On complex Langevin dynamics and zeroes of the fermion determinant

Gert Aarts

with Erhard Seiler, Dénes Sexty and Nucu Stamatescu

Swansea University
Prifysgol Abertawe

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:

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

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

$$K(z) = \nabla_z \rho(z) / \rho(z) \qquad K_x = \mathrm{Re}\, K(z) \qquad K_y = \mathrm{Im}\, K(z)$$

equivalence: $\langle O \rangle_{\rho(t)} \stackrel{?}{=} \langle O \rangle_{P(t)}$

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

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

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 $Z = \int DU \det M(U) e^{-S_{\rm YM}}$

$\det M(U) = 0$ for some $U \in$ 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

- $\dot{O}(z;t) = \tilde{L}O(z;t)$ $\qquad \tilde{L} = [\nabla_z + K(z)]\,\nabla_z$
- 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

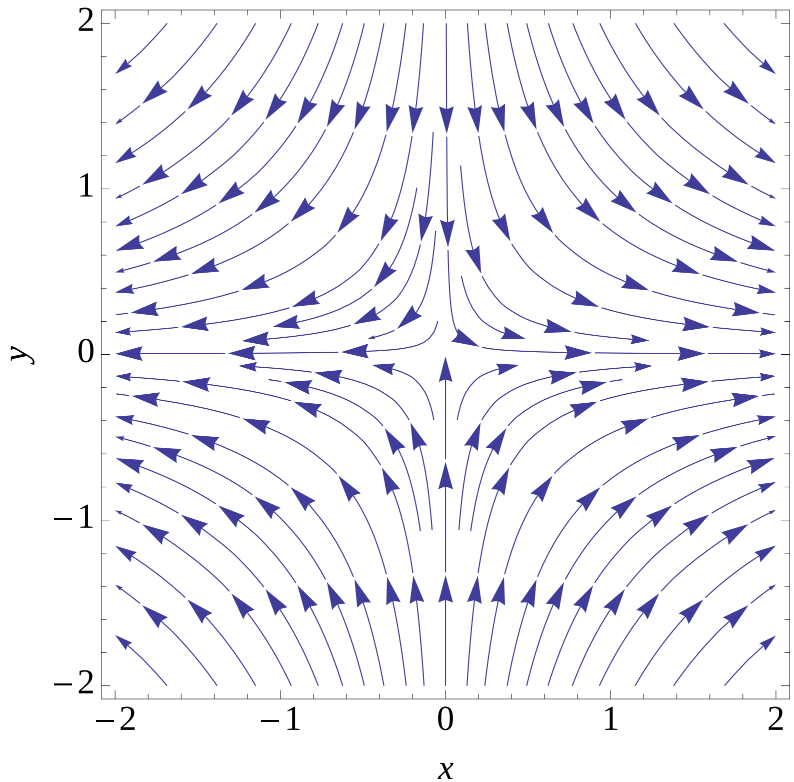
- outside the distribution
- on the edge of the distribution
- inside the distribution

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

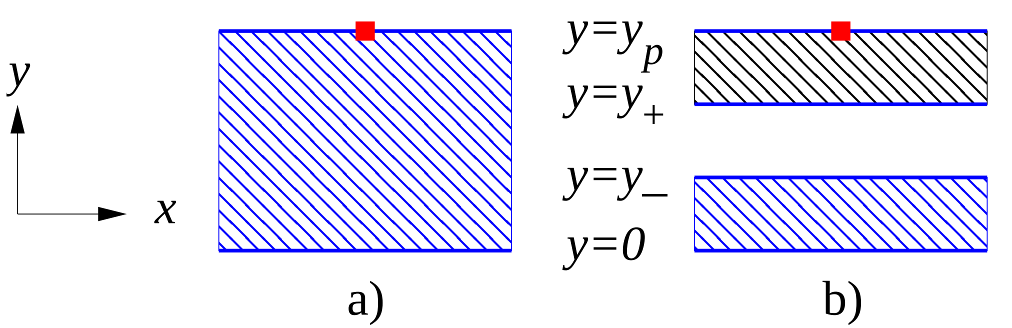
properties of distribution $P(x, y)$ for generic case

