$$

Studied with reweighting
[De Pietri, Feo, Seiler, Stamatescu '07]

$$
R=e^{\sum_{x} C \operatorname{Tr} P_{x}+C^{\prime} \operatorname{Tr} P^{-1}}
$$

CLE study using gaugecooling [Seiler, Sexty, Stamatescu (2012)]

Phase diagram mapped out [Aarts, Attanasio, Jaeger, Sexty (2016)]

Fermion density:

$$
n=\frac{1}{N_{\tau}} \frac{\partial \ln Z}{\partial \mu}
$$

average phase:

$$
\langle\exp (2 i \phi)\rangle=\left|\frac{\operatorname{det} M(\mu)}{\operatorname{det} M(-\mu)}\right|
$$


$\operatorname{det}(1+C P)^{2}=1+C^{3}+C \operatorname{Tr} P+C^{2} \operatorname{Tr} P^{-1}$
Sign problem is absent at small or large $\mu$

Reweigthing is impossible at $1 \leq \mu \leq 2$
CLE works all the way to saturation

## Mapping the phase diagram of HDQCD

Hopping parameter expansion of the fermion determinant Spatial fermionic hoppings are dropped Full gauge action
$\operatorname{Det} M(\mu)=\prod_{x} \operatorname{det}\left(1+C P_{x}\right)^{2} \operatorname{det}\left(1+C^{\prime} P_{x}^{-1}\right)^{2}$

Strategy to map $T-\mu$ plane
fixed $\beta=5.8 \rightarrow a \approx 0.15 \mathrm{fm} \quad$ Unitarity norm is mostly under control

$$
k=0.04
$$

onset transition at $\mu=-\ln (2 \kappa)$

$$
\begin{gathered}
N_{t} *\left(6^{3}, 8^{3}, 10^{3}\right) \text { lattice } \\
N_{t}=2 . .28
\end{gathered}
$$

Temperature scanning

$$
T=48-671 \mathrm{MeV}
$$



Exploring the phase diagram of HeavyDenseQCD
[Aarts, Attanasio, Jäger, Sexty (2016)]
Spatial fermionic hoppings are dropped - unmovable quarks Full gauge action


## Comparison with reweighting for full QCD

[Fodor, Katz, Sexty, Török (2015)]

Reweighting from ensemble at

$$
R=\operatorname{Det} M(\mu=0)
$$





## 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)]
Other strategies:
Measure the Stress-momentum tensor using gradient flow
[Suzuki, Makino (2013-)]
Shifted boundary conditions
[Giusti, Pepe, Meyer (2011-)]
Non-equilibrium quench
[Caselle, Nada, Panero (2018)]

First integrate along the temperature axis, then explore $\mu>0$
Taylor expansion [Bielefeld-Swansea (2002-)]
Simulating at imaginary $\mu$ to calculate susceptibilities [de Forcrand, Philipsen (2002-)]

## Pressure of the QCD Plasma at non-zero density

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

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

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

$$
\begin{aligned}
& c_{2}=\frac{1}{2} \frac{N_{T}}{N_{s}^{3}} \frac{\partial^{2} \ln Z}{\partial \mu^{2}} \\
& c_{4}=\frac{1}{24} \frac{1}{N_{s}^{3} N_{T}} \frac{\partial^{4} \ln Z}{\partial \mu^{4}}
\end{aligned}
$$

Measuring the coefficients of the Taylor expansion

$$
\begin{aligned}
\frac{\partial^{2} \ln Z}{\partial \mu^{2}}= & N_{F}^{2}\left\langle T_{1}^{2}\right\rangle+N_{F}\left\langle T_{2}\right\rangle \\
\frac{\partial^{4} \ln Z}{\partial \mu^{4}}= & -3\left(\left\langle T_{2}\right\rangle+\left\langle T_{1}^{2}\right\rangle\right)^{2}+3\left\langle T_{2}^{2}\right\rangle+\left\langle T_{4}\right\rangle \\
& +\left\langle T_{1}^{4}\right\rangle+4\left\langle T_{3} T_{1}\right\rangle+6\left\langle T_{1}^{2} T_{2}\right\rangle
\end{aligned}
$$

