Complex Langevin with meromorphic drift

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part of collective effort involving G. Aarts, J. Pawlowski, D. Sexty, I.-O.Stamatescu,....

1. Sign problem

Functional measure $\rho \propto e^{-S}$ in Euclidean QFT not always positive:

- Real time Feynman integral
- Topological terms – nonzero vacuum angle θ
- Finite density - chemical potential
- $\ldots$

ρ Signed or Complex measure.

General Idea:

(L. L. Salcedo 1993, 1997, 2007; Weingarten 2002)

Replace

complex (signed) measure ρ on $\mathcal{M}$ by

probability measure P on complexification $\mathcal{M}_c$

such that for holomorphic observables $\mathcal{O}$

$$\boxed{\langle \mathcal{O} \rangle \equiv \int_{\mathcal{M}} \mathcal{O} \rho d\mu = \int_{\mathcal{M}_c} \mathcal{O} dP \,.}$$

Note: P underdetermined.

General recipe

Complex Langevin (G. Parisi 1983, J. Klauder 1983): Works 'in principle'.

Recent successes include:

- HDM approximation for QCD (β not too small) (E. S., D. Sexty, I.-O. Stamatescu 2012)
- Full QCD (β not too small) (D. Sexty 2013)

Important tool: Gauge cooling

2. Conditions for Correctness

'Flat' case: defined on $\mathcal{M} = \mathbb{R}^n$ or $\mathcal{M} = U(1)^n$.
analytic extension of $\mathcal{M}$: $\mathcal{M}_c$.

Complex Langevin on $\mathcal{M}_c$

$$dz = K dt + dw, \quad K = -\nabla S$$

dw real Wiener increment $dw = \eta(t)dt$, η white noise).

$$\begin{aligned} dx =& K_x dt + dw, \quad & K_x = \mathrm{Re}\, K \\ dy =& K_y dt, & K_y = \mathrm{Im}\, K \end{aligned}$$

real stochastic process on $\mathcal{M}_c$.

Result (formal)

$$\boxed{\langle \mathcal{O} \rangle_{\rho(t)} = \langle \mathcal{O} \rangle_{P(t)} \quad \forall t \geq 0}$$

LHS: evolution of complex measure ρ;
RHS: evolution of probability measure P
Requirements:

- agreement of initial conditions
- holomorphy of drift $K \equiv K_x + iK_y$
- sufficient decay of $P\mathcal{O}$ at imaginary infinity
  Needed because derivation uses
  integration by parts without boundary terms

How smooth is $P(x,y)$*?*

Expect:

Elliptic regularity in $x \Longrightarrow P$ smooth in x.

No noise in imaginary part $\Longrightarrow P$ may have kinks in y.

Problems

Problems arise if assumptions don't hold:

#1: Slow decay

#2: Drift K has poles

3. Problem #1: slow decay

Typical:

$\mathcal{M}$ compact, $\mathcal{M}_c$ noncompact

Example: $\mathcal{M} = SU(N)$, $\mathcal{M}_c = SL(N, \mathbb{C})$

Note:

Holomorphic functions grow $\Longrightarrow$

Drift K grows; observables $\mathcal{O}$ as well $\Longrightarrow$

Large excursions possible

"Skirts", "tails" of distribution P on $\mathcal{M}_c$.

Integration by parts without boundary terms:

Questionable

Simple example

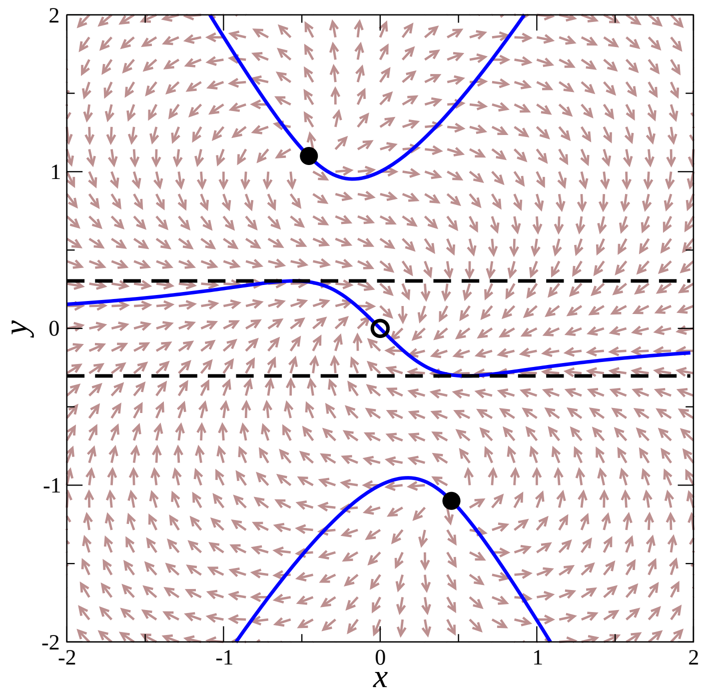
Quartic model: $\mathcal{M} = \mathbb{R}$, $\mathcal{M}_c = \mathbb{C}$:

$$S = \frac{1}{2}\sigma x^2 + \frac{1}{4}\lambda x^4, \quad \sigma = A + iB, \ \ \lambda = 1\,.$$

(G. Aarts, P. Giudice, E. S. 2013)

Lucky case

$3A^2 > B^2$: Process confined in strip.



$\sigma = 1 + i, \lambda = 1$. Solid lines: $K_y = 0$.

CLE results correct

4. Problem #2: poles in drift

If ρ has zeroes in $\mathcal{M}_c$

$\Longrightarrow$ drift only meromorphic (positive integer residues)

$\Longrightarrow$ Problem:

$\dot{\mathcal{O}} = L\mathcal{O}$ does not preserve holomorphy of $\mathcal{O}$, justification of CLE destroyed.

Full QCD:

Fermion determinant

$$\det(\not{D}_U + M)$$

generically vanishes for some $U \in SL(3,\mathbb{C})$.

But: D. Sexty 2013 finds in QCD: eigenvalues avoid 0.

How poles affect justification

Integration by parts:

$$\frac{\partial}{\partial\tau}F(t,\tau) = -\int_{\mathbb{R}^2} L^T P(x,y;t-\tau)\mathcal{O}(x+iy;\tau)dxdy + \int_{\mathbb{R}^2} P(x,y;t-\tau)L\mathcal{O}(x+iy;\tau)dxdy = 0\,??$$

Possibly spoiled by boundary terms near poles (and ∞)

Existence of integrals?

Experience says 'yes'.

Assume single pole at $z = z_p$. First integrate over

$$G_\epsilon \equiv \{z = x + iy \,|\, |z - z_p| > \epsilon\}\,, \quad \epsilon \to 0 \quad \text{later}$$

Integration by parts over G_ϵ:
bulk terms cancel; remainder R_ϵ:

$$R_\epsilon \equiv -\int_{\partial G_\epsilon} P(x,y;t-\tau)\, n_x \partial_x \mathcal{O}(x+iy;\tau) + \int_{\partial G_\epsilon} \mathcal{O}(x+iy;\tau)(n_x\partial_x + \vec{n}\cdot\vec{K})P(x,y;t-\tau)ds\,. \quad (1)$$

where $\vec{n}$ outer normal, $\tilde{G}_\epsilon \equiv \{z = x+iy \,|\, |z-z_p| \leq \epsilon\}$.

A priori:

limit $\epsilon \to 0$ may be zero, finite or divergent.

Experience: Never divergent; $P(x_p, y_p) = 0$

Typically: $\mathcal{O}(z;t)$ has essential singularity at z_p.

