On complex Langevin dynamics and zeroes of the fermion determinant

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with Erhard Seiler, Dénes Sexty and Nucu Stamatescu
Complex Langevin dynamics

- solved the sign problem in a selection of theories including QCD with heavy quarks

  see talks by Attanasio, Jäger, Sexty, ...

- presence of the fermion determinant causes a theoretical problem

  absence of holomorphicity of the Langevin drift

- requires a reconsideration of the formal derivation

- understanding/assessment applicable to generic cases
Outline

- formal derivation revisited
- interplay between poles and distribution
- extract generic lessons
- sequence of models
- conclusions
Formal derivation revisited

complex weight: $\rho(x) \in \mathbb{C}$  

two expectation values:

$$\langle O \rangle_{\rho(t)} = \int dx \, \rho(x, t) O(x) \quad \langle O \rangle_{P(t)} = \int dx \, dy \, P(x, y; t) O(x + iy)$$

with Fokker-Planck equations for the distributions

$$\dot{\rho}(x, t) = \nabla_x \left[ \nabla_x - K(x) \right] \rho(x, t)$$

$$\dot{P}(x, y; t) = \left[ \nabla_x \left( \nabla_x - K(x) \right) - \nabla_y K_y \right] P(x, y; t)$$

and Langevin drift terms

$$K(z) = \nabla_z \rho(z) / \rho(z) \quad K_x = \text{Re} K(z) \quad K_y = \text{Im} K(z)$$

equivalence:

$$\langle O \rangle_{\rho(t)} \equiv \langle O \rangle_{P(t)}$$

GA, ES, IOS, 0912.3360 (PRD), + James 1101.3270 (EPJC)
Formal derivation revisited

equivalence \[ \langle O \rangle_{\rho(t)} = \langle O \rangle_{P(t)} \] provided

- holomorphicity of drift and observables
- fast decay of distribution \( P(x, y) \) at \( y \to \pm \infty \)

proof requires partial integration at \( |y| \to \infty \) without boundary terms
Formal derivation revisited

\[ \langle O \rangle_\rho(t) = \langle O \rangle_P(t) \]

provided

- holomorphicity of drift and observables
- fast decay of distribution \( P(x, y) \) at \( y \to \pm \infty \)

proof requires partial integration at \( |y| \to \infty \) without boundary terms

zero in measure:

\[ \rho(x = z_p) = 0 \]

- drift \( K(z) = \nabla_z \rho(z)/\rho(z) \) has pole at \( z = z_p \)
- meromorphic, not holomorphic \( \Rightarrow \) reconsider derivation

example: QCD

\[ Z = \int DU \det M(U)e^{-S_{\text{YM}}} \]

\[ \det M(U) = 0 \text{ for some } U \in \text{SL}(N, \mathbb{C}) \]
Formal derivation revisited

- exclude region around the pole: \(|z - z_p| > \epsilon\)
- derivation goes through
- new potential boundary terms at \(z \sim z_p\)
- study behaviour of \(P(x, y)O(x + iy)\) around \(z \sim z_p\)

note: time evolution of holomorphic observables

\[ \dot{O}(z; t) = \tilde{L}O(z; t) \quad \tilde{L} = \left[ \nabla_z + K(z) \right] \nabla_z \]

solution

\[ O(z; t) = e^{\tilde{L}t}O(z; 0) = \sum_k \frac{t^k}{k!} \tilde{L}^k O(z; 0) \]

\(O(z; t)\) formally has essential singularity at \(z = z_p\)

counteracted by \(P(x, y) \to 0\) as \(z \to z_p\)

and nontrivial angular dependence (see below)
Poles and the distribution

three logical possibilities: poles are

- outside the distribution
- on the edge of the distribution
- inside the distribution

zero at $z_p$ of order $n_p$

$$\rho(x) = (x - z_p)^{n_p} e^{-S(x)}$$

generic flow around a pole: drift

$$K(z) = \frac{\rho'(z)}{\rho(z)} = \frac{n_p}{z - z_p} - S''(z)$$

- attractive/repulsive directions
- angular dependence

multiple circlings of the pole not expected (see below)
Pole in simple, generic model

properties of distribution $P(x, y)$ for generic case

$$\rho(x) = (x - z_p)^n p e^{-\beta x^2} \quad \beta \in \mathbb{R} \quad z_p = x_p + iy_p \in \mathbb{C}$$

follow analysis of GA, Giudice, ES, 1306.3075 (Annals of Physics)

- stripes in $xy$ plane where $P(x, y) = 0$
- decay at $|y| \to \infty$ no problem
- $y_p^2 < 2n_p/\beta$ : $P(x, y) \neq 0$ when $0 < y < y_p$
- $y_p^2 > 2n_p/\beta$ : $P(x, y) \neq 0$ when $0 < y < y_- < y_p$

pole on edge

pole outside distribution
Pole in simple, generic model

- pole outside: CL reproduces exact results, formal derivation holds
- pole on edge: depends on parameter values, i.e. on properties of distribution

