Complex Langevin dynamics: distributions and gauge theories

Gert Aarts
QCD phase diagram

QCD partition function

\[ Z = \int DU D\bar{\psi} D\psi e^{-S_{YM} - S_F} = \int DU \det D e^{-S_{YM}} \]

at nonzero quark chemical potential

\[ [\det D(\mu)]^* = \det D(-\mu^*) \]

- fermion determinant is complex
- straightforward importance sampling not possible
- sign problem

⇒ phase diagram has not yet been determined non-perturbatively
Outline

- complex Langevin dynamics: exploring a complexified field space
- distributions in simple models
- connection with Lefschetz thimbles
- gauge theories: from SU($N$) to SL($N, \mathbb{C}$)
- summary and outlook
Complex integrals

- consider simple integral

\[ Z(a, b) = \int_{-\infty}^{\infty} dx \, e^{-S(x)} \quad S(x) = ax^2 + ibx \]

- complete the square/saddle point approximation: into complex plane

- lesson: don’t be real(istic), be more imaginative

radically different approach:

- complexify all degrees of freedom \( x \to z = x + iy \)
- enlarged complexified space
- new directions to explore
Complexified field space

complex weight $\rho(x)$
dominant configurations in the path integral?

real and positive distribution $P(x, y)$: how to obtain it?
$\Rightarrow$ solution of stochastic process

$\Rightarrow$ complex Langevin dynamics

Parisi 83, Klauder 83
Complex Langevin dynamics

does it work?

- for real actions: stochastic quantization
  - equivalent to path integral quantization
    - Parisi & Wu 81

- for complex actions: no formal proof
  - troubled past: “disasters of various degrees”
    - Ambjørn et al 86

nevertheless, recent examples in which CL

- can handle severe sign and Silver Blaze problems
- gives the correct result
- analytical understanding under control
- first results for gauge theories and QCD
Complex Langevin dynamics

various scattered results since mid 1980s
here:

finite density results obtained with Nucu Stamatescu, Erhard Seiler, Frank James, Denes Sexty, Lorenzo Bongiovanni, Jan Pawlowski, Pietro Giudice, Kim Splittorff

0807.1597 [GA, IOS]
0810.2089, 0902.4686 [GA]
0912.3360 [GA, ES, IOS]
0912.0617, 1101.3270 [GA, FJ, ES, IOS]
1005.3468, 1112.4655 [GA, FJ]
1006.0332 [GA, KS]
1211.3709 [ES, DS, IOS]
1212.5231 [GA, FJ, JP, ES, DS, IOS]

1306.3075 [GA, PG, ES]
1307.7748 [DS] 1308.4811 [GA]
1311.1056 [GA, LB, IOS, ES, DS]
reviews: 1302.3028 [GA], 1303.6425 [GA, LB, IOS, ES, DS]
Real Langevin dynamics

partition function \( Z = \int dx \, e^{-S(x)} \) \( S(x) \in \mathbb{R} \)

- Langevin equation
  \[
  \dot{x} = -\partial_x S(x) + \eta, \quad \langle \eta(t)\eta(t') \rangle = 2\delta(t - t')
  \]

- associated distribution \( \rho(x, t) \)
  \[
  \langle O(x(t)) \rangle_\eta = \int dx \, \rho(x, t) O(x)
  \]

- Langevin eq for \( x(t) \) ⇔ Fokker-Planck eq for \( \rho(x, t) \)
  \[
  \dot{\rho}(x, t) = \partial_x \left( \partial_x + S'(x) \right) \rho(x, t)
  \]

- stationary solution: \( \rho(x) \sim e^{-S(x)} \)
Fokker-Planck equation

- stationary solution typically reached exponentially fast

\[
\dot{\rho}(x, t) = \partial_x \left( \partial_x + S'(x) \right) \rho(x, t)
\]

- write

\[
\rho(x, t) = \psi(x, t) e^{-\frac{1}{2}S(x)}
\]

\[
\dot{\psi}(x, t) = -H_{\text{FP}} \psi(x, t)
\]