Behavior of $\mathcal{O}(z;t)$ and $P(x,y,t)$ angle dependent.

5. How bad are poles?

Three possibilities:

(a) Pole outside support of P

(b) Pole at the boundary of support of P

(c) Pole really inside inside support of P (so far not encountered)

Three Toy models:

(1) $\rho(x) = (x - z_p)^{n_p} \exp(-\beta x^2)$

"one-pole model"

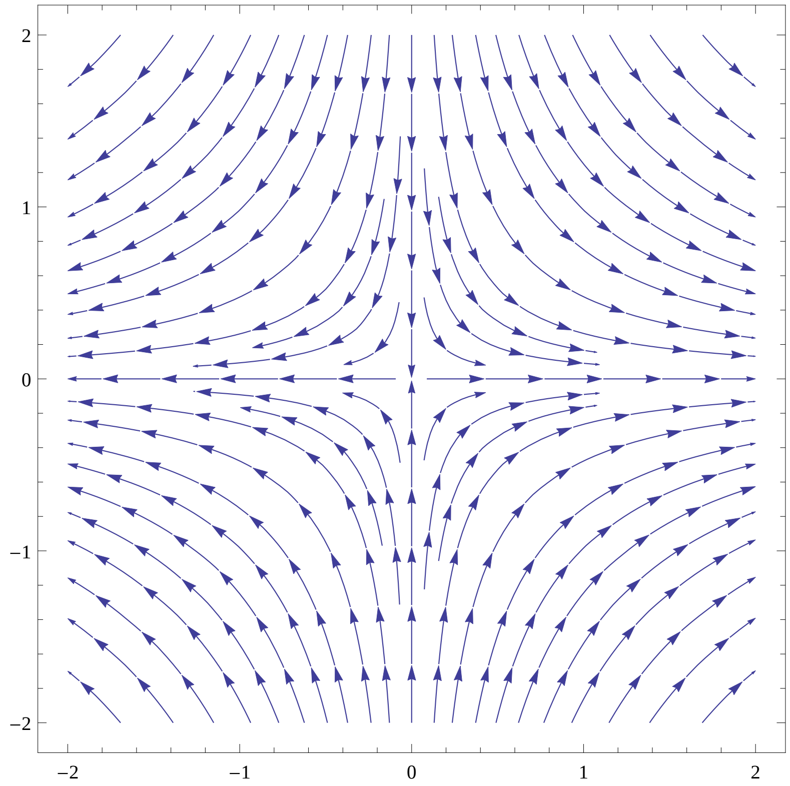
(2) $\rho(x) \equiv \exp(-S) = (1 + \kappa \cos(x - i\mu))^{n_p} \exp[\beta \cos(x)]$

"$U(1)$ one-plaquette model"

(3) $\ln \rho = \beta \sum_{i=1}^{3} \left(\mathrm{e}^{\alpha_i} \mathrm{e}^{imw_i} + \mathrm{e}^{-\alpha_i} \mathrm{e}^{-imw_i} \right) + \ln \mathrm{Det} + \ln \mathrm{H}$

"$SU(3)$ one-plaquette model"

Flow near pole



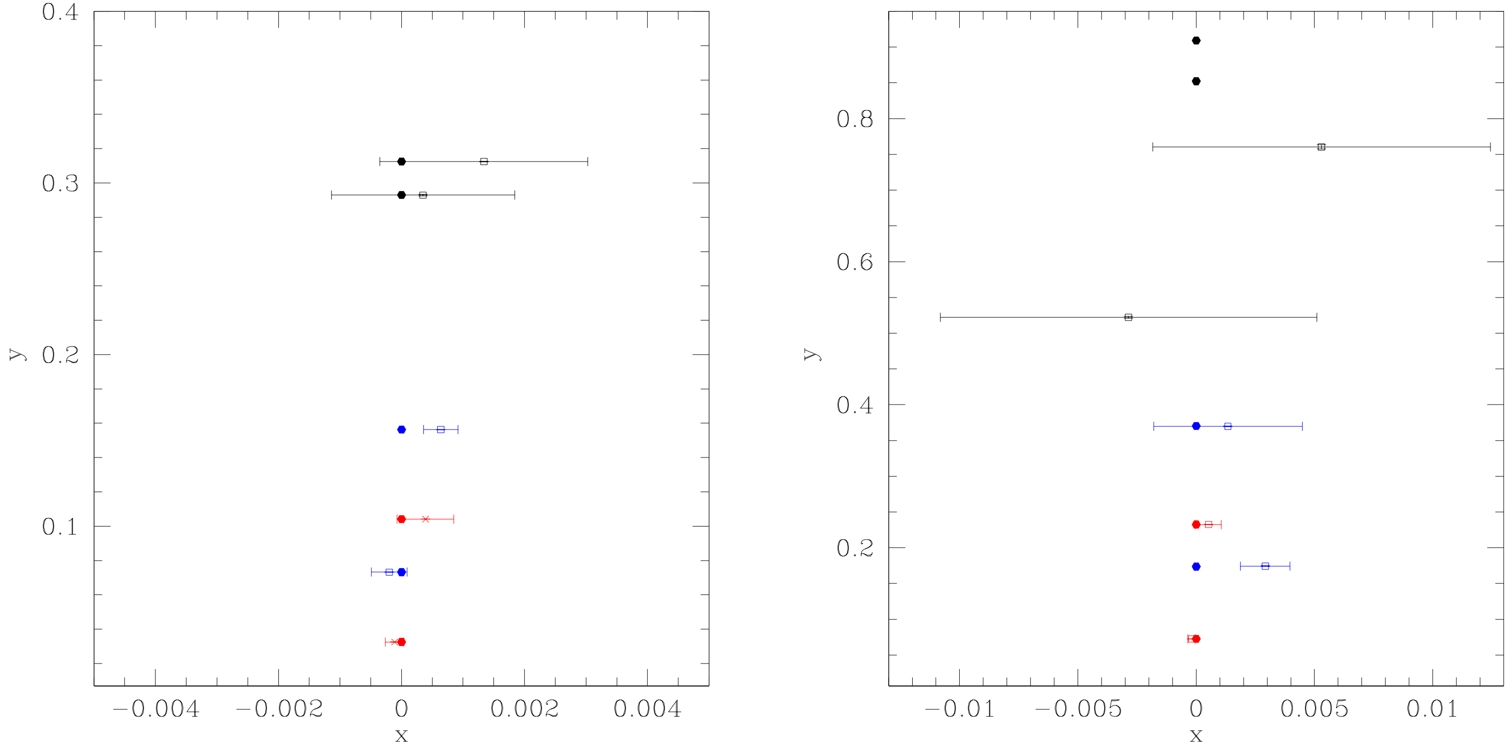
Pattern characteristic for any pole with positive residue.

Crossing of horizontal line through pole difficult.

