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

 $S = -\frac{1}{4} \operatorname{Tr} F_{\mu\nu} F^{\mu\nu} + \sum_{i=1}^{6} \overline{\psi}_{f} (i \gamma^{\mu} D_{\mu} + m_{f}) \psi_{f}$

1 gauge coupling 6 quark masses

Confinement mechanism?

Scattering cross sections?

Phases transition to Quark-gluon plasma?

Compressibility of quark matter? (in neutron stars)

Critical point at nonzero density?

Color superconducting phases?

Mass of hadrons?

Equation of state?

Quarkyonic phase?

Exotic phases:

.... 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





For these lectures we focus on thermodynamics at nonzero density











compare with: Phase diagram of water



much better known....

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

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



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?

Path integral formulation of Quantum Mechanics

Quantum Mechanics with

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q})$$

Time evolution given by $i\partial_t \Psi(x,t) = \hat{H} \Psi(x,t)$ $|\Psi(x,t)\rangle = e^{-it\hat{H}} |\Psi(x,0)\rangle$ Schrödinger eq.

Equivalent formulation

Transition amplitude:

ude:
$$\langle q_2 | e^{-it\hat{H}} | q_1 \rangle = \int_{q_1}^{q_2} D q e^{iS[q(t)]}$$

 $\int_{q_1}^{q_2} Dq =$ normalized sum for all fur

Path integral:

normalized sum for all functions with correct bound. cond.

 $q(t_1 \leq t \leq t_2)$ $q(t_1) = q_1 q(t_2) = q_2$



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



Thermodynamics with Path integral

Thermodynamics $e^{-it\hat{H}} \rightarrow e^{-\beta\hat{H}}$

Imaginary time - Wick rotation

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



 $\langle q_1 | e^{-\beta \hat{H}} | q_2 \rangle = \int_{q_1}^{q_2} D q e^{-S_E[q(t)]} \qquad S_E[q(t)] = \int_{t=0}^{t=\beta} dt \left(\frac{1}{2} m \dot{q}(t)^2 + V(q(t)) \right)$ We want $Z = \operatorname{Tr}(e^{-\beta H}) \quad \langle X \rangle = \operatorname{Tr}(X e^{-\beta H})$

Periodical boundary conditions in temporal directions

System of size $L_s^{3,}L_t \rightarrow \text{Temperature} = 1/L_t$

Temperature only appears as the inverse temporal size.

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

Lattice QCD



Discretised action:

Discretise action on a cubic-space time lattice

$$F^{a}_{\mu\nu} = \partial_{\mu} A^{a}_{\nu} - \partial_{\nu} A^{a}_{\mu} + g f_{abc} A^{b}_{\mu} A^{c}_{\nu}$$

Gluon fields
$$A^{a}_{\mu}(x) \rightarrow U_{\mu}(x) = \exp\left[i \int dx A^{a}_{\mu}(x) \lambda_{a}\right]$$

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

Site variables

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

fermions: $\overline{\psi}(i\gamma^{\mu}D_{\mu}+m)\psi \rightarrow \overline{\psi}(i\gamma^{\mu}D_{\mu}^{L,F}+m)\psi$ $D_{\nu}^{L,F}\psi(x) = \frac{1}{a} (U_{\nu}(x)\psi(x+\hat{\nu})-\psi(x))$

Lattice QCD



Discretise action on a cubic-space time lattice

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

Path integral:

$$\int DA_{\mu} \rightarrow \int \prod_{x,\mu} dU_{\mu}(x)$$

finite number of integrals with respect to the Haar measure of the 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 $a \rightarrow 0, V \rightarrow \infty$

Gauge transformations on the lattice



Gauge transformations

$$A_{\mu}(x) \rightarrow -\frac{i}{g} (\partial_{\mu} \Omega(x)) \Omega^{-1}(x) + \Omega(x) A_{\mu}(x) \Omega(x)^{-1}$$

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

on the lattice

$$U_{\mu}(x) \rightarrow \Omega(x) U_{\mu}(x) \Omega^{-1}(x + a_{\mu})$$

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

Symmetry group: $SU(3)^{N_s^3N_t}$

Finite volume of gauge orbits

No need for gauge fixing No ghosts

Observables have to be gauge invariant:

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

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

Lattice observables



Plaquette $U_{\mu\nu} = U_{\mu}(x) U_{\nu}(x+\mu) U_{\mu}^{-1}(x+\nu) U_{\nu}^{-1}(x)$

Related to Field strength tensor $~F_{\mu
u}$

Wilson loops $W_{m,n,\mu\nu}$ $W_{1,1,\mu\nu} = U_{\mu\nu}$ $\log \langle W_{R,T} \rangle =$ energy of static quark pair at dist. R \rightarrow String tension Polyakov loop $P = \prod_{i=0}^{N_i - 1} U_i$