- Fokker-Planck hamiltonian:

\[
H_{\text{FP}} = Q^\dagger Q = \left[ -\partial_x + \frac{1}{2}S'(x) \right] \left[ \partial_x + \frac{1}{2}S'(x) \right] \geq 0
\]

\[
Q\psi(x) = 0 \quad \Leftrightarrow \quad \psi(x) \sim e^{-\frac{1}{2}S(x)}
\]

\[
\psi(x, t) = c_0 e^{-\frac{1}{2}S(x)} + \sum_{\lambda > 0} c_\lambda e^{-\lambda t} \rightarrow c_0 e^{-\frac{1}{2}S(x)}
\]
Complex Langevin dynamics

partition function $Z = \int dx \, e^{-S(x)} \quad S(x) \in \mathbb{C}$

- complex Langevin equation: complexify $x \rightarrow z = x + iy$

  \[
  \begin{align*}
  \dot{x} &= -\text{Re} \, \partial_z S(z) + \eta \\
  \dot{y} &= -\text{Im} \, \partial_z S(z)
  \end{align*}
  \]

  \[
  \langle \eta(t)\eta(t') \rangle = 2\delta(t - t')
  \]

- associated distribution $P(x, y; t)$

  \[
  \langle O(x + iy)(t) \rangle = \int dx \, dy \, P(x, y; t) \, O(x + iy)
  \]

- Langevin eq for $x(t), y(t) \iff$ FP eq for $P(x, y; t)$

  \[
  \dot{P}(x, y; t) = [\partial_x (\partial_x + \text{Re} \, \partial_z S) + \partial_y \text{Im} \, \partial_z S] \, P(x, y; t)
  \]

- generic solutions? semi-positive FP hamiltonian?
Field theory

scalar field:

- (discretized) Langevin dynamics in “fifth” time direction

\[ \phi_x(n + 1) = \phi_x(n) + \epsilon K_x(n) + \sqrt{\epsilon} \eta_x(n) \]

- drift:

\[ K_x = -\delta S[\phi]/\delta \phi_x \]

- Gaussian noise:

\[ \langle \eta_x(n) \rangle = 0 \quad \langle \eta_x(n) \eta_x(n') \rangle = 2\delta_{xx'}\delta_{nn'} \]
Field theory

scalar field:

- (discretized) Langevin dynamics in “fifth” time direction

\[ \phi_x(n+1) = \phi_x(n) + \epsilon K_x(n) + \sqrt{\epsilon} \eta_x(n) \]

- drift: \[ K_x = -\delta S[\phi]/\delta \phi_x \]

- Gaussian noise: \[ \langle \eta_x(n) \rangle = 0 \quad \langle \eta_x(n) \eta_x'(n') \rangle = 2\delta_{xx'}\delta_{nn'} \]

gauge/matrix theories:

\[ U(n+1) = R(n) U(n) \quad R = \exp \left[ i \lambda_a (\epsilon K_a + \sqrt{\epsilon} \eta_a) \right] \]

Gell-mann matrices \( \lambda_a \) (\( a = 1, \ldots N^2 - 1 \))

- drift: \[ K_a = -D_a(S_B + S_F) \quad S_F = -\ln \det M \]

- complex action: \( K^\dag \neq K \iff U \in SL(N, \mathbb{C}) \)
Results

even without rigorous mathematical proof
many promising results at nonzero $\mu$:

- 1d QCD
- 3d SU(3) spin models
- 4d Bose gas (severe sign and Silver Blaze problem)
- heavy dense QCD

however, also notable failures

- 3d XY model at nonzero $\mu$

also problems for

- Minkowski integrals, $e^{iS}$

Berges, Borsanyi, Stamatescu, Sexty 05 – 08
Distributions

emerging insight: crucial role played by distribution $P(x, y)$

- does it exist?
  usually yes, constructed by brute force by solving the CL process
direct solution of FP equation extremely hard
  GA, ES & IOS 09, Duncan & Niedermaier 12, GA, PG & ES 13

- what are its properties?
  localization in $x - y$ space, fast/slow decay at large $|y|$
  essential for mathematical justification of approach
  GA, ES, IOS (& FJ) 09, 11

- smooth connection with original distribution when
  $\mu \sim 0$?
  GA, FJ, JP, ES, DS & IOS 12

study with histograms, scatter plots, flow
Distributions

distribution in well-behaved example
One-dimensional QCD

- exactly solvable
  
  - phase quenched: transition at $\mu = \mu_c$, full: no transition

- severe sign problem when $|\mu| > |\mu_c|$

- chiral condensate:
  write as integral over spectral density

\[
\Sigma = \int d^2 z \frac{\rho(z; \mu)}{z + m} \quad \mu_c = \text{arcsinh } m
\]

- $\rho(z; \mu)$ complex and oscillatory
  
  - condensate independent of $\mu$: Silver Blaze
  
  - solve with complex Langevin

Gibbs 86, Bilic & Demeterfi 88

Ravagli & Verbaarschot 07

Silver Blaze

GA & Splittorff 10
One-dimensional QCD

- exact results reproduced
- discontinuity at \( \mu_c = 0 \) in thermodynamic limit \( n \to \infty \)

\[ \mu_c = \text{arcsinh } m \]