5.a *One-pole model with* $z_p = i$

$$\rho(x) = (x-i)^{n_p}\exp(-\beta x^2)$$

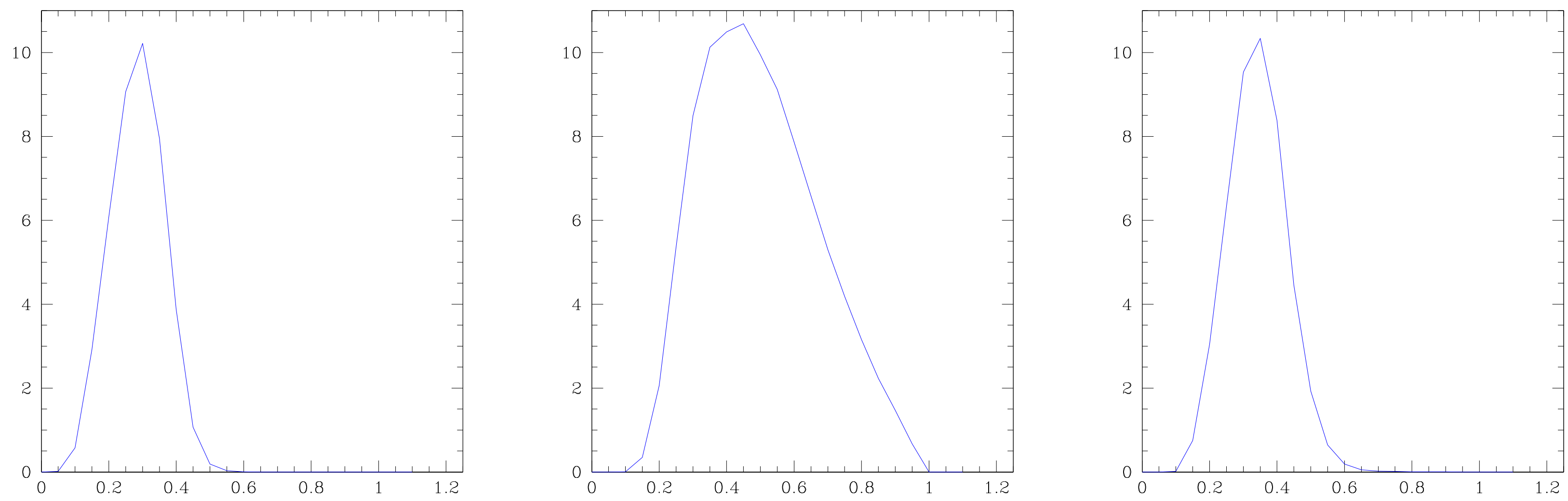
Data for $\langle z\rangle$ and $\langle z^3\rangle$



$n_p = 1$ $n_p = 2$

Black: $\beta = 1.6$, Blue: $\beta = 3.2$, Red: $\beta = 4.8$

Histograms $\int P(x,y)dx$ vs y



$\beta = 1.6\,, n_p = 1$ CL Reasonable

$\beta = 1.6,\ n_p = 2$ CL Bad

$\beta = 3.2, n_p = 2$ CL Reasonable

n_p larger: $\Longrightarrow$ P pushed towards pole

β larger: $\Longrightarrow$ P pushed away from pole

5.b One plaquette $U(1)$ *model*

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

Poles:

(1) $\kappa \leq 1$: $z_P = \pm\pi + i \cosh^{-1}(\kappa^{-1})$

(2) $\kappa > 1$: $z_P = \pm\frac{2\pi}{3} + i\mu$

Three examples:

$\kappa = 0.5, \beta = 1, \mu = 1$

$\kappa = 2, \beta = 0.3, \mu = 1$: the worst case

$\kappa = 2, \beta = 5, \mu = 1$

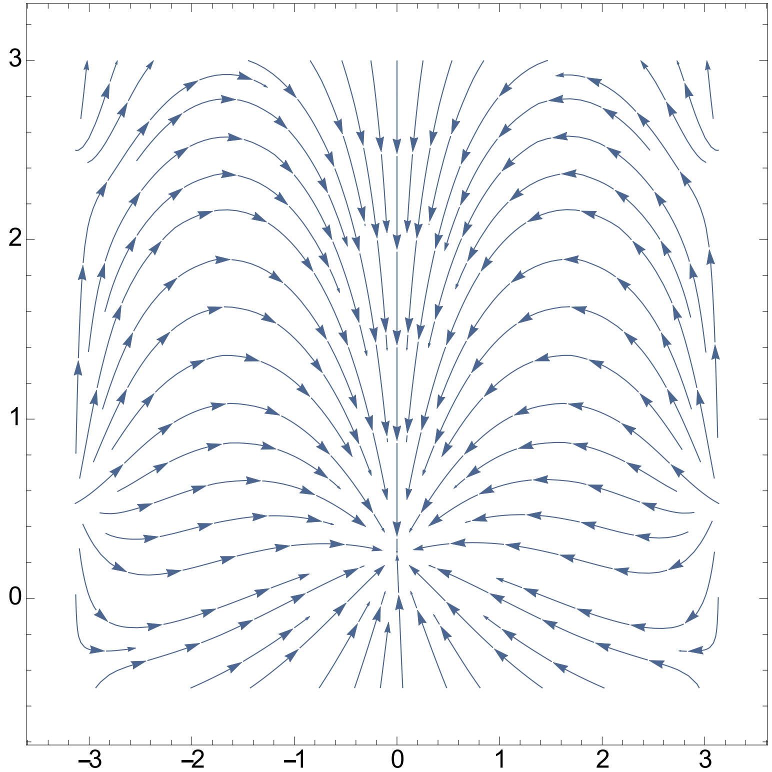
Determinant

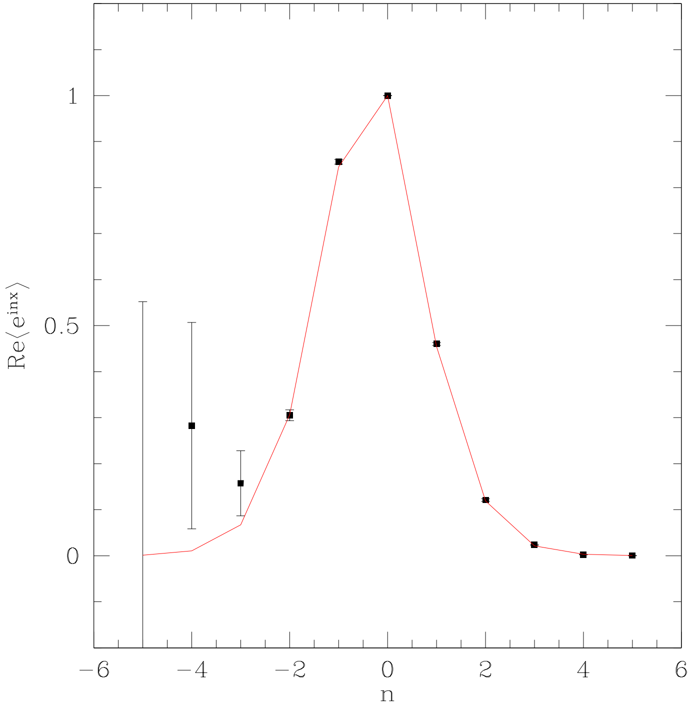
$$D(z) \equiv 1 + \kappa \cos(z - i\mu)$$