 $L = \langle \operatorname{Tr} P \rangle \simeq e^{-F_q(T)/T} \quad \text{energy of a static quark}$ $T = 0 \text{ confinement} \rightarrow F(q) = \infty \rightarrow L = 0$ $T = \text{Large deconfinement} \rightarrow L \neq 0$

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 $C = \{\phi_i\}$ (or $\{U_v\}$ for QCD)

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

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

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

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

observable averaged on configurations

Scale setting in lattice QCD

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

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

We can set the inverse coupling in the action:

$$S_G = \frac{1}{g^2} \sum_{\text{plaquettes}} \operatorname{Re} \operatorname{Tr}(U_{\mu\nu})$$

In practice we use

$$\beta = \frac{2N_c}{g^2}$$

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 $W_{RT} \simeq e^{-\alpha RT}$

(Nowadays e.g. "Gradient Flow" is used for scale setting.)

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)



So in lattice QCD β 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 $Z = \int d \psi d \overline{\psi} e^{\overline{\psi}(i \gamma^{\mu} \partial_{\mu} + m) \psi}$ $\int d \eta d v e^{\eta M v} = \det M$ M = Dirac matrix

In gauge theories: $\partial_v \rightarrow \partial_v + ig A_v = D_v$ covariant derivative

quarks: $\overline{\psi}(i \gamma^{\mu} D_{\mu} + m) \psi \rightarrow \ln \det (1 + \kappa \sum_{\pm \mu} (1 + \gamma_{\mu}) U_{\mu}(x) \delta_{y, x + \hat{\mu}})$ large matrix $N = 10^5 - 10^7$ source of most of the problems with lattice QCD...

Fermion doubling

The dispersion relation for a particle should be:

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

Is this satisfied for fermions on the lattice? Let's use free fermions: $U_v = 1$

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

symmetrized derivative as antihermiticity is needed

$$\partial = \frac{1}{2} (\partial_F + \partial_B)$$

momentum on the lattice
$$\psi(x) \simeq e^{ikx}$$
 $k = \frac{2\pi}{N}i$
 $\frac{i}{2a}(e^{ik(x+\hat{v})} - e^{ik(x-\hat{v})}) = i\sin(ka)e^{ikx} = ik_{LAT}e^{ikx}$

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

$$\Delta e^{ikx} = e^{ik(x+\hat{v})} - 2e^{ikx} + e^{ik(x-\hat{v})} = 4\sin^2\left(\frac{ka}{2}\right)e^{ikx} = k_{LAT}^2 e^{ikx}$$



4 dimensional lattice \rightarrow 2⁴=16 fermion modes $k=(0,0,0,0), k=(0,0,0,\pi/a),...$

Fermion doubling – Solutions Wilson fermions

Introduce new term in fermion action to suppress unwanted doublers

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

Add a new term to lift energy of edge modes:

 $S_{W} = \frac{r}{2} \overline{\psi} \Delta \psi \qquad Second \text{ derivative} \\ \Delta \psi = \psi(x + \hat{\mu}) - 2 \psi(x) + \psi(x - \hat{\mu})$

Acts as "momentum dependent mass" $M(p) = m + \frac{2r}{a} \sum_{v} \sin^2(k_v a/2)$

As the continuum limit is neared Edge modes (doublers) become very heavy $m_{doubler} \simeq O(1/a)$ Physical modes have O(a) mass contribution

Price to pay:

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

Fermion doubling – Solutions

Staggered fermions

One notes 4-fold symmetry of the naive fermion action $\psi_{i,a}(x) \rightarrow \psi_a(x)$ throw away 3 of them 16 fermion flavours ("tastes") \rightarrow 4 fermion tastes

Still needs some rooting:

If we had 2 degenerate fermion flavors in continuum $Z = \int d \psi_1 d \overline{\psi}_1 d \psi_2 d \overline{\psi}_2 e^{\overline{\psi}_1(i \gamma^{\mu} \partial_{\mu} + m) \psi_1} e^{\overline{\psi}_2(i \gamma^{\mu} \partial_{\mu} + m) \psi_2} = (\det M)^2$

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

 $\det M \quad \Rightarrow \quad (\det M)^{1/4}$

In reality taste breaking effects vanish only in the continuum limit

Improved actions for lattice QCD



Carrying out continuum extrapolation $a \rightarrow 0$ Simulate at multiple lattice spacings Fitting some observable $O(a)=O_0+O_1a+O_2a^2+...$

Change action such that O_1 is eliminated

Gauge improvement

Syr

Include larger loops in action

manzik action:
$$S = -\beta \left(\frac{5}{3} \sum \text{ReTr} \square -\frac{1}{12} \sum \text{Re} \operatorname{Tr} \square \right)$$