- sign problem severe when \( |\mu_c| < |\mu| \)
- condensate independent of \( \mu \): Silver Blaze
One-dimensional QCD

elegant analytical solution:

- original distribution:
  \[ \rho(x) \sim e^{n(\mu - \mu_c)}e^{inx} \]
  when \( n \to \infty \)

- real distribution sampled by complex Langevin:
  \[ P(x, y) = \begin{cases} 
    1 & \mu - \mu_c < y < \mu + \mu_c \\
    0 & \text{elsewhere} 
  \end{cases} \]

Kyoto, November 2013 – p. 16
Quartic model

\[ Z = \int_{-\infty}^{\infty} dx \, e^{-S} \]
\[ S(x) = \frac{\sigma}{2} x^2 + \frac{\lambda}{4} x^4 \]

often used toy model: complex mass parameter \( \sigma = A + iB \)

essentially analytical proof:

- CL gives correct result for all observables \( \langle x^n \rangle \) when \( A > 0 \) and \( A^2 > B^2/3 \)
- based on properties of the distribution \( P(x, y) \)
- \( P(x, y) = 0 \) outside strip: \( |y| > y_- \)

\[ y_- = \frac{1}{2\lambda} \left( A - \sqrt{A^2 - B^2/3} \right) \]

- follows from FPE
Quartic model

\[ Z = \int_{-\infty}^{\infty} dx \ e^{-S} \quad S(x) = \frac{\sigma}{2} x^2 + \frac{\lambda}{4} x^4 \quad \sigma = A + iB \]

- numerical solution of FPE for \( P(x, y) \)
  \( \sim 150^2 \times 150^2 \) matrix problem
- distribution is localised in a strip around real axis
Quartic model

interesting connection to Lefschetz thimbles

Witten 10

Cristoforetti, Di Renzo, Mukherjee & Scorzato 12, 13

Fujii, Honda, Kato, Kikukawa, Komatsu & Sano 13

generalisation of steepest descent
integrate along path in complex plane where
$\text{Im } S(z) = \text{cst}$, the thimble $\mathcal{J}$
residual sign problem due to curvature of thimble

\[
Z = e^{-i \text{Im } S_{\mathcal{J}}} \int_{\mathcal{J}} dz \ e^{-\text{Re } S(z)} \\
= e^{-i \text{Im } S_{\mathcal{J}}} \int ds \ J(s) e^{-\text{Re } S(z(s))}
\]

with complex Jacobian $J(s) = z'(s) = x'(s) + iy'(s)$
Quartic model

- thimbles can be computed analytically
- pass through stationary points $\partial_z S = 0$ & $\text{Im } S(z) = \text{cst}$

3 stationary points: only 1 thimble (for $A > 0$)
introducing along thimble gives correct result, with inclusion of complex Jacobian
Quartic model

compare thimble and FP distribution $P(x,y)$

- thimble and $P(x,y)$ follow each other
- however, weight distribution quite different

intriguing result: CLE finds the thimble – is this generic?

Kyoto, November 2013 – p. 17
Gauge theories

SU($N$) gauge theory: complexification to SL($N$, $\mathbb{C}$)

- links $U \in \text{SU}(N)$: CL update

\[ U(n+1) = R(n) U(n) \quad R = \exp \left[ i\lambda_a \left( \epsilon K_a + \sqrt{\epsilon} \eta_a \right) \right] \]

Gell-mann matrices $\lambda_a$ ($a = 1, \ldots, N^2 - 1$)

- drift: $K_a = -D_a(S_B + S_F)$, $S_F = -\ln \det M$
Gauge theories

SU\( (N) \) gauge theory: complexification to SL\((N, \mathbb{C})\)

- links \( U \in SU(N) \): CL update
  \[
  U(n+1) = R(n)U(n) \quad R = \exp \left[ i\lambda_a \left( \epsilon K_a + \sqrt{\epsilon}\eta_a \right) \right]
  \]
  Gell-mann matrices \( \lambda_a \) \((a = 1, \ldots N^2 - 1)\)

- drift:
  \[
  K_a = -D_a(S_B + S_F) \quad S_F = -\ln \det M
  \]

- complex action: \( K^\dagger \neq K \iff U \in SL(N, \mathbb{C}) \)