Two regions

$$G_{\pm} \equiv \{z \in \mathbb{C} | \pm \mathrm{Re} D(z) > 0\}$$

(a) $\kappa = 0.5, \beta = 1, \mu = 1, n_p = 1$

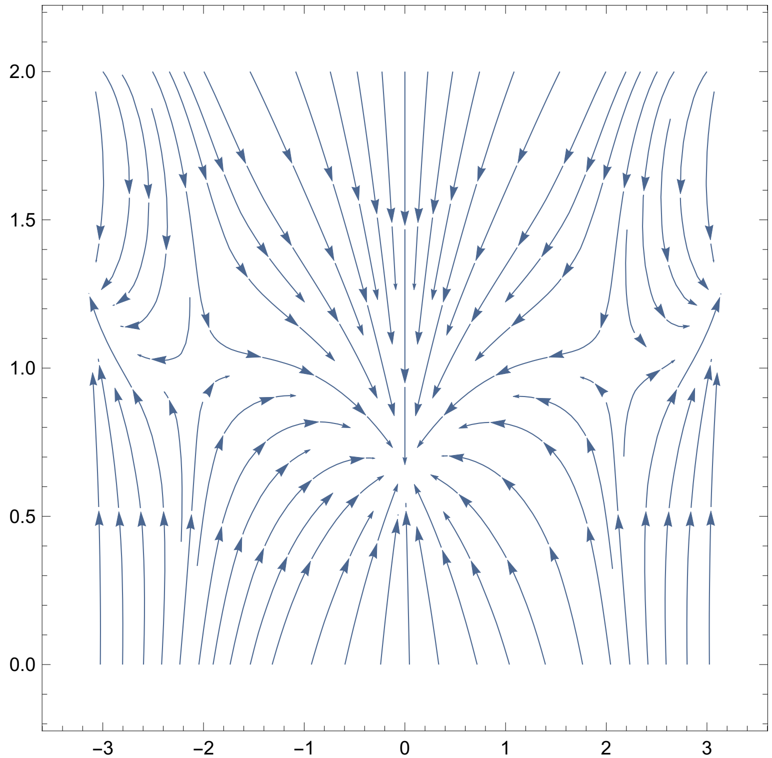


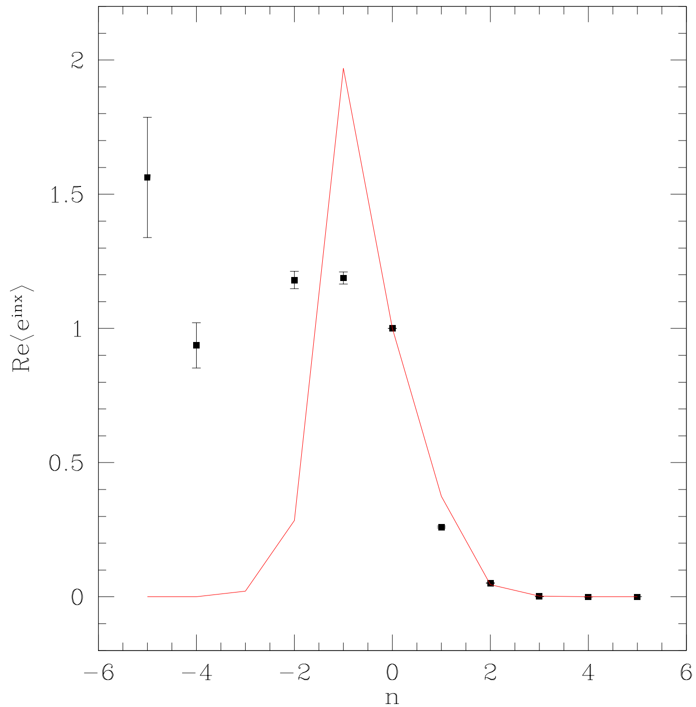


Left: flow pattern; only 1 attractive fixed point; large excursions upwards possible.

Right: $\langle e^{inz} \rangle$; red: exact

(b) $\kappa = 2, \beta = 0.3, \mu = 1, n_p = 1$

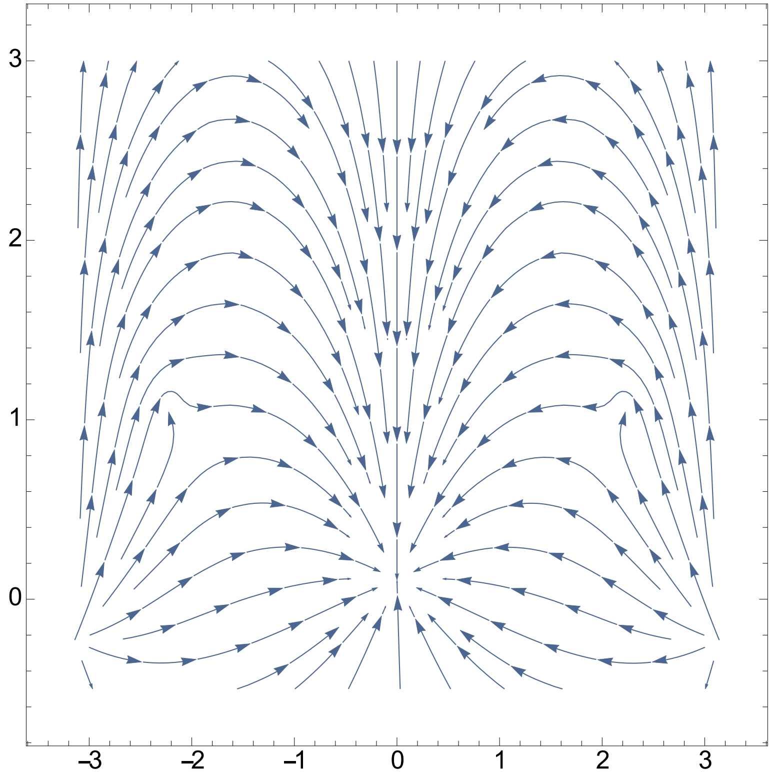


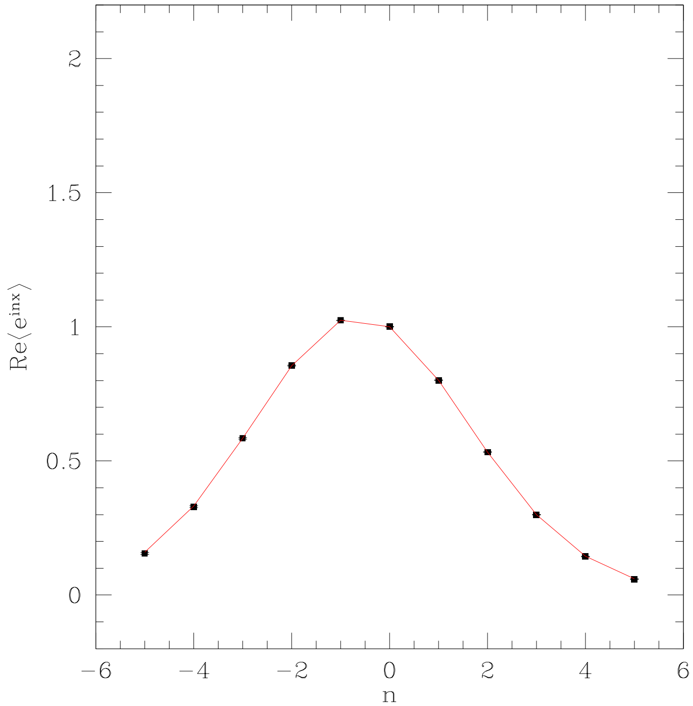


Left: flow pattern; secondary attractive fixed point at $\pm\pi + 1.3422i$. Right: $\langle e^{inz} \rangle$; red: exact

Note: Process confined to strip; no slow decay!

