Langevin with meromorphic drift: problems and partial solutions

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based on work with I. O. Stamatescu

part of collective effort involving furthermore G. Aarts, L. Bongiovanni, P. Giudice, J. Pawlowski, D. Sexty ....

Overview

1. Introduction
2. Reminder: formal justification
3. Poles in the drift cause problems
4. Solutions are possible: toy models
5. Cures for real sign problem
6. Attempted cures for phase problem
7. Outlook

1. Sign problem

Functional measure ρ in Euclidean QFT not always positive:

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

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 $\mathcal{O}$

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

Underdetermined.

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

Successes

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

More on this: talk by I.-O. Stamatescu

2. Formal justification

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

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).

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

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

Evolution of observables $\mathcal{O}$: By Ito calculus

$$\dot{\mathcal{O}} = L\mathcal{O}$$

L real Langevin operator

$$L \equiv [\nabla_x + K_x]\,\nabla_x + K_y \nabla_y$$

$\mathcal{O}(z)$ holomorphic: $\nabla_y \mathcal{O} = i\nabla_x \mathcal{O} \Longrightarrow$

$$L\mathcal{O} = L_c \mathcal{O}$$

L_c complex Langevin operator

$$L_c \equiv [\nabla_x + K]\nabla_x = [\nabla_z + K]\nabla_z$$

.

Evolution of densities:

$$\frac{\partial}{\partial t} P(x,y;t) = L^T P(x,y;t)\,; \quad P(x,y;0) = \delta(x-x_0)\delta(y)\,,$$

$L^T \equiv \nabla_x[\nabla_x - K_x] - \nabla_y K_y$ real Fokker-Planck operator.

$$\frac{\partial}{\partial t}\rho(x;t) = L_c^T \rho(x;t)\,; \quad \rho(x;0) = \delta(x-x_0),$$

$L_c^T \equiv \nabla_x\,[\nabla_x + K)]$ complex Fokker-Planck operator.

Relation of evolutions

$$\langle \mathcal{O} \rangle_{P(t)} \equiv \frac{\int \mathcal{O}(x) P(x,y;t) dx\, dy}{\int P(x,y;t) dx\, dy}, \quad \langle \mathcal{O} \rangle_{\rho(t)} \equiv \frac{\int \mathcal{O}(x) \rho(x;t) dx}{\int \rho(x;t) dx}.$$

Two time evolutions:

$$\partial_t \langle \mathcal{O} \rangle_{\rho(t)} = \int dx \mathcal{O}(x)\, L^T \rho(x;t)$$

$$\partial_t \langle \mathcal{O} \rangle_{P(t)} = \int dx dy \mathcal{O}(x+iy) L^T P(x,y;t)\,.$$

Consistent?

Result (not rigorous)

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

Requirements:

- Agreement of initial conditions
- holomorphy of drift $K \equiv K_x + iK_y$
- sufficient decay of $P\mathcal{O}$ at imaginary infinity

Idea of proof

Interpolate between evolutions of P and $\mathcal{O}$:

1. Initial conditions agree.

2. Let $\mathcal{O}(x+iy;t) \equiv \exp[tL]\,\mathcal{O}(x+iy)$ be unique solution of DE

$$\partial_t \mathcal{O}(x+iy;t) = L\mathcal{O}(x+iy;t) \quad (t \geq 0)\,;$$

3. Consider $F(t,\tau) \equiv \int P(x,y;t-\tau)\mathcal{O}(x+iy;\tau)$.
Interpolates between $\langle \mathcal{O} \rangle_{P(t)}$ and $\langle \mathcal{O} \rangle_{\rho(t)}$:

$$F(t,0) = \langle \mathcal{O} \rangle_{P(t)}; \quad F(t,t) = \langle \mathcal{O} \rangle_{\rho(t)}$$

Formally: $F(t,\tau)$ independent of τ:

$$\frac{\partial}{\partial\tau}F(t,\tau) = -\int L^T P(x,y;t-\tau)\mathcal{O}(x+iy;\tau)dxdy$$
$$+\int P(x,y;t-\tau)L\mathcal{O}(x+iy;\tau)dxdy$$