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

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
- $y_p^2 < 2n_p/\beta$: $\quad P(x, y) \neq 0$ when $0 < y < y_p$
- $y_p^2 > 2n_p/\beta$: $\quad P(x, y) \neq 0$ 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

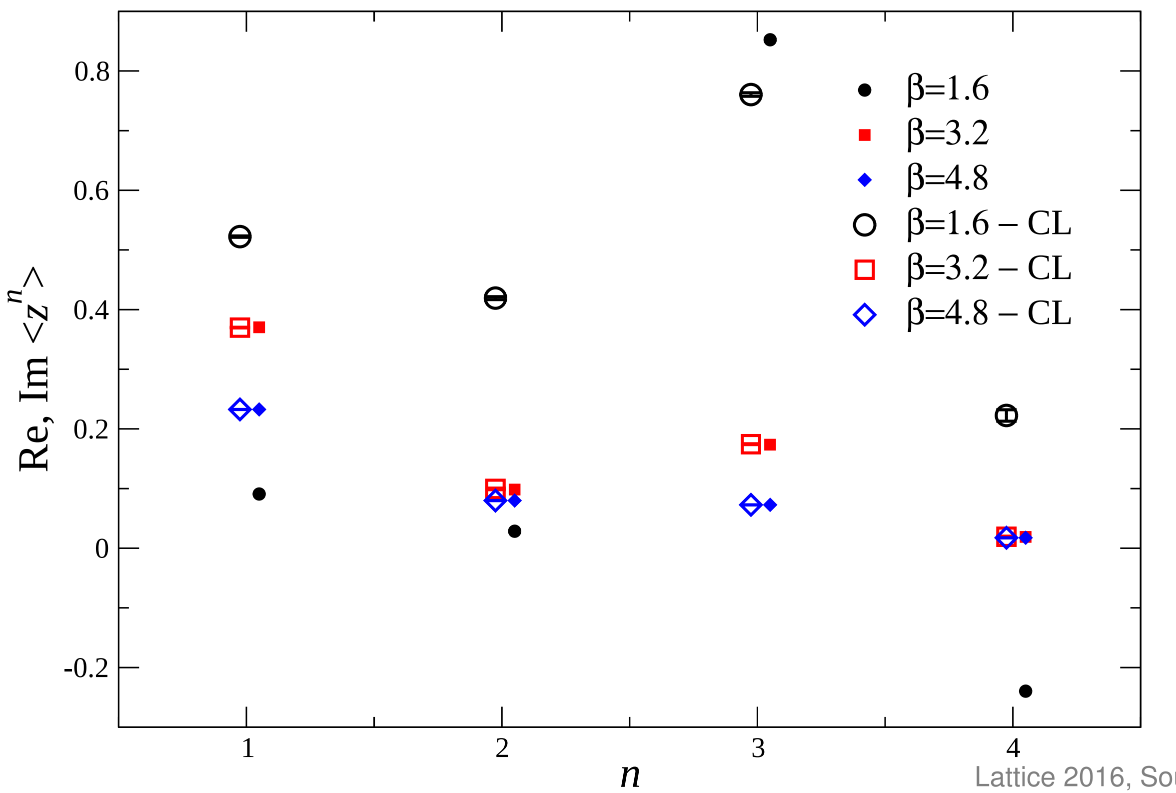
example: $z_p = i$ $n_p = 2$ $\beta = 1.6, 3.2, 4.8$