Example: \( z_p = i \quad n_p = 2 \quad \beta = 1.6, 3.2, 4.8 \)

\[ \langle z^n \rangle \]

for \( n = 1, 2, 3, 4 \)

- \( \beta = 1.6 \quad \times \)
- \( \beta = 3.2 \quad \checkmark \)
- \( \beta = 4.8 \quad \checkmark \)
Pole in simple, generic model

compare distributions: \( P(x, y) \neq 0 \) for \( 0 < y < y_p = 1 \)

- small \( \beta \): \( P(x, y) \neq 0 \) right up to the pole
- larger \( \beta \): much faster decay

small \( \beta \): boundary terms at \( z = z_p \) due to partial integration
\( \Rightarrow \) CL not valid
Pole in simple, generic model

partially integrated distribution

\[ P_y(y) = \int dx \, P(x, y) \]

- small \( \beta \): \( P(x, y) \to 0 \) linearly
- larger \( \beta \): \( P(x, y) \to 0 \) exponentially

boundary terms for small \( \beta \): CL not valid
no boundary terms for larger \( \beta \): CL valid

consistent with formal derivation
Towards more realistic models

- carry over the essence to more realistic models
- devise diagnostics applicable also in QCD

**U(1) one-link model** (used many times)

\[ \rho(x) = [1 + \kappa \cos(x - i\mu)]^{np} \exp(\beta \cos x) \]

findings (roughly): \[ \kappa < 1: \text{CL } \checkmark \]

\[ \kappa > 1: \text{CL } \times \]
Towards more realistic models

- carry over the essence to more realistic models
- devise diagnostics applicable also in QCD

**U(1) one-link model**

(used many times)

GA, IOS, 0807.1597 (JHEP), Mollgaard, Splittorff, 1309.4335 (PRD)

\[
\rho(x) = [1 + \kappa \cos(x - i\mu)]^{n_p} \exp(\beta \cos x)
\]

findings (roughly):

\( \kappa < 1: \text{CL } \checkmark \)
\( \kappa > 1: \text{CL } \times \)

consider

\( \beta = 0.3 \quad \kappa = 2 \quad \mu = 1 \quad n_p = 1, 2, 4 \)

- poles at \( z_p = \pm x_p + i\mu \)
- distribution \( P(x, y) \neq 0 \) in strip only, \( y_- < y < y_+ \)
- strong \( n_p \) dependence on correctness
U(1) one-link model

\[ \beta = 0.3 \quad \kappa = 2 \quad \mu = 1 \quad n_p = 1, 2, 4 \]

\[ \text{Re} \langle e^{ikz} \rangle \quad \text{for} \quad k = -2, -1, 1, 2 \]

strong dependence on order of zero, \( n_p \)
$n_p = 2$: classical flow

- distribution contained in strip, poles inside strip
- but poles pinch the distribution: two $\sim$ disconnected regions $\Rightarrow$ zero acts as bottleneck, even in $\mathbb{C}$
- no circling of poles
U(1) one-link model

partially integrated distribution

\[ P_x(x) = \int dy \, P(x, y) \]

- small \( n_p \): \( P(x, y) \rightarrow 0 \) linearly at pole
- larger \( n_p \): \( P(x, y) \rightarrow 0 \) rapidly

boundary terms for small \( n_p \): CL not valid
no boundary terms for larger \( n_p \): CL valid
Extend to more realistic models

- complexified configuration space not accessible
- use complex determinant $D$ with weight $D^{n_p}$ instead

Determinant in U(1) model for $n_p = 2$:

- $n_p = 1$
- $n_p = 2$
- $n_p = 4$

Pole pinches the distribution, $P \to 0$ at $\text{Re det } D = 0$
Extend to more realistic models

- two disconnected regions:
  \[ \text{Re det } D \leq 0 \]

- treat as separate regions with constrained partition functions \( Z_{\pm} \)

- positive/negative weights

\[ w_{\pm} = \frac{Z_{\pm}}{Z_+ + Z_-} \]

- typically \( w_- \ll w_+ \)
SU(3) effective one-link model

see also poster by Nucu Stamatescu at XQCD16

same structure observed in more realistic models

scatter plot of complex determinant

- model designed to understand heavy dense QCD
- pole pinches the distribution, even in $\mathbb{C}$
- separate analysis of pos/neg parts possible
Extend to more realistic models

analysis of determinant

- easy to extend to heavy dense QCD
- full QCD numerically more intensive

but same principle holds

- two disjunct distributions
- zero/pole acts as a bottle neck
- higher order of zero (larger $n_p$):
  - stronger drift towards and then away from pole
  - stronger pinching
  - typically better agreement with expected results

see next talk by Dénes Sexty and poster by Nucu Stamatescu at XQCD16
Summary

- zero of order $n_p$ $[\text{det } D]^{n_p}$

- formal derivation revisited, meromorphic drift

- common features in all models
  - pole pinches the distribution
  - two disjunct regions
  - can be analysed separately
  - larger $n_p$ typically yields better results

- not specific to simple models

- $\text{Re } \text{det } D$ is relevant variable, accessible in (HD)QCD

see next talk by Dénes Sexty