Symmetry of discretisation: plaquette action scales with $O(a^2)$

Symanzik sets the coefficient of $O(a^2)$ term in the action to zero at tree level loop effects $\rightarrow O(g^2 a^2)$ 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

$$V_{\mu} = (1 - \alpha)U_{\mu} + \alpha \sum staples$$

 $U'_{\mu} = \operatorname{Proj}_{SU(3)} V_{\mu}$

Stout

$$U'_{\mu} = e^{iQ_{\mu}}U_{\mu}$$
 $Q_{\mu} = \rho \sum$ staples

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



Chiral symmetry on the lattice

 $\overline{\psi} \rightarrow e^{i\Theta_{\gamma_5}} \overline{\psi} \quad \overline{\psi} \rightarrow \overline{\psi} e^{i\Theta_{\gamma_5}}$ Fermion action $S_F = \int \overline{\psi}(x) D(x, y) \psi(y)$ is invariant if $\{\gamma_5, D\} = 0$

In continuum the kinetic term respects symmetry mass term gives an explicit breaking

Nielsen-Ninomiya theorem:

On the lattice a local discretisation that satisfies $\{\gamma_5, D\}=0$ 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

$$\{\gamma_5, D\} = 0 \longrightarrow \{\gamma_5, D\} = a D \gamma_5 D$$

In the continuum limit Reduces to usual chiral symmetry

Corresponding lattice transformations:

$$\psi \rightarrow e^{i\Theta\gamma_5(1-\frac{a}{2}D)}\psi \qquad \overline{\psi} \rightarrow \overline{\psi} e^{i\Theta\gamma_5(1-\frac{a}{2}D)}$$

A Dirac operator satisfying this can be constructed:

$$D = \frac{1}{a} (1 + \gamma_5 \operatorname{sign}(\gamma_5 A))$$

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: $Z = \int DU e^{-S_g}$

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

Cost to update all links: $O(N_s^3 N_t)$

With fermions:

 $Z = \int DU e^{-S_g} \det M[U_v]$

Determinant depends on all link variables — > Nonlocal action Cost of determinant: $O(N^3) = O(N_s^9 N_t^3)$ Cost to update all links: $O(N_s^{12}N_t^4)$

Action change very expensive, not parallelisable

Hybrid Monte Carlo with pseudofermions

HMC: introduce momenta for all fields with trivial kinetic terms

$$S[\phi_i] \rightarrow H_{HMC}[\phi_i, p_i] = S[\phi_i] + \sum \frac{p_i^2}{2}$$

 $\rho^{-\beta S_{HMC}}$ Gaussian distribution for all momenta

0 to t = 1

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

$$\dot{\phi}_i = \frac{\partial H}{\partial p_i} = p_i$$
 $\dot{p}_i = -\frac{\partial H}{\partial \phi} = -\frac{\partial S[\phi]}{\partial \phi_i}$ with stepsize Δt from $t = 0$ to $t = 1$

-forget momenta: new configuration of ϕ

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

 Δt large \rightarrow energy conservation imprecise, $e^{-\Delta S} < 1 \rightarrow$ acceptance small

Hybrid Monte Carlo with pseudofermions



Cost to update all links: $\approx O((N_s^3 N_t)^{5/4} m_q^{-\alpha})$

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: $\approx O((N_s^3 N_t)^{5/4} m_q^{-\alpha})$ $\alpha \approx 4-6$

 $(N_s^3 N_t)^{5/4}$ 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

 $Z = \int DU \, e^{-S_g} \det M[U_v]$

Determinant depends on all link variables — 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:

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

Gaussian noise
$$\langle \eta(\tau) \rangle = \mathbf{0}$$

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

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 $\Delta \tau \rightarrow 0$

Fermions in lattice QCD

 $Z = \int DU \, e^{-S_g} \det M[U_v]$

Determinant depends on all link variables — 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: $\langle \eta_a \eta_b \rangle = 2 \delta_{ab}$ Fermionic Drift from noise vectors: $\langle \psi_{ai}^*(x) \psi_{bj}(x) \rangle = \delta_{ab} \delta_{ij} \delta_{xy}$ $K_{axv,F} = D_{axv} (\ln \det M^{N_F}) = N_F \operatorname{Tr} ((D_{axv} M) M^{-1}) = N_F \langle \psi^*(D_{axv} M) M^{-1} \psi \rangle$ 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
- Stepsize needs to be extrapolated to zero

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

Chemical potential in the continuum

Fermion action:
$$S = \int_{0}^{1/T} \int d^{3}x \,\overline{\psi}(\gamma_{\nu}\partial_{\nu} + m) \psi$$

This action has the symmetry: $\psi \rightarrow e^{i\alpha} \psi \quad \overline{\psi} \rightarrow e^{-i\alpha} \overline{\psi}$ Corresponding conserved charge: $N = \int d^3 x \, \overline{\psi} \, \gamma_4 \, \psi = \int d^3 x \, \psi^+ \, \psi$

We want grand canonical potential $Z = e^{-\beta(H-\mu N)}$

$$\frac{\mu N}{T} = \int_0^\beta d\tau \int d^d x \,\mu \,\overline{\psi} \,\gamma_4 \,\psi$$