(c) $\kappa = 2, \beta = 5, \mu = 1, n_p = 1$

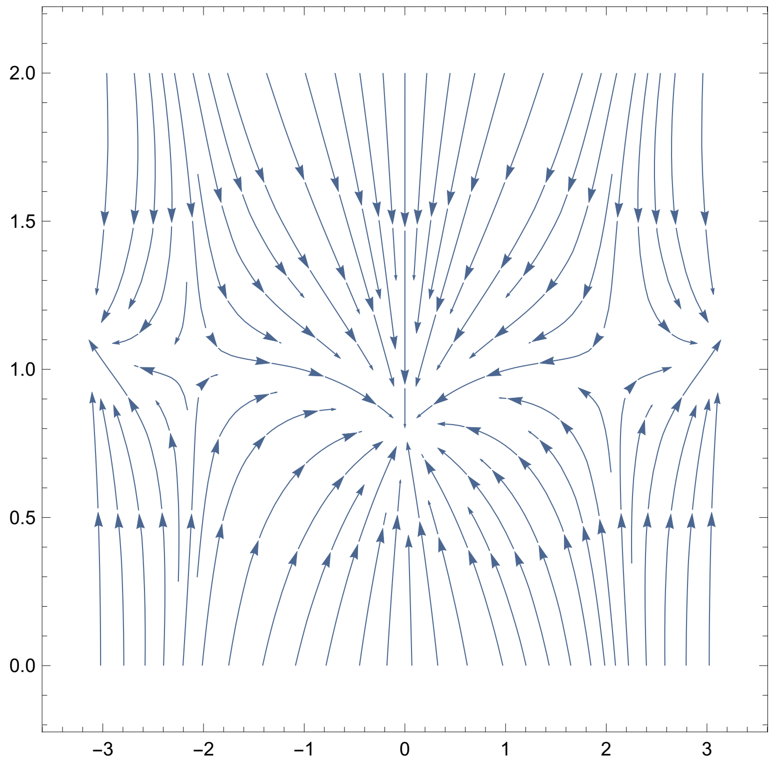


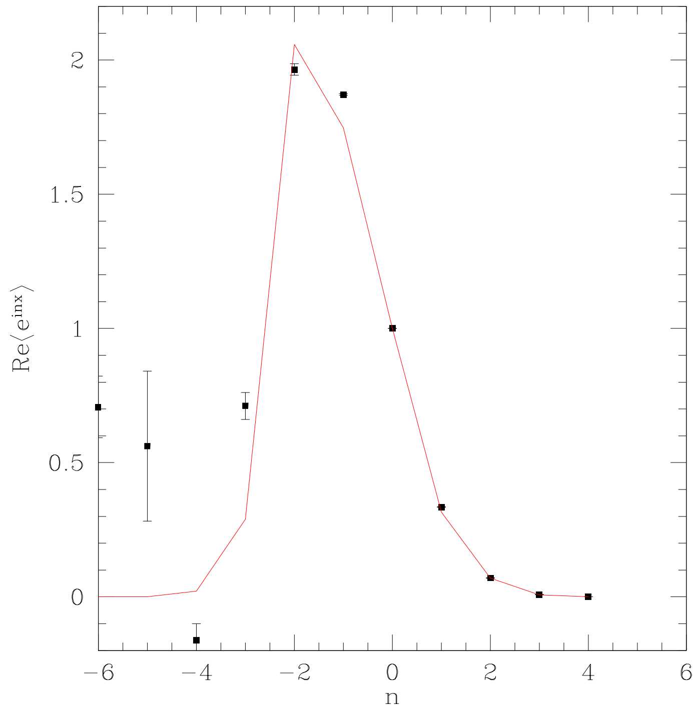


Left: flow pattern; only one attractive fixed point.

Right: $\langle e^{inz} \rangle$; red: exact

(d) $\kappa = 2, \beta = 0.3, \mu = 1, n_p = 2$

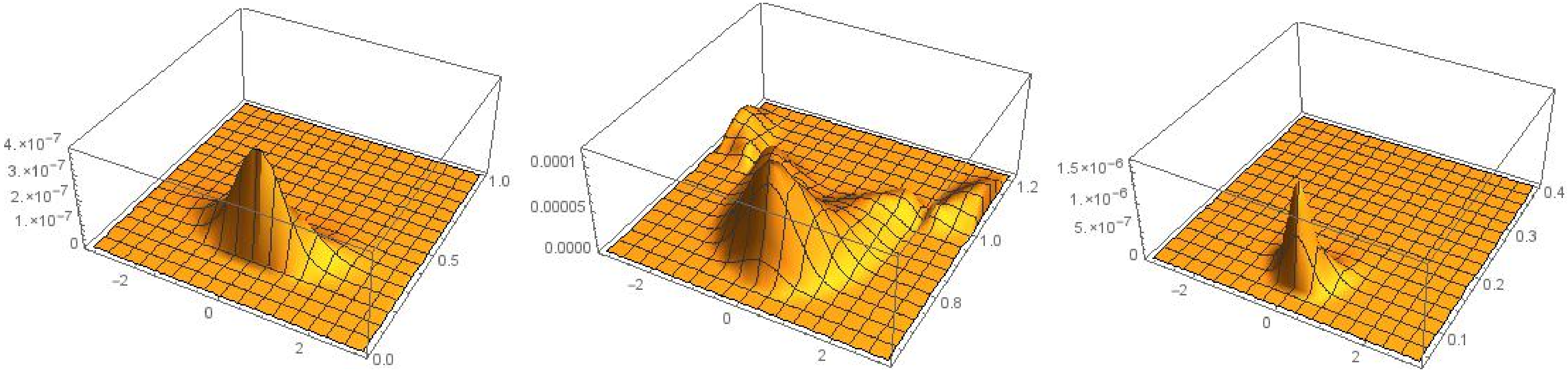




Left: flow pattern; secondary attractive fixed point at $\pm\pi + 1.25457i$. Right: $\langle e^{inz} \rangle_+$; red: exact

Note: Process still confined to strip; better than $n_p = 1$.

Histograms for $n_p = 2$



Left: $\kappa = 0.5, \beta = 1, \mu = 1$

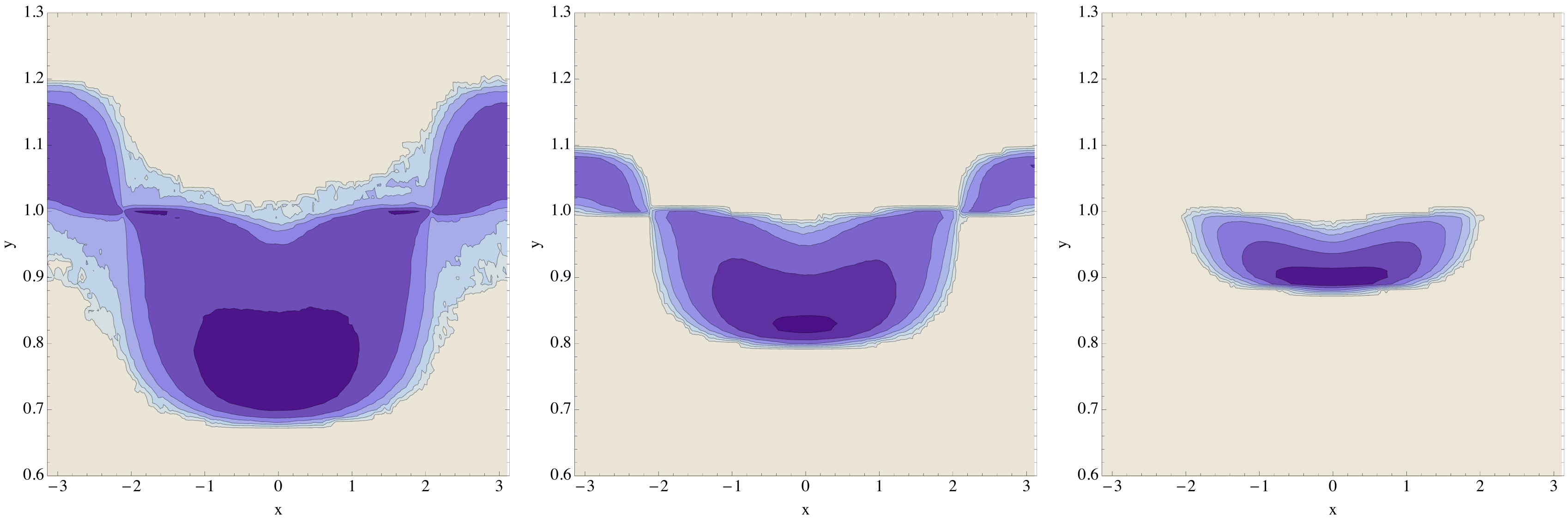
Middle: $\kappa = 2, \beta = 0.3, \mu = 1$