$\langle z^n \rangle$

for

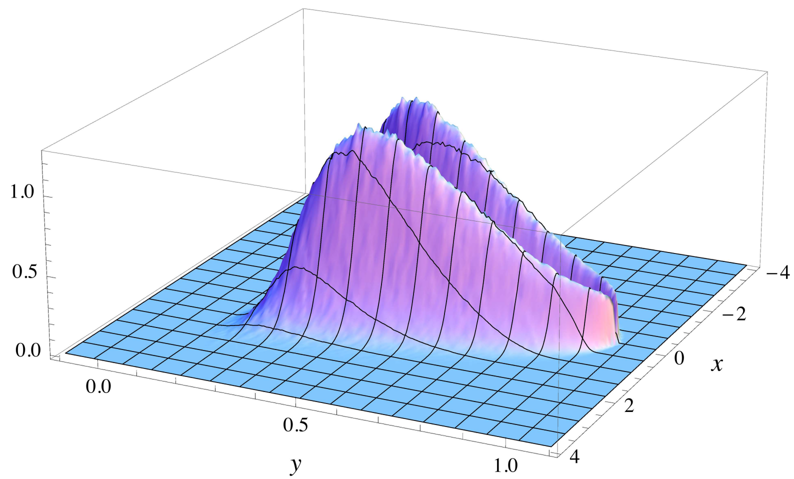
$n = 1, 2, 3, 4$

$\beta = 1.6$ ✗
$\beta = 3.2$ ✓
$\beta = 4.8$ ✓

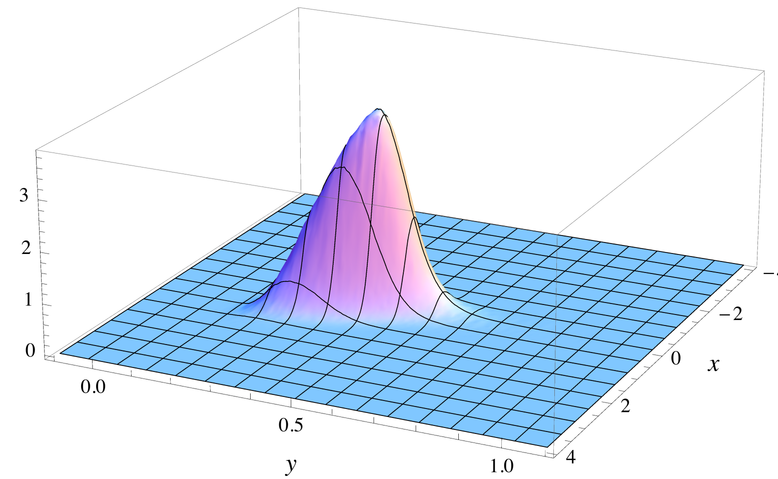


Pole in simple, generic model

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



$\beta = 1.6$



$\beta = 3.2$

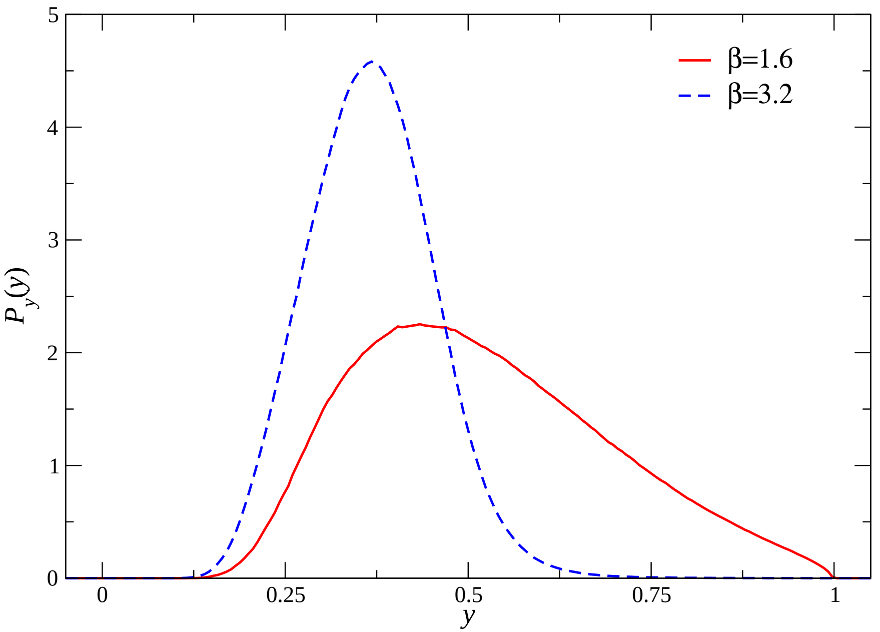
- small β: $P(x,y) \neq 0$ right up to the pole
- larger β: much faster decay