So the action becomes: $S = \int_0^{1/T} \int d^3 x \, \overline{\psi} (\gamma_v (\partial_v + i A_\mu) + \mu \, \overline{\gamma_4} + m) \, \psi = \int \overline{\psi} \, M \, \psi$

At
$$\mu = 0$$
 γ_5 -Hermiticity: $(\gamma_5 M)^+ = \gamma_5 M$
 $(\det M)^* = \det M^+ = \det (\gamma_5 M \gamma_5) = \det M \rightarrow \det M$ is real

At
$$\mu \neq 0$$
 $M^+(\mu) = \gamma_5 M(-\mu^*) \gamma_5$

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

$$S = \int_0^{1/T} \int d^4 x \,\overline{\psi} (\gamma_{\nu} (\partial_{\nu} + i A_{\mu}) + \mu \gamma_4 + m) \psi = \int \overline{\psi} M \psi$$

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

Chemical potential appears as imaginary Abelian gauge field in temporal direction

Imaginary chemical potential — Determinant is real again

Chemical potential in the continuum

U(1) symmetric bosons

 $S = \int d^4 x (|\partial_{\nu} \phi|^2 + m^2 |\phi|^2) + \lambda |\phi|^4 \qquad \text{Symmetry: } \phi \Rightarrow e^{i\alpha} \phi$ Conserved charge: $N = \int d^3 x i (\phi^* \partial_4 \phi - (\partial_4 \phi^*) \phi)$

$$Z = e^{-\beta(H-\mu N)} \quad \text{Leads to:}$$

$$S = \int d^4 x \Big[(\partial_4 + \mu) \phi^* (\partial_4 - \mu) \phi + \partial_i \phi^* \partial_i \phi + m^2 |\phi^2| + \lambda |\phi^4| \Big]$$

$$S = \int d^4 x \Big[|\partial_\nu \phi^2| + (m^2 - \mu^2) |\phi^2| + \mu \Big[\phi^* \partial_4 \phi - (\partial_4 \phi^*) \phi \Big] + \lambda |\phi^4| \Big]$$

Bosons also have a quadratic term in the chemical potential Linear term is imaginary $S(\mu)=S(-\mu)^*$

Imaginary $\mu \rightarrow$ Action is real

Chemical potential on the lattice

How does μ appear in lattice QCD? adding $\mu \overline{\phi} \gamma_4 \psi$ to the action \rightarrow ultraviolet divergences Instead we add it as an imaginary Abelian vectorfield Forward hopping terms: $e^{iA_4} = e^{a\mu}$ Backward hopping terms: $e^{-iA_4} = e^{-a\mu}$

 $M^+(\mu) = \gamma_5 M(-\mu^*) \gamma_5$ remains valid on the lattice

Complex determinant at nonzero $\ \mu$

 μ Couples to conserved charge — \blacktriangleright no divergences appear



Closed loops don't change Forward loops gain factor $e^{a\mu Nt}$ Backward loops gain factor $e^{-a\mu Nt}$ $a N_t = \frac{1}{T} \rightarrow a\mu N_t = \frac{\mu}{T}$

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

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

Probability of visiting C

$$p(C) \sim W[C]$$

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

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

Toy model with sign problem

$$Z = \int_{-\infty}^{\infty} e^{-(\sigma x^2 + i\lambda x)} dx$$

$$\langle x^2 \rangle = \frac{1}{Z} \int x^2 e^{-(\sigma x^2 + i\lambda x)} dx = ?$$

 $-a \leq x_i \leq a$

Sampling method: draw uniform random

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





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



 $\sim 10^{46}$ samples to have 10% relative error

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



Theta therm

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

THE GREASE STRUCTURE COLOR

Inbalanced Fermi gas



And everything else with complex action $w[C] = e^{-S[C]}$ w[C] is positive $\leftarrow \Rightarrow S[C]$ is real

Sign problems

Real-time evolution in QFT

"strongest" sign problem

Non-zero density

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

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

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

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

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

$$Z = \operatorname{Tr} e^{-\beta(H-\mu N)} = \sum_{n} Z_{n} e^{\beta\mu n}$$

$$Z = \operatorname{Tr} e^{-\beta(H-\mu N)} = \int dE \rho_{\mu}(E) e^{-\beta E}$$

$$Z = \operatorname{Tr} e^{-\beta(H-\mu N)} = \sum_{C} W[C] = \sum_{S} \left(\sum_{C \in S} W[C] \right)$$

$$Subsets$$

How to solve the sign problem?