Right: $\kappa = 2, \beta = 5, \mu = 1$

Worst case:

$\kappa = 2, \beta = 0.3, \mu = 1$

Logarithmic contour plots for $\kappa = 2, \beta = 0.3, \mu = 1$

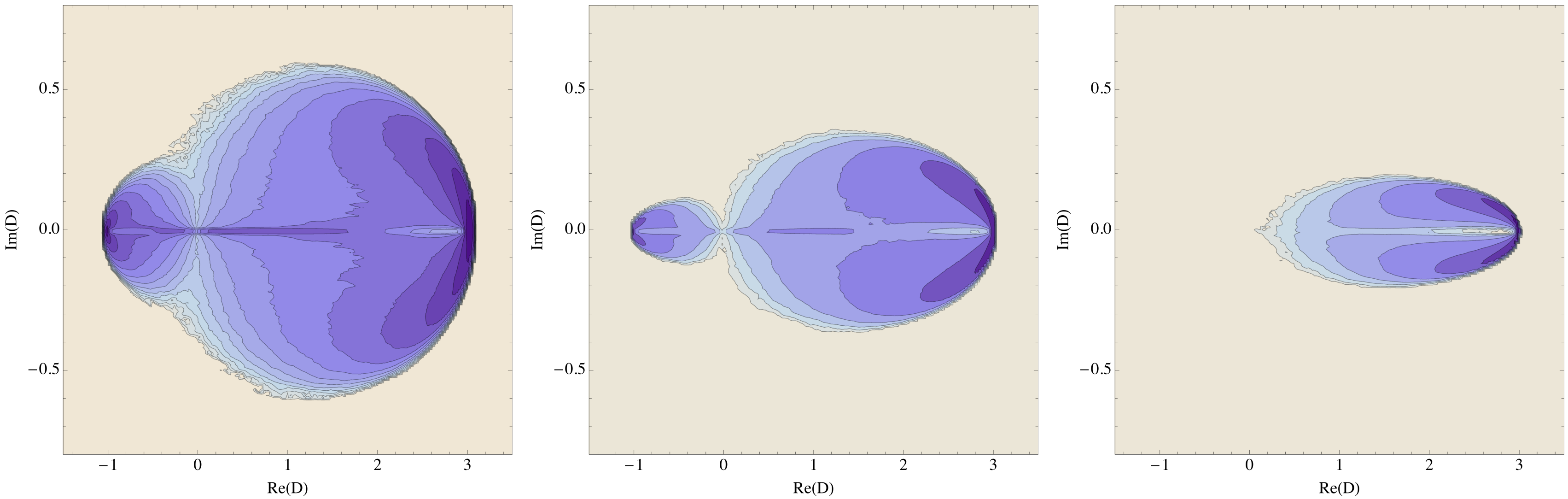


$n_p = 1$ $n_p = 2$ $n_p = 4$

Worst case:

$\kappa = 2, \beta = 0.3, \mu = 1$

Logarithmic contour plots for 'determinant'



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Restricting to $G_\pm$

G_- bad region? Restricting averages to $G_\pm$:

$$\langle\mathcal{O}\rangle_\pm \equiv \int_{x+i\mu\in G_\pm} \rho(x+i\mu)\mathcal{O}(x+i\mu)dx$$
$$= \int_{G_\pm} P(x,y)\mathcal{O}(x+iy)dxdy$$

CLE simulates different systems.

Note: $n_p \uparrow \implies$ relative weight of $G_- \downarrow$:

Let $r_- \equiv \int_{G_-}\rho / \int_{\mathbb{R}}\rho$

$n_p = 1 : r_- = -0.09551$

$n_p = 2 : r_- = 0.02733$

5.c $SU(3)$ one-plaquette model

Definitions: Always $w_1 + w_2 + w_3 = 0$

$$H = \sin^2 \tfrac{w_2 - w_3}{2} \sin^2 \tfrac{w_3 - w_1}{2} \sin^2 \tfrac{w_1 - w_2}{2}$$

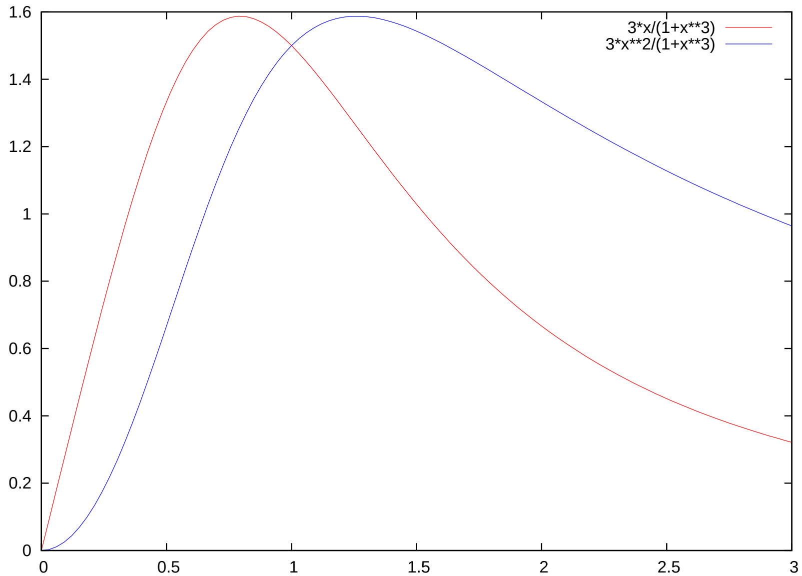
$$\mathrm{Det} = \left(\mathrm{D}\, \tilde{\mathrm{D}}\right)^2$$

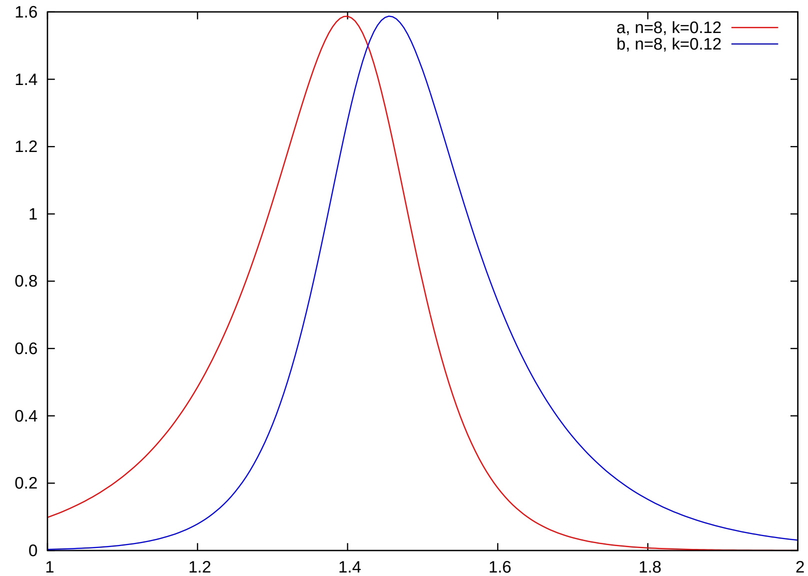
$$D = 1 + C\mathrm{tr}U + C^2\mathrm{tr}U^{-1} + C^3 = \left(1 + C^3\right)\left(1 + a\,P + b\,P'\right)$$

$$\tilde{D} = 1 + \tilde{C}\mathrm{tr}U^{-1} + \tilde{C}^2\mathrm{tr}U + \tilde{C}^3 = \left(1 + \tilde{C}^3\right)\left(1 + \tilde{a}\,P' + \tilde{b}\,P\right) .$$

$$a = \tfrac{3C}{1+C^3},\ b = C\,a, \quad \tilde{a} = \tfrac{3\tilde{C}}{1+\tilde{C}^3}, \tilde{b} = \tilde{C}\,\tilde{a}$$

$$C = 2\kappa \mathrm{e}^{\mu},\ \tilde{C} = 2\kappa \mathrm{e}^{-\mu}, \quad P = \tfrac{1}{3}\mathrm{tr}U,\ P' = \tfrac{1}{3}\mathrm{tr}U^{-1} .$$