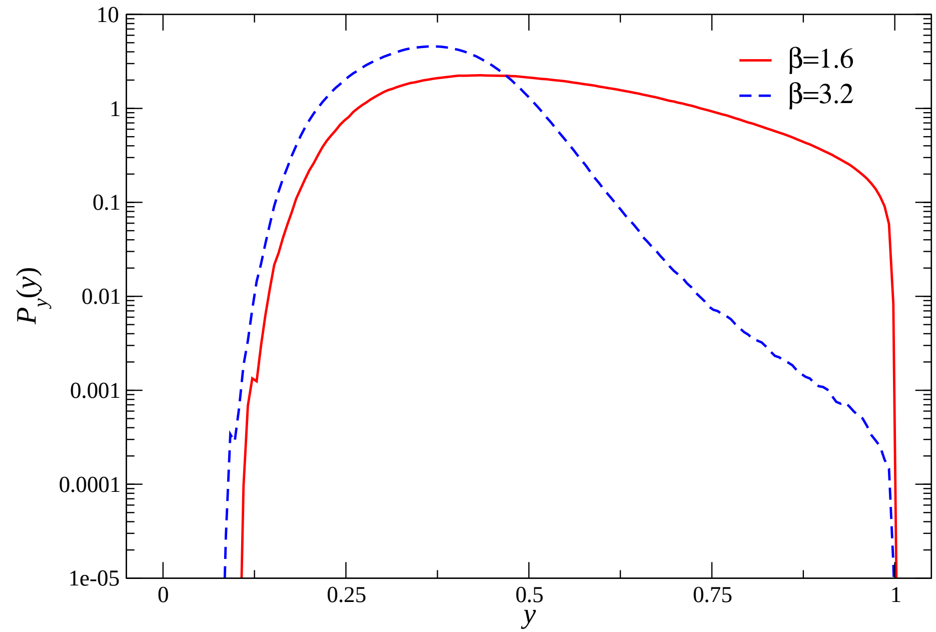
small β: boundary terms at $z = z_p$ due to partial integration

$\Rightarrow$ CL not valid

Pole in simple, generic model

partially integrated distribution $P_y(y) = \int dx\, P(x,y)$





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

consistent with formal derivation

boundary terms for small β: CL not valid
no boundary terms for larger β: CL valid

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): $\kappa < 1$: CL ✓ $\kappa > 1$: CL ✗

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): $\kappa < 1$: CL ✓ $\kappa > 1$: CL ✗