- deviation from SU\( (N) \): unitarity norms
  \[
  \frac{1}{N} \text{Tr} \left( UU^\dagger - \mathbb{I} \right) \geq 0 \quad \frac{1}{N} \text{Tr} \left( UU^\dagger - \mathbb{I} \right)^2 \geq 0
  \]
Gauge theories

deviation from SU(3): unitarity norm

\[ \frac{1}{3} \text{Tr} \, UU^\dagger \geq 1 \]

heavy dense QCD, $4^4$ lattice with $\beta = 5.6, \, \kappa = 0.12, \, N_f = 3$
Gauge theories

controlled evolution: stay close to SU($N$) submanifold when

- small chemical potential $\mu$
- small non-unitary initial conditions
- in presence of roundoff errors
Gauge theories

controlled evolution: stay close to SU($N$) submanifold when

- small chemical potential $\mu$
- small non-unitary initial conditions
- in presence of roundoff errors

in practice this is not the case

$\Rightarrow$ unitary submanifold is unstable!

- process will not stay close to SU($N$)
- wrong results in practice, e.g. jumps when $\mu^2$ crosses 0
- also seen in abelian XY model
Unstable gauge theories

what is the origin? can this be fixed?

- gauge freedom: link at site $k$

\[ U_k \rightarrow \Omega_k U_k \Omega_{k+1}^{-1} \]

\[ \Omega_k = e^{i \omega^k_a \lambda_a} \]

- in SU($N$): $\omega^k_a \in \mathbb{R}$

- in SL($N$, $\mathbb{C}$): $\omega^k_a \in \mathbb{C}$

- choose $\omega^k_a$ purely imaginary, orthogonal to SU($N$) direction

control unitarity norm

\[ \frac{1}{N} \text{Tr} \left( UU^\dagger - \mathbb{1} \right) \geq 0 \]

- gauge cooling

ES, DS & IOS 12

GA, LB, ES, DS & IOS 13

Kyoto, November 2013 – p. 21
Gauge cooling

cooling update at site $k$

$$U_k \rightarrow \Omega_k U_k$$

unitarity norm: distance

$$\Omega_k = e^{-\alpha f_a^k} \lambda_a \quad \alpha > 0$$

$$U_{k-1} \rightarrow U_{k-1} \Omega_{k}^{-1}$$

after one update, $\mathcal{d} \rightarrow \mathcal{d}'$

linearise

$$\mathcal{d}' - \mathcal{d} = -\frac{\alpha}{N} (f_a^k)^2 + \mathcal{O}(\alpha^2) \leq 0$$

reduce distance from $\text{SU}(N)$
Gauge cooling

what is $f_a^k$?

$$\Omega_k = e^{-\alpha f_a^k \lambda_a} \quad \mathcal{d}' - \mathcal{d} = -\alpha/N (f_a^k)^2 + \ldots$$

- choose $f_a^k$ as the gradient of the unitarity norm
  $$f_a^k = 2 \text{Tr} \lambda_a \left( U_k U_k^\dagger - U_{k-1}^\dagger U_{k-1} \right)$$

- if $U \in \text{SU}(N)$: $f_a^k = 0$, $\mathcal{d} = 0$, no effect

cooling brings the links as close as possible to $\text{SU}(N)$
Gauge cooling

- simple example: one-link model

\[
S = \frac{1}{N} \text{Tr} U \quad U \rightarrow \Omega U \Omega^{-1}
\]

\[
d' = \frac{1}{N} \text{Tr} \left(UU^\dagger - \mathbb{1} \right) \quad f_a = 2 \text{Tr} \lambda_a \left(UU^\dagger - U^\dagger U \right)
\]

- note: \( c = \text{Tr} U/N, \quad c^* = \text{Tr} U^\dagger/N \) invariant under cooling

- cooling dynamics:

\[
d' - d \equiv \dot{d} = -\frac{\alpha}{N} f_a^2 = -\frac{16\alpha}{N} \text{Tr} UU^\dagger [U, U^\dagger]
\]

- in SU(2)/SL(2,\mathbb{C}):\n
\[
\dot{d} = -8\alpha \left( d^2 + 2 \left( 1 - |c|^2 \right) d + c^2 + c^{*2} - 2|c|^2 \right)
\]
Gauge cooling

SU(2)/SL(2,\mathbb{C}) one-link model

\[ \dot{c} = -8 \alpha \left( d^2 + 2 \left( 1 - |c|^2 \right) d + c^2 + c^*^2 - 2|c|^2 \right) \]

- \( c = \frac{1}{2} \text{Tr } U, \quad c^* = \frac{1}{2} \text{Tr } U^\dagger \) invariant under cooling