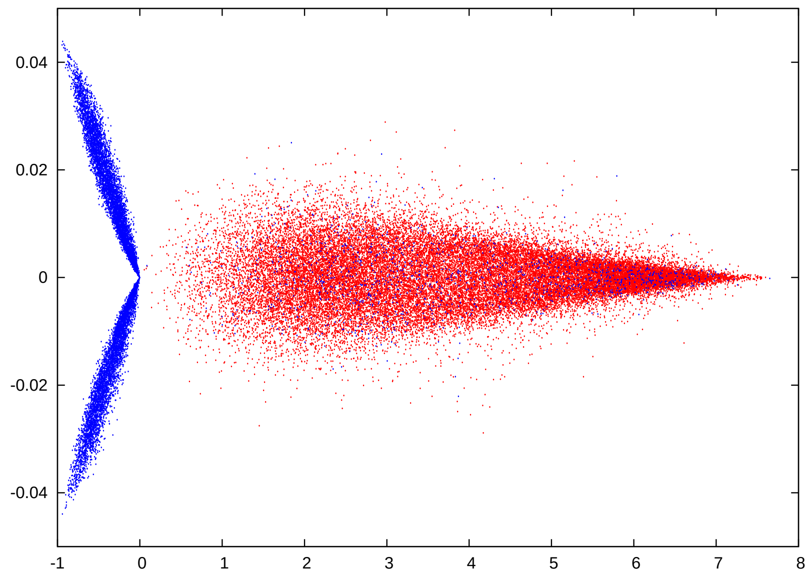


Coefficients $a = 3C/(1+C^3),\ b = 3C^2/(1+C^3)$

left vs. C, right vs. μ (for $N_\tau = 8$)

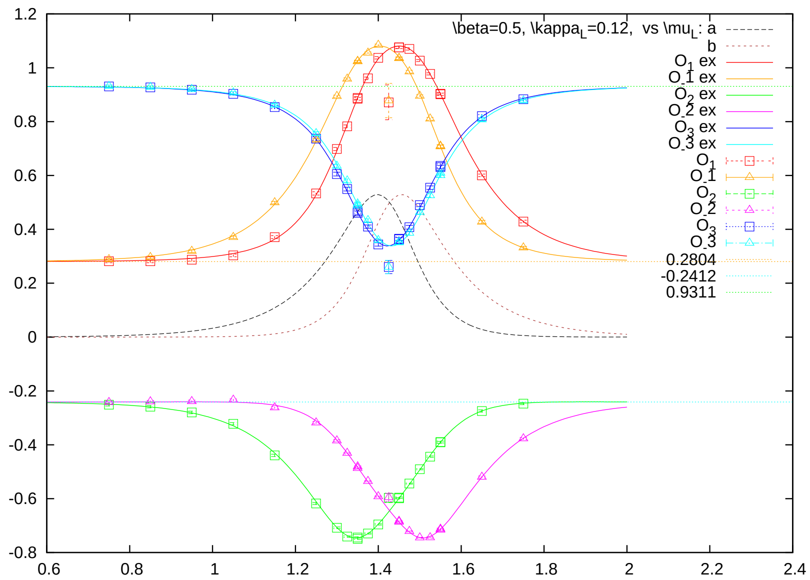
Note: a, b bounded (unlike κ in $U(1)$).

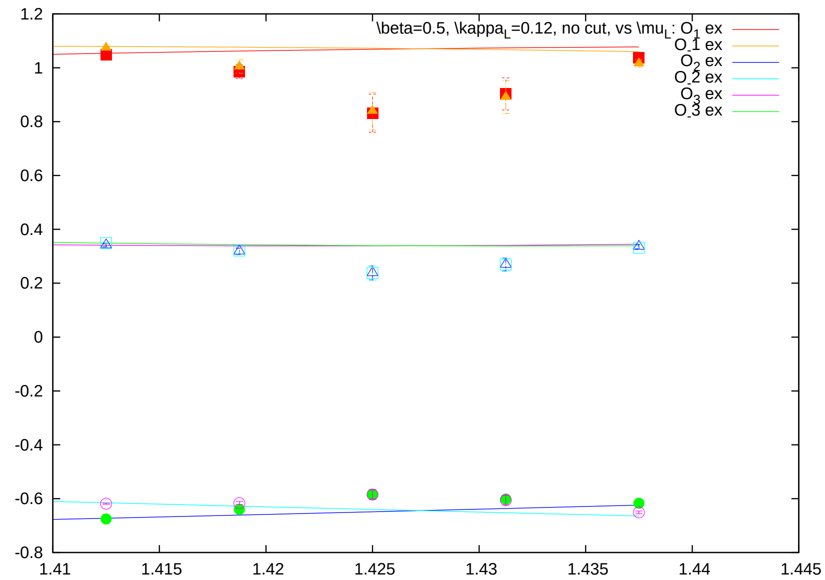
Scatter plot of determinant



Worst case; ‘whisker’ ($\mathrm{Re}\det < 0$) less important than ‘ears’ in $U(1)$