consider $\beta = 0.3$ $\kappa = 2$ $\mu = 1$ $n_p = 1, 2, 4$

- 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

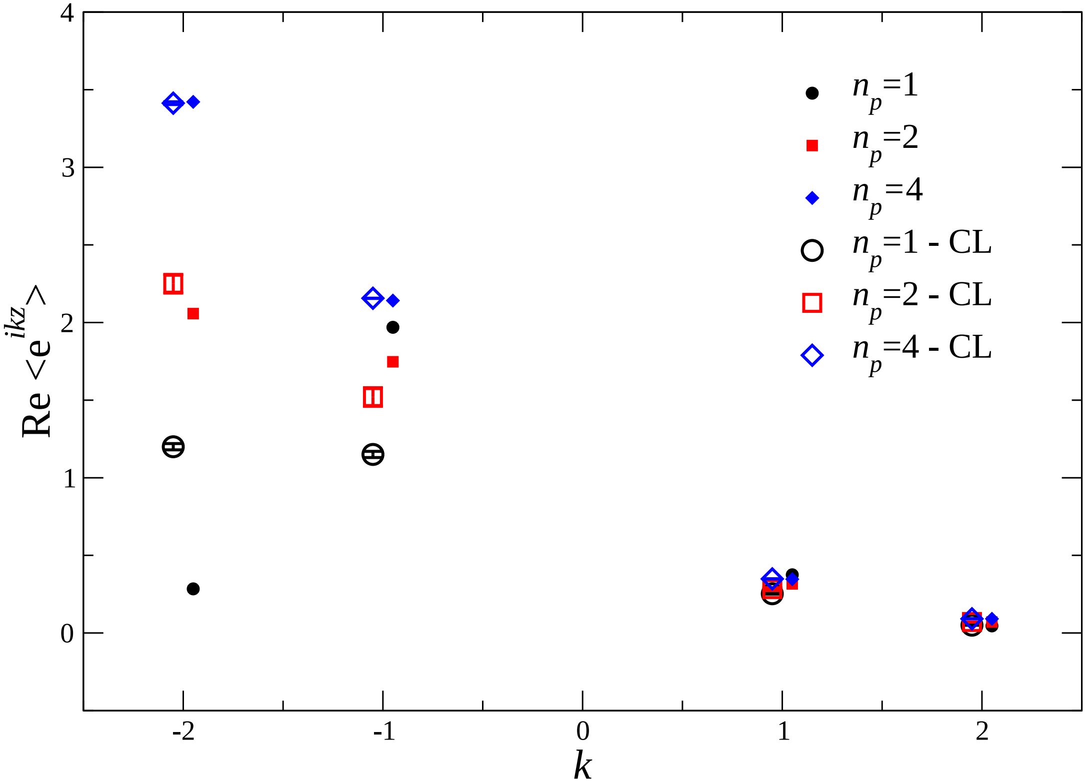
U(1) one-link model

$\beta = 0.3 \qquad \kappa = 2 \qquad \mu = 1 \qquad n_p = 1, 2, 4$

$n_p = 1$ ✗

$n_p = 2$ ✗

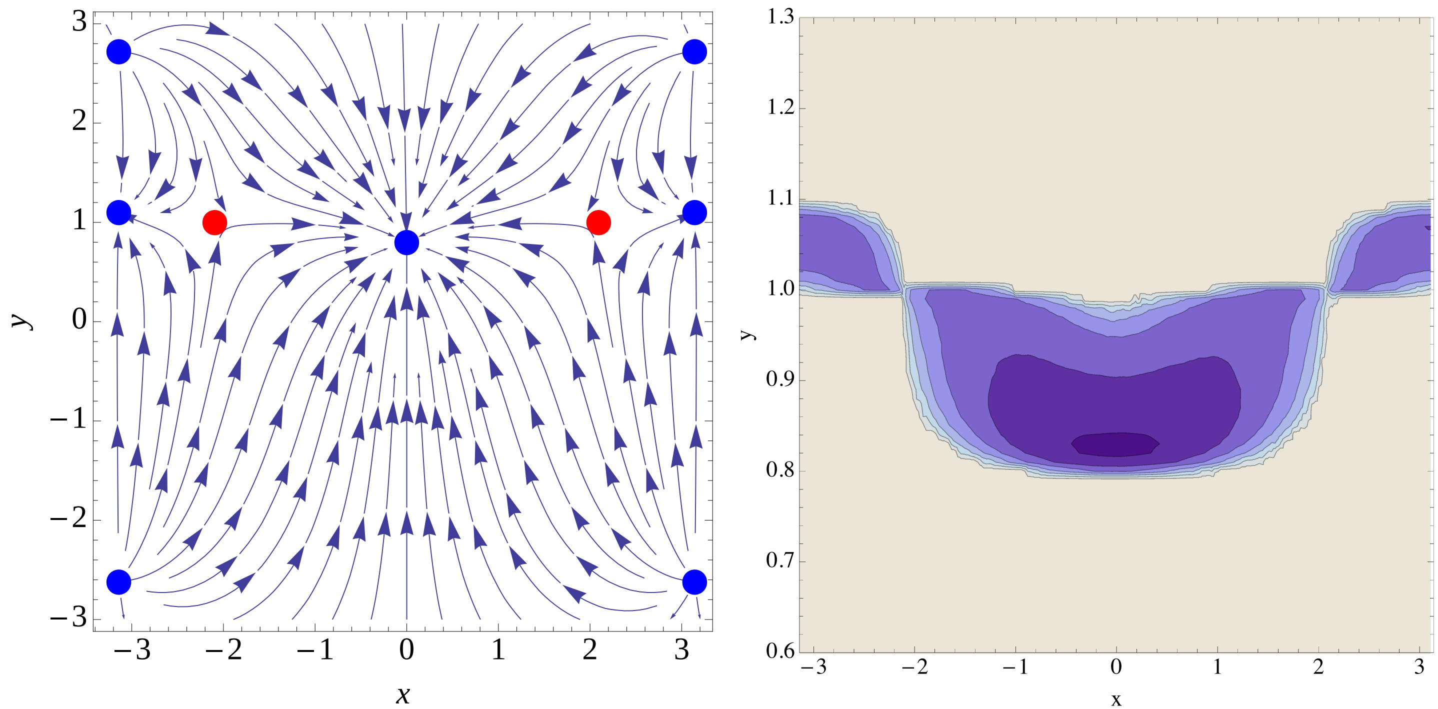