$$
\begin{aligned}
T_{1} / N_{F}= & \operatorname{Tr}\left(M^{-1} \partial_{\mu} M\right) \\
T_{i+1}=\partial_{\mu} & T_{i} \\
T_{2} / N_{F}= & \operatorname{Tr}\left(M^{-1} \partial_{\mu}^{2} M\right)-\operatorname{Tr}\left(\left(M^{-1} \partial_{\mu} M\right)^{2}\right) \\
T_{3} / N_{F}= & \operatorname{Tr}\left(M^{-1} \partial_{\mu}^{3} M\right)-3 \operatorname{Tr}\left(M^{-1} \partial_{\mu} M M^{-1} \partial_{\mu}^{2} M\right) \\
& +2 \operatorname{Tr}\left(\left(M^{-1} \partial_{\mu} M\right)^{3}\right) \\
T_{4} / N_{F}= & \operatorname{Tr}\left(M^{-1} \partial_{\mu}^{2} M\right)-4 \operatorname{Tr}\left(M^{-1} \partial_{\mu} M M^{-1} \partial_{\mu}^{3} M\right) \\
& -3 \operatorname{Tr}\left(M^{-1} \partial_{\mu}^{2} M M^{-1} \partial_{\mu}^{2} M\right)-6 \operatorname{Tr}\left(\left(M^{-1} \partial \mu M\right)^{4}\right) \\
& +12 \operatorname{Tr}\left(\left(M^{-1} \partial_{\mu} M\right)^{2} M^{-1} \partial_{\mu}^{2} M\right)
\end{aligned}
$$

## Pressure of the QCD Plasma using CLE

If we can simulate at $\quad \mu>0$

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

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

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

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

## Pressure with improved action

In deconfined phase
Symanzik gauge action
stout smeared staggered fermions



| $\beta$ | $c_{2}$ Taylor exp. | $c_{4}$ Taylor exp. | $c_{6}$ Taylor exp. | $c_{2}$ CLE | $c_{4}$ CLE | $c_{6}$ CLE |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 3.7 | $2.206 \pm 0.009$ | $0.156 \pm 0.016$ | $0.016 \pm 0.013$ | $2.33 \pm 0.1$ | $0.13 \pm 0.02$ | $0.002 \pm 0.001$ |
| 3.9 | $2.312 \pm 0.007$ | $0.150 \pm 0.007$ | $0.001 \pm 0.005$ | $2.36 \pm 0.04$ | $0.14 \pm 0.01$ | $0.002 \pm 0.001$ |

Good agreement at small $\mu$ 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

$$
B_{3}=\frac{\left\langle O^{3}\right\rangle}{\left\langle O^{2}\right\rangle^{3 / 2}}
$$

$O=P-\langle P\rangle$ with $P=\sqrt{P_{\text {bare }} P_{\text {bare }}^{-1}}$
no renormalization zero crossing defines transition


## Shift method



Define $T_{c}(\mu)$ as $\phi\left(T_{c}(\mu), \mu\right)=C$
e.g. $B_{3}$, chiral condensate,
baryon number susceptibility

Works well for small $\mu$ Critial point at $\mu_{4}$ ?

Lattice spacing: $a=0.065 \mathrm{fm}$
Pion mass: $\quad m_{\pi}=1.3 \mathrm{GeV}$
Volumes: $8^{3}, 12^{3}, 16^{3}$

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 $\mu / T$


## Complex Langevin

Theoretically
Good understanding of the failure modes (boundary terms, poles) Monitoring prescriptions allow for independent detection of failure unitarity norm, eigenspectrum, histograms, boundary terms
Is a cutoff allowed? (Dynamical stabilization)
How to cure problems? - No general answer, hit and miss

In practice
Many lattice models solved, crosschecked with alternative methods
(Bose gas, SU(3) Spin model, HDQCD, kappa exp., cond. mat. systems...)
Some remain unsolved (xy model, Thirring,... )

Full QCD
High temperatures seem to be unproblematic checks with reweighting, Taylor expansion
Status of low T and near T_c is unclear - more work needed
Results for full QCD above transition (at large pion masses) phase diag, EoS and improved actions

## Summary

Nonzero density on the lattice is hampered by the sign problem

Extrapolation methods (reweighting, Taylor exp, imaginary mu)
Can reach to $\mu_{B}$ up to $\mu_{B}<3 T \quad\left(\mu_{q}<T\right)$

Lattice results for EoS, charge fluctuations No sign of critical point in this region

Using analiticity:
Lefschetz thimbles, sign-improved manifolds
Encouraging results for simple theories
Complex Langevin:
Monitoring of process is required (boundary terms, histograms...) Solid results for high Temperature QCD (at large pion masses) Low temperatures still present a problem