- if \( c = c^* \): \( U \) gauge equivalent to SU(2) matrix

\[ \dot{d} = 8 \alpha (d + 2 - 2c^2)d \quad \quad d(t) \sim e^{-16\alpha(1-c^2)t} \rightarrow 0 \]

- if \( c \neq c^* \): \( U \) not gauge equivalent to SU(2) matrix

\[ d(t) \rightarrow d_0 = |c|^2 - 1 + \sqrt{1 - c^2 - c^*^2 + |c|^4} > 0 \]

minimal distance from SU(2) reached exponentially fast
Langevin with gauge cooling

complex Langevin dynamics with gauge cooling:

- alternate CL updates with gauge cooling updates
- monitor unitarity norm
- stay fairly close to SU($N$)

models

- Polyakov chain (exactly solvable)

$$S = \beta_1 \text{Tr} \, U_1 \ldots U_{N_\ell} + \beta_2 \text{Tr} \, U_{N_\ell}^{-1} \ldots U_1^{-1} \quad \beta_{1,2} \in \mathbb{C}$$

- heavy dense QCD  
  ES, DS & IOS 12

- full QCD  
  Denes Sexty 1307.7748

- SU(3) with a $\theta$-term  
  GA, LB, ES, DS, IOS 1311.1056
Langevin with gauge cooling

SU(2) Polyakov loop model

SU(2) Polyakov chain, $N_{\text{links}} = 30$, $\beta = (1+i \sqrt{3})/2$

$\text{Tr}(U U^\dagger)/2 - 1$

- no cooling
- $\alpha = 0.001$ (10 gc steps)
- $\alpha$ adaptive (10 gc steps)

Langevin time

evolution of unitarity norm
Langevin with gauge cooling

SU(2) Polyakov loop model

histograms of observables

- without cooling: broad distributions, no rapid decay
- with some cooling: reduced
- with sufficient adaptive cooling: narrow distributions
Langevin with gauge cooling

SU(2) Polyakov loop model

- Observables depend on gauge cooling
- Exact results are reproduced when distributions are narrow and unitarity norm close to 0
Langevin with gauge cooling

in QCD:

- unitary submanifold very unstable
- gauge cooling essential
- first results promising  
  Denes Sexty 1307.7748

many things to sort out

- cooling not effective at small $\beta \lesssim 5.7$
- larger lattices required
- fermion matrix inversion
- stepsize dependence
- ...

here: SU(3) with a $\theta$ term  
  GA, LB, ES, DS, IOS 1311.1056
**SU(3) with a $\theta$ term**

pure SU(3) Yang-Mills theory (no fermions)

$$S = S_{\text{YM}} - i\theta Q$$

$$Q = \frac{g^2}{64\pi^2} \int d^4 x \, F^{a}_{\mu\nu} \tilde{F}^{a}_{\mu\nu}$$

on the lattice:

$$S = S_{W} - i\theta_L \sum_x q_L(x)$$

$q_L(x) = \text{discretised lattice version}$

- $\theta_L$ bare parameter, requires renormalisation
- lattice $Q_L = \sum_x q_L$ is not topological (top. cooling)
- complex action for real $\theta_L$, real action for imaginary $\theta_L$

imaginary $\theta_L$: real Langevin and hybrid Monte Carlo (HMC)
real $\theta_L$: use complex Langevin
**SU(3) with a \( \theta \) term**

very preliminary results: \( 6^4 \) lattice, \( \theta_L^2 = 0, \pm 1, \pm 4 \)

**test of analyticity in \( \theta_L^2 \):** \[ \langle \text{plaquette} \rangle \]

no \( \theta_L \) dependence: smooth analytic behaviour (as expected)
SU(3) with a $\theta$ term

very preliminary results: $6^4$ lattice, $\theta_L^2 = 0, \pm 1, \pm 4$

histograms: better localisation at larger $\beta$ values
SU(3) with a $\theta$ term

topological charge:
- $\theta_L$ real/imaginary: $\langle Q_L \rangle$ imaginary/real
- small $\theta_L$: linear dependence $\langle q_L \rangle = i\theta_L \chi_L + \mathcal{O}(\theta_L^3)$

$\chi_L$ lattice topological susceptibility

Running average: preliminary result agrees with expectation
Summary and outlook

complex Langevin dynamics can handle

- sign problem
- Silver Blaze problem
- phase transition
- thermodynamic limit

in a variety of theories, but correct result not guaranteed so far

- better mathematical and practical understanding
- connection with Lefschetz thimbles
- gauge cooling for SU($N$) gauge theories
- first application to QCD and $\theta$ term

lots of work to do!