$n_p = 4$ ✓



$\mathrm{Re}\langle e^{ikz}\rangle$ for $k = -2, -1, 1, 2$

strong dependence on order of zero, n_p

U(1) one-link model

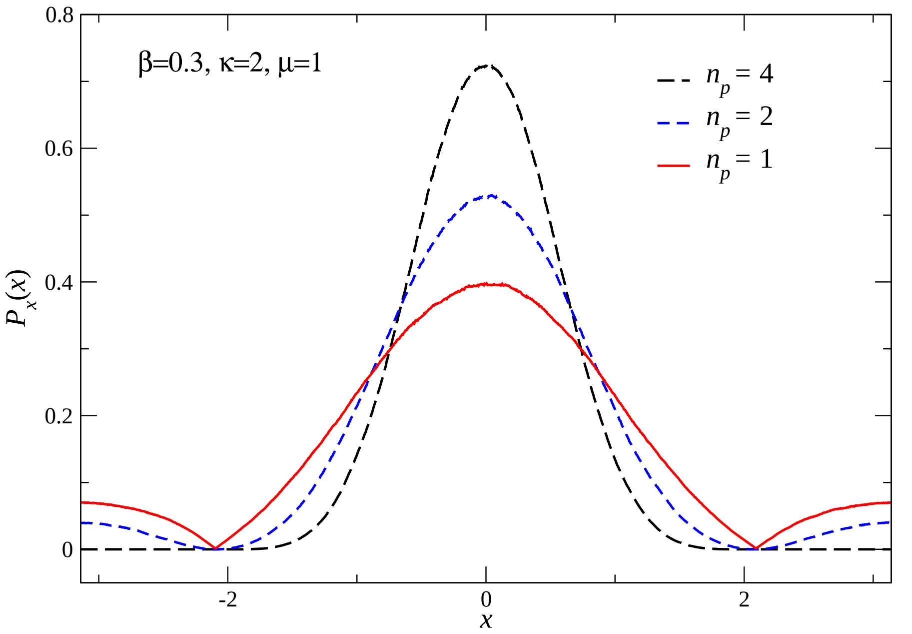


$n_p = 2$: classical flow histogram (logarithmic scale)

- 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 $\quad P_x(x) = \int dy\, P(x,y)$