Extrapolation from a positive ensemble

Reweighting
$$\langle X \rangle_{W} = \frac{\sum_{c} W_{c} X_{c}}{\sum_{c} W_{c}} = \frac{\sum_{c} W'_{c} (W_{c}/W'_{c}) X_{c}}{\sum_{c} W'_{c} (W_{c}/W'_{c})} = \frac{\langle (W/W') X \rangle_{W}}{\langle W/W' \rangle_{W'}}$$

Taylor expansion

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

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 μ , canonical ens. all break down around

$$\frac{\mu_q}{T} \approx 1 - 1.5 \qquad \frac{\mu_B}{T} \approx 3 - 4.5$$



 $\mu_B \approx 450 - 600 \,\mathrm{MeV}$



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

using Imaginary mu, Reweighting, Canonical ensemble

Agreement only at $\mu/T < 1$



Reweighting

$$\langle F \rangle_{\mu} = \frac{\int DU e^{-S_{E}} det M(\mu) F}{\int DU e^{-S_{E}} det M(\mu)} = \frac{\int DU e^{-S_{E}} det M(\mu=0) \frac{det M(\mu)}{det M(\mu=0)} F}{\int DU e^{-S_{E}} det M(\mu=0) \frac{det M(\mu)}{det M(\mu=0)}}$$

$$=\frac{\langle F \det M(\mu)/\det M(\mu=0)\rangle_{\mu=0}}{\langle \det M(\mu)/\det M(\mu=0)\rangle_{\mu=0}}$$

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

 $\Delta f(\mu, T)$ =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 $\mu/T \approx 1$

Reweighting

Overlap problem

If the two ensembles are far,

most configurations are far from the peak of the target distribution

Reweighting factor

det $M(\mu)$ has long tailed distribution

Most configs have small weight, averages are dominated by a few configs

even errorbars are untrustworthy

 $\det M(0)$

Explicit calculation of determinant Is expensive $O(N_s^9 N_t^3)$

Sign problem has exponential volume depence

Volume is limited



Silver blaze

At low temperature, system is in the ground state

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

No dependence on the chemical potential

If chemical potential reaches mass of the lightes excitation ——— onset transition

Reweighting from phase quanched theory $\int DU e^{-S_g} |\det M(\mu)|$ we have u and d quarks: $|\det M(\mu)|^2 = \det M(\mu) \det M(-\mu)$. u and d has opposite chemical potentials Phasequenched theory \checkmark nonzero isospin chemical potential pions have nonzero isospin charge

Silver blaze in QCD

Lightest excitation in phasequenched theory:pionOnset: $\mu_{c,PQ} = m_{\pi}/2$ Lightest excitation in baryon chemical pot. theory: protonOnset: $\mu_c = m_n/3$

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

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

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

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

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

Pressure:

$$\frac{p}{T^4} = \frac{\ln Z}{V T^3}$$

density
$$= \frac{1}{2} \frac{1}{N_s^3 N_t} \frac{\partial \ln Z}{\partial \mu}$$

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

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

μ dependence of observable: $\partial_{\mu} \left(\frac{1}{Z} \int DU e^{-S} X \right) \simeq \langle X n \rangle$ At higher order again correlators, fluctuations appear Measuring the coefficients of the Taylor expansion

$$\frac{\partial^2 \ln Z}{\partial \mu^2} = N_F^2 \langle T_1^2 \rangle + N_F \langle T_2 \rangle$$
$$\frac{\partial^4 \ln Z}{\partial \mu^4} = -3 \left[\langle T_2 \rangle + \langle T_1^2 \rangle \right]^2 + 3 \langle T_2^2 \rangle + \langle T_4 \rangle$$
$$+ \langle T_1^4 \rangle + 4 \langle T_3 T_1 \rangle + 6 \langle T_1^2 T_2 \rangle$$

$$\begin{split} T_{1}/N_{F} &= \mathrm{Tr}(M^{-1}\partial_{\mu}M) \\ T_{i+1} &= \partial_{\mu}T_{i} \\ T_{2}/N_{F} &= \mathrm{Tr}(M^{-1}\partial_{\mu}^{2}M) - \mathrm{Tr}((M^{-1}\partial_{\mu}M)^{2}) \\ T_{3}/N_{F} &= \mathrm{Tr}(M^{-1}\partial_{\mu}^{3}M) - 3\,\mathrm{Tr}(M^{-1}\partial_{\mu}MM^{-1}\partial_{\mu}^{2}M) \\ &+ 2\,\mathrm{Tr}((M^{-1}\partial_{\mu}M)^{3}) \\ T_{4}/N_{F} &= \mathrm{Tr}(M^{-1}\partial_{\mu}^{2}M) - 4\,\mathrm{Tr}(M^{-1}\partial_{\mu}MM^{-1}\partial_{\mu}^{3}M) \\ &- 3\,\mathrm{Tr}(M^{-1}\partial_{\mu}^{2}MM^{-1}\partial_{\mu}^{2}M) - 6\,\mathrm{Tr}((M^{-1}\partial_{\mu}M)^{4}) \\ &+ 12\,\mathrm{Tr}((M^{-1}\partial_{\mu}M)^{2}M^{-1}\partial_{\mu}^{2}M) \end{split}$$