Some observables

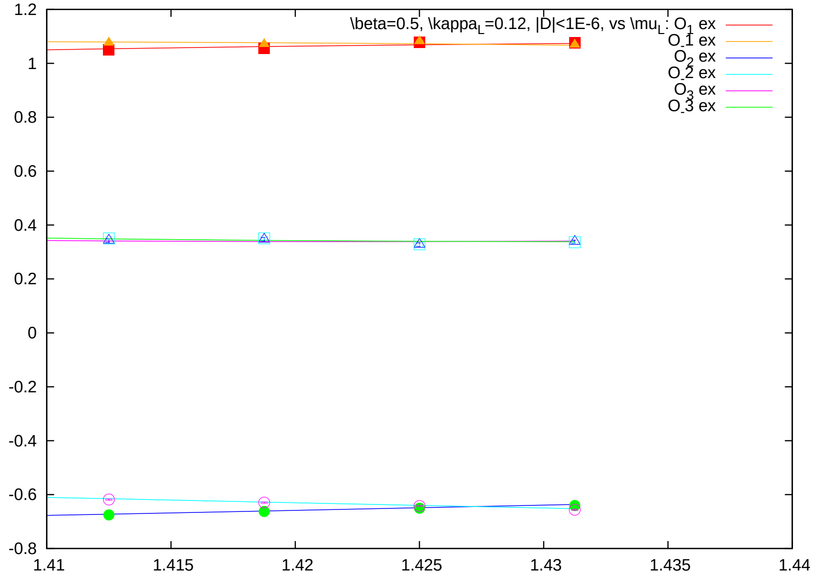


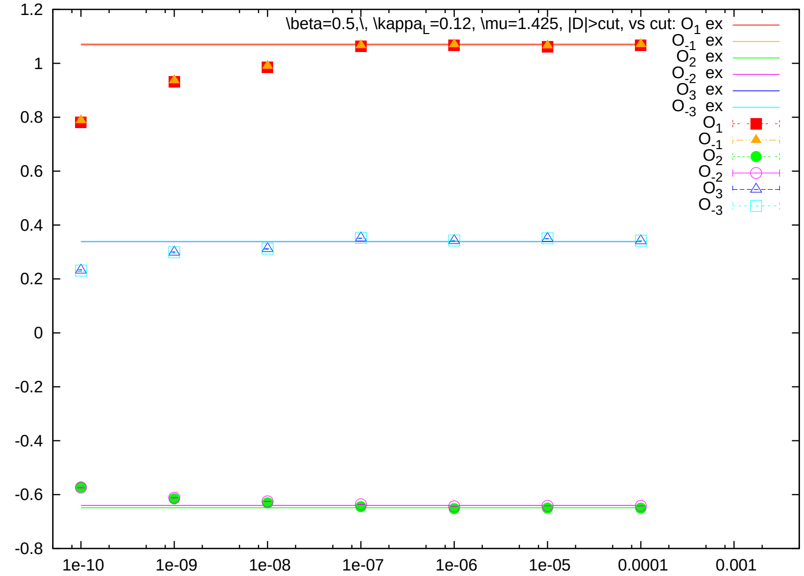


Left: Various observables vs μ

Right: Blowup of “dangerous region”

Restriction to G_+





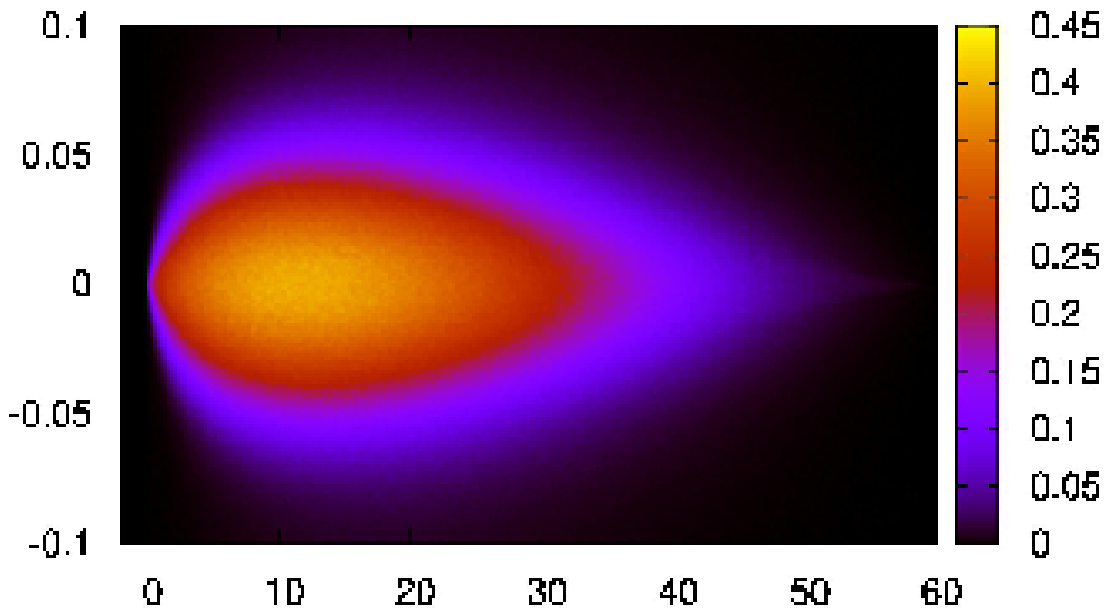
Left: Restriction to trajectories keeping distance 10^{-6} from pole

Right: Expectation values vs d_c

Upshot: G_- quite unimportant compared to $U(1)$!

HDQCD

Scatter plot of local determinant:

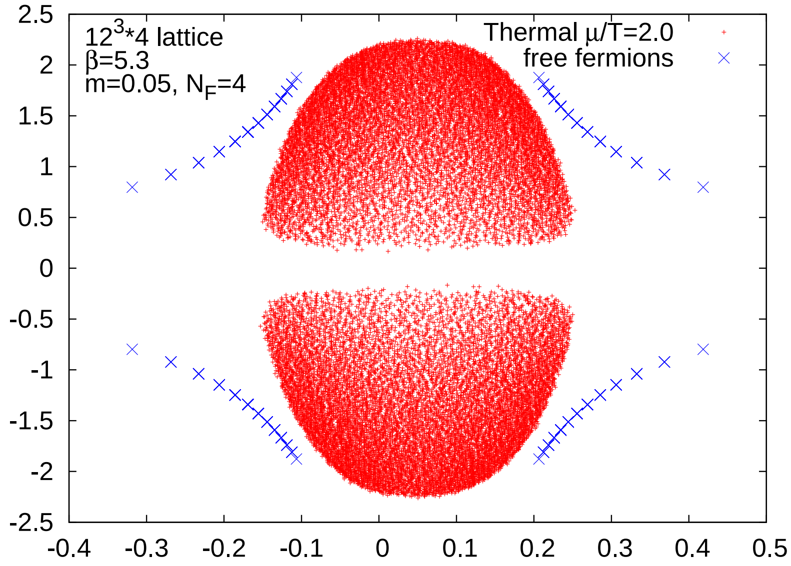


$\beta = 6.0 \; \kappa = 0.12 \; , \mu = 1.425$

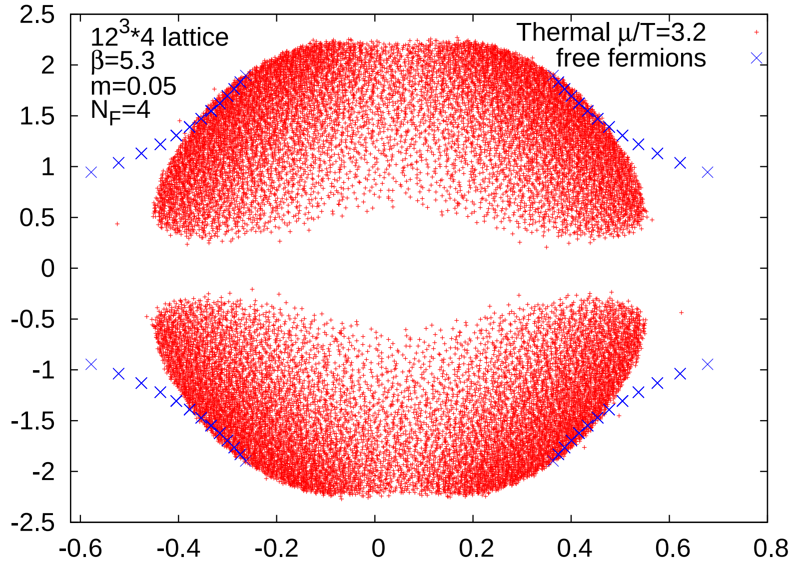
Full QCD

Spectrum of staggered fermion operator

($12^3 \times 4$ lattice, $\beta = 5.3, m = 0.05, N_f = 4$)



$\mu/T = 2.0$



$\mu/T = 3.2$

Zero avoided $\Longrightarrow$ Poles of drift avoided!

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- Increasing n_p:
  pushes $\mathrm{Im} z$ towards $\mathrm{Im} z_P$ (bad)
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