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

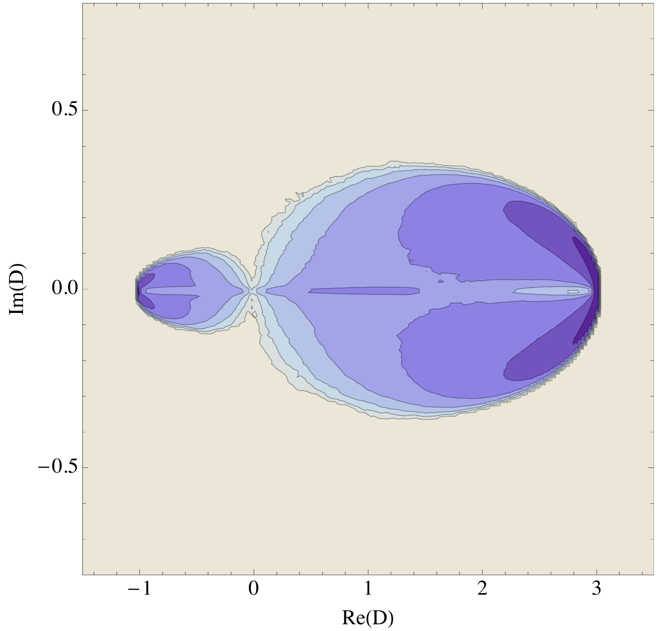
consistent with formal derivation

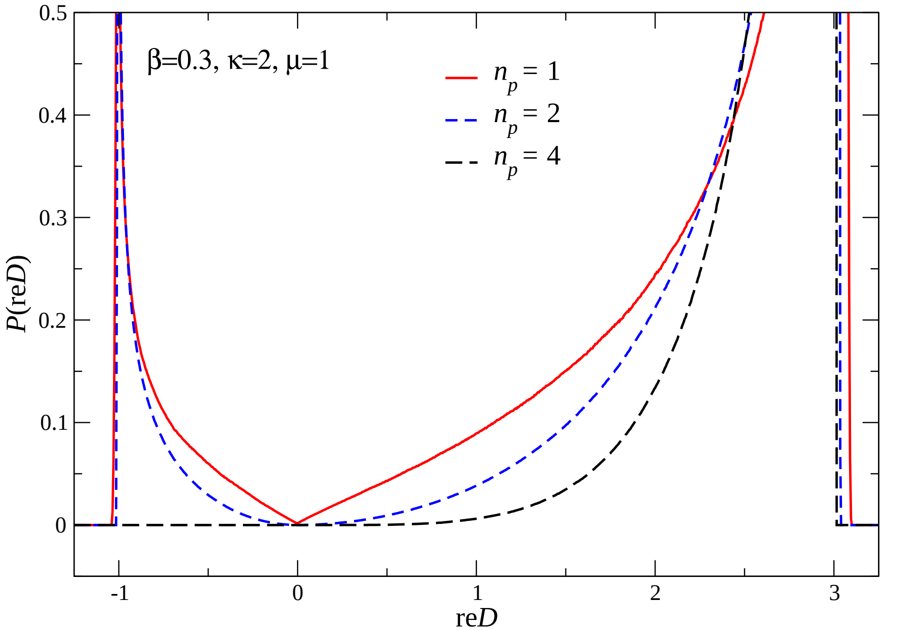
boundary terms for small n_p: CL not valid
no boundary terms for larger n_p: CL valid

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 $n_p = 2$:





histogram (logarithmic scale) re(D)

- pole pinches the distribution, $P \to 0$ at $\mathrm{Re}\det D = 0$

Extend to more realistic models

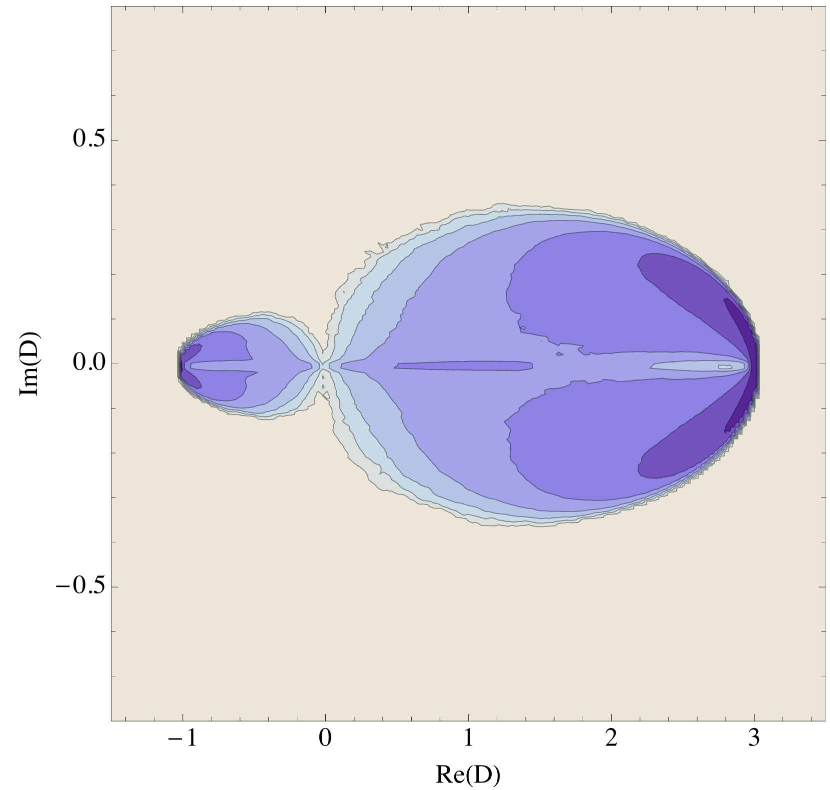
- two disconnected regions:

$$\mathrm{Re}\det D \lessgtr 0$$

- treat as separate regions with constrained partition functions $Z_\pm$
- positive/negative weights

$$w_\pm = \frac{Z_\pm}{Z_+ + Z_-}$$

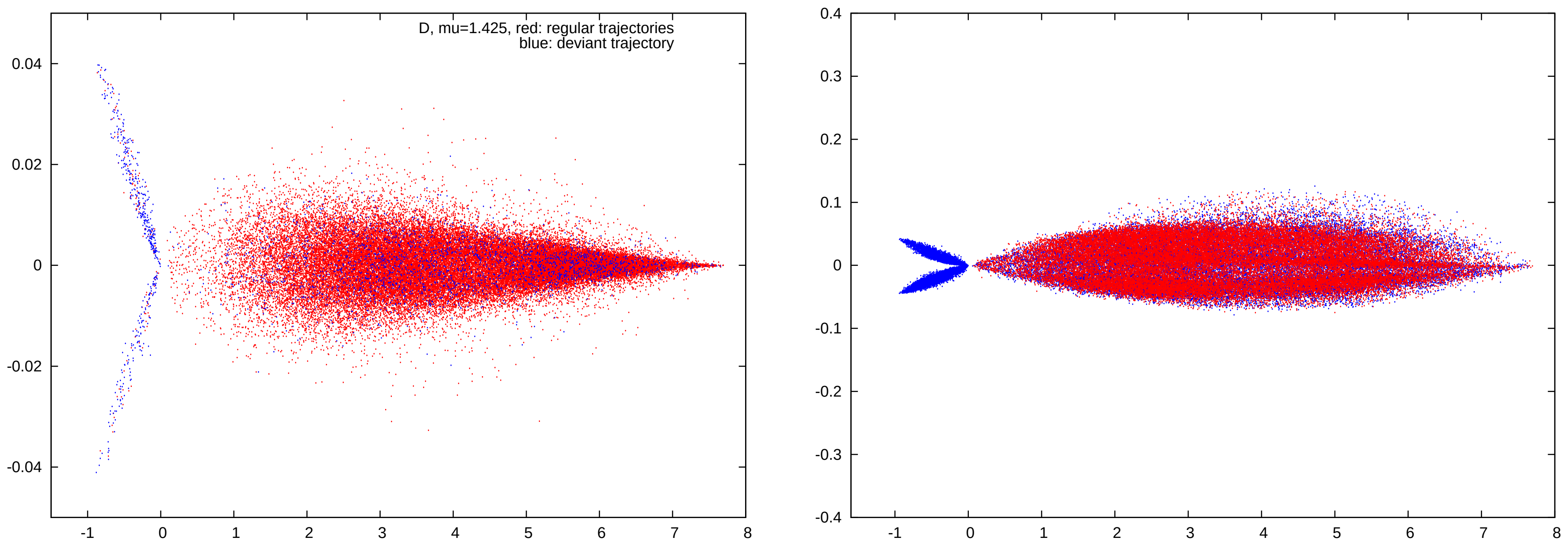
- typically $w_- \ll w_+$



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 $\qquad [\det D]^{n_p}$
- 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
- $\mathrm{Re}\det D$ is relevant variable, accessible in (HD)QCD

see next talk by Dénes Sexty