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

Baryon: μ^{B} Strangeness: μ^{S} Electric: μ^{Q}

Higher order fluctuations

$$\chi^{B,Q,S}_{i,j,k} = \frac{\partial^{i+j+k} (p/T^4)}{(\partial \mu^B)^i (\partial \mu^Q)^j (\partial \mu^S)^k}$$

Fluctuations are expected to diverge in the victinity of a critical point Subject of intense experimental and theoretical work



[[]Fig: BW collaboration]

Up to 8th order fluctuations calculated on the lattice

Freezout temperature

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

$$R_{12}^{B}(T,\mu_{B}) = \frac{M_{B}}{\sigma_{B}^{2}} = \frac{\chi_{1}^{B}(T,\mu_{B})}{\chi_{2}(T,\mu_{B})} \qquad R_{31}^{B}(T,\mu_{B}) = \frac{S_{B}\sigma_{B}^{3}}{M_{B}}\frac{\chi_{3}^{B}(T,\mu_{B})}{\chi_{1}(T,\mu_{B})}$$

 $R_{31}(R_{12}) \rightarrow$ no need to measure *T*, μ

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

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



Fit function unknown \longrightarrow systematic error Loses predictivity around $\mu_B/T \simeq 3$ $\mu_q/T \simeq 1$

Transition Temperature

At zero μ transition is crossover Ambigous definitions nevertheless converge in cont.lim.

Pseudocritical line:

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





Critical endpoint?

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

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



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

Various estimators for Taylor expansions

Could also signal other singularities on complex plane: Lee-Yang zeroes, Roberge-Weiss

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 $U_t \rightarrow z U_t$ $z = e^{i2\pi k/N_c}$ center of SU(N)

Spontaneously broken in first order transition

quarks give explicit breaking



Center symmetry and imaginary chemical potential

$$U_t \rightarrow z U_t \qquad U_t^{-1} = z^{-1} U_t \qquad z = e^{i2\pi k/N}$$

Chemical potential dependence of Dirac matrix Can be transformed to a single time-slice

with μ_I temporal links in the Dirac matrix get extra factor: $U_t \Rightarrow e^{iN_t\mu_I}U_t$ $U_t^{-1} \Rightarrow e^{-iN_t\mu_I}U_{N_t}^{-1}$ equivalent to center transformation if $\frac{\mu_I}{T} = \frac{2\pi k}{N}$

Roberge-Weiss symmetry:

$$Z\left(\frac{\mu}{T}\right) = Z\left(\frac{\mu}{T} + \frac{i2\pi k}{N_c}\right)$$

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





[Figs: Aarts]

3D Columbia plot



Columbia plot extended with μ^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

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

Probability of visiting C

$$p(C) \sim W[C]$$

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

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

Langevin Equation (aka. stochatic quantisation)

Given an action S(x)

Stochastic process for x:

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

Gaussian noise
$$\langle \eta(\tau) \rangle = \mathbf{0}$$

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

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 $\Delta \tau \rightarrow 0$

Complex Langevin Equation

Given an action S(x)

Stochastic process for x:
$$\frac{dx}{d\tau} = -\frac{\partial S}{\partial x} + \eta(\tau) \qquad \begin{array}{c} \text{Gaussian noise} \\ \langle \eta(\tau) \rangle = 0 \\ \langle \eta(\tau) \eta(\tau') \rangle = \delta(\tau - \tau) \end{array}$$

Averages are calculated along the trajectories:

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

$$\frac{dx}{d\tau} = -\frac{\partial S}{\partial x} + \eta(\tau)$$
The field is complexified
real scalar \rightarrow complex scalar

link variables: SU(N) \longrightarrow SL(N,C) compact non-compact $det(U)=1, \ \underline{U^{+} \neq U^{-1}}$

Analytically continued observables

$$\frac{1}{Z} \int P_{comp}(x) O(x) dx = \frac{1}{Z} \int P_{real}(x, y) O(x + iy) dx dy$$
$$\langle x^2 \rangle_{real} \rightarrow \langle x^2 - y^2 \rangle_{complexified}$$

Lefschetz Thimble

Transform integral by shifting contour

$$\int_{-\infty}^{\infty} dx \, e^{S(x)} F(x) = \int_{C} dz \, e^{S(z)} F(z) = \int dt \left(\frac{dz}{dt}\right) e^{S(z(t))} F(z(t))$$

Better than the original contour if

 $e^{\operatorname{Re}(S(z(t)))}$ peak + fast decay $e^{i\operatorname{Im}(S(z(t)))}$ milder sign problem than original

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

Thanks to Cauchy-Riemann equations

Lefschetz thimble is a contour which starts from saddle points $\partial_z S(z_0) = 0$

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

 $z \rightarrow z_0$ for $t \rightarrow \infty$

+: stable thimble ◀ ► steepest descent -: unstable thimble ◀ ► steepest ascent

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

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:

$$\sum_{k} m_{k} T_{k} \rightarrow T_{0}$$

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

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

Lefschetz thimble

Shift integration contour into complex plane

Look for critical points, Find contributing thimbles

Reweight the residual sign problem

$$\frac{1}{Z} \int P_{comp}(x) O(x) dx = \frac{1}{Z} \int_{T} P_{comp}(z) O(z) dz$$





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


Sign optimized manifolds

Transform integral by shifting contour

$$\int_{-\infty}^{\infty} dx \, e^{S(x)} F(x) = \int_{C} dz \, e^{S(z)} F(z) = \int dt \left(\frac{dz}{dt}\right) e^{S(z(t))} F(z(t))$$

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 — F 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

 $S = \sum_{x,v} \frac{N_F}{a^2} (1 - \cos(A_{xv})) + \sum_{x,y} \bar{\psi}_x D_{xy} (A, \mu) \psi_y$ [Alexandru et. al. (2018)] $D_{xy}(A,\mu)$ = staggered fermion matrix, det $(D) \in \mathbb{C}$

Parametrize new manifold as:

$$\widetilde{A}_0 = A_0 + i(\lambda_0 + \lambda_1 \cos(A_0) + \lambda_2 \cos(2A_0))$$

$$\widetilde{A}_1 = A_1 \qquad \widetilde{A}_2 = A_2$$

Search for the minimum of

 $\langle \overline{e^{i \varphi}} \rangle_{PO}$ num

nerically, 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, simulation on 4^4 has to have $\langle e^{i\varphi} \rangle \approx 0.999$

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 $S_p = i\beta\cos(\varphi) + ip\varphi$ Langevin equation: $\frac{d\varphi}{d\tau} = -i\beta\sin\varphi + ip + \eta(\tau)$

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 complex ϕ 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

link variables: SU(N) \longrightarrow SL(N,C) compact non-compact $det(U)=1, U^{+} \neq U^{-1}$

Gauge degrees of freedom also complexify

Infinite volume of irrelevant, unphysical configurations

Process leaves the SU(N) manifold exponentially fast already at $\ \mu \ll 1$

Unitarity norm: Distance from SU(N) $\sum_{i} Tr(U_{i}U_{i}^{+})$ $\sum_{ij} |(UU^{+}-1)_{ij}|^{2}$ $Tr(UU^{+}) + Tr(U^{-1}(U^{-1})^{+}) \ge 2N$

Gauge cooling [Seiler,Sexty,Stamatescu '13]

Minimize unitarity norm Distance from SU(N)

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

Gauge transformation along Steepest descent



Gauge cooling keeps 'skirts' from developing

ensuring correct results



Empirical observation: Cooling is effective for

a<a_{max}

but remember, $\beta \rightarrow \infty$ in cont. limit $a_{max} \approx 0.1 - 0.2 \, fm$ Argument for correctness of CLE results

If there is fast decay $P(x, y) \rightarrow 0$ 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

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

measure has zeros (*Det* M=0) complex logarithm has a branch cut → 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 What we want What we get with CLE

$$\int dx \rho(x) O(x) = \int dx \, dy \, P(x, y) O(x+iy)$$

Interpolating function:

$$F(t,\tau) = \int P(x,y,t-\tau)O(x+iy,\tau)dxdy$$

$$F(t,0) = \langle O(x+iy) \rangle_{P(t)} \qquad F(t,t) = \dots = \langle O(x) \rangle_{\rho(t)}$$

 $\partial_{\tau} F(t,\tau) = 0 \implies \text{CLE is correct}$

Boundary terms as a volume integral

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

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

$$\partial_{\tau} F_{O}(Y,t,\tau=0) = B_{O}(Y,t,\tau=0) = \int_{-Y}^{Y} P(x,y,t) L_{c}O(x+iy) - \int_{-Y}^{Y} (L^{T}P)O(x+iy,0)$$

Observable with a cutoff easy to do in many dimensions

Vanishes as process equilibrates

 $L_c O(x+iy)$ consistency conditions \approx Schwinger-Dyson eqs.

Order of limits crucial

 $\lim_{t \to \infty} \lim_{Y \to \infty} \int_{-Y}^{Y} P(x, y, t) L_c O(x + iy) \text{ can be undefined}$

One plaquette model

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

Full QCD

Boundary term for spatial plaquettes



Unambigous detection of boundary terms Observable cheap also for lattice systems

Correcting CLE using boundary terms



Interpolation function

$$F(t,\tau) = \sum A_n \exp(-\omega_n \tau)$$

Ansatz $F(t,\tau) = A_0 + A_1 \exp(-\omega_1 \tau)$

Higher order boundary terms $\frac{\partial^{n} F(t,\tau)}{\partial \tau^{n}} = B_{n} = \langle L_{c}^{n} O \rangle$

Systematic error of CLE $F(t,0)-F(t,t)=B_1^2/B_2$



Test in U(1) toy model

Measuring $B_{1,}B_{2}$ allows correction of results when CLE fails

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

eta,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)



 B_2 is very noisy, hard to measure

Step in the right direction

Ø	β, μ^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 d=3

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

Can be solved exactly using dual variables (worldlines)

CLE fails in one of the phases



[plot from: Aarts and James (2010)]

Test in U(1) toy model

Measuring $B_{1,}B_{2}$ allows correction of results when CLE fails

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

eta,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)



 B_2 is very noisy, hard to measure

Step in the right direction

Ø	β, μ^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)



Bose Gas at zero temperature [Aarts '08]

Silver Blaze problem:

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

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

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

Complexification with Langevin method:

Complex scalar field — Two real fields — Two complex fields



Silver Blaze:

Cancellations should destroy the apparent chemical potential dependence

 $\langle n \rangle = \frac{1}{\Omega} \frac{\partial \ln Z}{\partial \mu}$

$$|\Phi|^{2} = \sum_{a=1,2} \left((\Phi_{a}^{R})^{2} - (\Phi_{a}^{I})^{2} + 2i\Phi_{a}^{R}\Phi_{a}^{I} \right)$$



Sign problem

Complex action: $Z = \int Z$ Phase quenched theoryZ

$$Z = \int D \phi e^{-S} = \int D \phi |e^{-S}| e^{i\phi}$$
$$Z = \int D \phi |e^{-S}|$$

Average phase factor

$$\langle e^{i\phi} \rangle_{pq} = \frac{Z_{full}}{Z_{pq}} = e^{-\Omega \Delta f} \rightarrow 0$$

Sign problem is exponentially hard in thermodinamic limit



Phase quenched action $V(|\phi|) = \frac{1}{2}(m^2 - \mu^2)|\phi|^2 + \lambda |\phi|^4$ 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 — Marks

Det
$$M(\mu) = \prod_{x} \det(1 + C P_{x})^{2} \det(1 + C' P_{x}^{-1})^{2}$$

 $P_{x} = \prod_{\tau} U_{0}(x + \tau a_{0}) \qquad C = [2 \kappa \exp(\mu)]^{N_{\tau}} \qquad C' = [2 \kappa \exp(-\mu)]^{N_{\tau}}$

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

Studied with reweighting [De Pietri, Feo, Seiler, Stamatescu '07] $R = e^{\sum_{x} C \operatorname{Tr} P_{x} + C' \operatorname{Tr} P^{-1}}$

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

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



 $\kappa \rightarrow 0, \mu \rightarrow \infty, \zeta = \kappa e^{\mu}$ fixed

d $C = (2\zeta)^{N_{\tau}}$





 $\det(1+CP)^2 = 1+C^3+C\operatorname{Tr} P+C^2\operatorname{Tr} P^{-1}$

Sign problem is absent at small or large $\ \mu$

Reweigthing is impossible at $1 \le \mu \le 2$

CLE works all the way to saturation

Mapping the phase diagram of HDQCD [Aarts, Attanasio, Jäger, Sexty (2016)]

Hopping parameter expansion of the fermion determinant Spatial fermionic hoppings are dropped Full gauge action

Det
$$M(\mu) = \prod_{x} \det(1 + C P_{x})^{2} \det(1 + C' P_{x}^{-1})^{2}$$

Strategy to map $T - \mu$ plane

fixed $\beta = 5.8 \rightarrow a \approx 0.15 \, \text{fm}$ Unitarity norm is mostly under control.

 $\kappa = 0.04$ onset transition at $\mu = -\ln(2\kappa)$

 $N_t * (6^3, 8^3, 10^3)$ lattice $N_t = 2..28$

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





Similar to but much simpler than full QCD



Comparison with reweighting for full QCD

[Fodor, Katz, Sexty, Török (2015)]

Reweighting from ensemble at $R = \text{Det } M(\mu = 0)$





Pressure of the QCD Plasma at non-zero density



[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 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

$$\frac{\partial^2 \ln Z}{\partial \mu^2} = N_F^2 \langle T_1^2 \rangle + N_F \langle T_2 \rangle$$
$$\frac{\partial^4 \ln Z}{\partial \mu^4} = -3 \left[\langle T_2 \rangle + \langle T_1^2 \rangle \right]^2 + 3 \langle T_2^2 \rangle + \langle T_4 \rangle$$
$$+ \langle T_1^4 \rangle + 4 \langle T_3 T_1 \rangle + 6 \langle T_1^2 T_2 \rangle$$

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

Pressure of the QCD Plasma using CLE

[Sexty (2019)]

If we can simulate at $\mu > 0$

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

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

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

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 $\ \mu$ 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

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

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

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 fm

Pion mass: $m_{\pi} = 1.3 \text{ GeV}$ Volumes: $8^3, 12^3, 16^3$

Finite size effects large

Consistent results

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?



 $\kappa_2 \approx 0.0012$

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



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 μ_B up to $\mu_B < 3T$ ($\mu_q < T$)

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