Integration by parts and holomorphy of $\mathcal{O}(z;t) \Rightarrow$

$$\boxed{\frac{\partial}{\partial\tau}F(t,\tau) = 0} \quad \Longrightarrow \quad \langle\mathcal{O}\rangle_{\rho(t)} = \langle\mathcal{O}\rangle_{P(t)} \quad \square$$

Assumption: no boundary terms

3. Problems: poles in drift

If ρ has zeroes in $\mathcal{M}_c$
$\Longrightarrow$ drift only meromorphic
$\Longrightarrow$ Obvious problem:
$\dot{\mathcal{O}} = L\mathcal{O}$ does not preserve holomorphy of $\mathcal{O}$.

Full QCD:
Fermion determinant

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

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

But see D. Sexty's talk.

Ambjørn, Flensburg & Peterson (1986) studied CLE for

$$\rho(x) \equiv \exp(-S) = \cos(x)\exp[\beta\cos(x)]\,.$$

and found “disaster”.

Unavoidable:

Real axis attractor $\Longrightarrow$ equilibrium density

$$P(x,y) = \delta(y)\sigma(x), \quad \sigma(x) \geq 0\,,$$

Incompatible with $\rho(x)$, CLE must fail!

Of course: RLE fails as well!

Flower, Otto&Callahan(1986):
'segregation phenomenon'
K. Fujimura et al (1994):
attempted cure adding $i\pi\delta(\cos x)$ to drift –
does not work in general.

We (2013) find:
Mathematically process not ergodic. Stationary FPE has two linearly independent solutions:

$$P_+(x) = \rho(x)\theta(\rho(x)) \quad \text{and} \quad P_-(x) = \rho(x)\theta(-\rho(x))\,;$$

Numerically: Get phase quenched result
$P \propto P_+(x) + P_+(x)$.

4. Solutions are possible

Simple real example:

$$\rho(x) = 1 + \kappa \cos x$$

For $\kappa \leq 1$: Real LE works. For $\kappa > 1$: Sign problem!

$$K(z) = -\tfrac{\sin z}{1+\kappa\cos z}$$

Claim:

$$P(x,y) \equiv (1+\cos x)\tfrac{1}{\sqrt{2\pi\sigma}} \exp\left[\tfrac{-y^2}{2\sigma}\right] , \quad \sigma = 2\log\kappa$$

solves problem for $\kappa > 1$:

$$\forall n \in \mathbb{Z}: \int_{-\pi}^{\pi} dx \rho(x) \mathrm{e}^{inx} = \int_{-\pi}^{\pi} dx \int_{-\infty}^{\infty} dy P(x,y) \mathrm{e}^{in(x+iy)}$$

P is equilibrium distribution for ‘complex Langevin process’

$$\begin{aligned} dx =& K_x dt + dw_x, \\ dy =& K_y dt + dw_y \end{aligned}$$

with

$$K_x = -\frac{\sin x}{1+\cos x}, \quad K_y = -\frac{y}{\sigma} \,.$$

But: $K_x + iK_y$ not holomorphic.

Similar solutions constructed for all $U(1)$ toy models.

5. Cures for real models

Cure #1: “Sign reweighting”

$$\rho(x) = \theta(\rho(x))P_+(x) - \theta(-\rho(x))P_-(x)$$

whereas simulation yields

$$\rho(x) = \theta(\rho(x))P_+(x) + \theta(-\rho(x))P_-(x)\,,$$

$\Longrightarrow$ the following reweighting should work:

$$\langle\mathcal{O}\rangle_{rew} \equiv \frac{\mathcal{O}(x+iy)\mathrm{sgn}\rho(x)\rangle}{\langle\mathrm{sgn}\rho(x)\rangle}\,.$$

$\langle\cdot\rangle$: ordinary Langevin average.

Works for toy models (cf. I.-O. Stamatescu’s talk)

Cure #2 for compact real models:

"Shifting poles"

Idea: Choose c s.t.

$$\sigma(x) \equiv \rho(x) + c \geq 0\,,$$

Consider $\mathcal{O}$ with $\int \mathcal{O} = 0$. Then

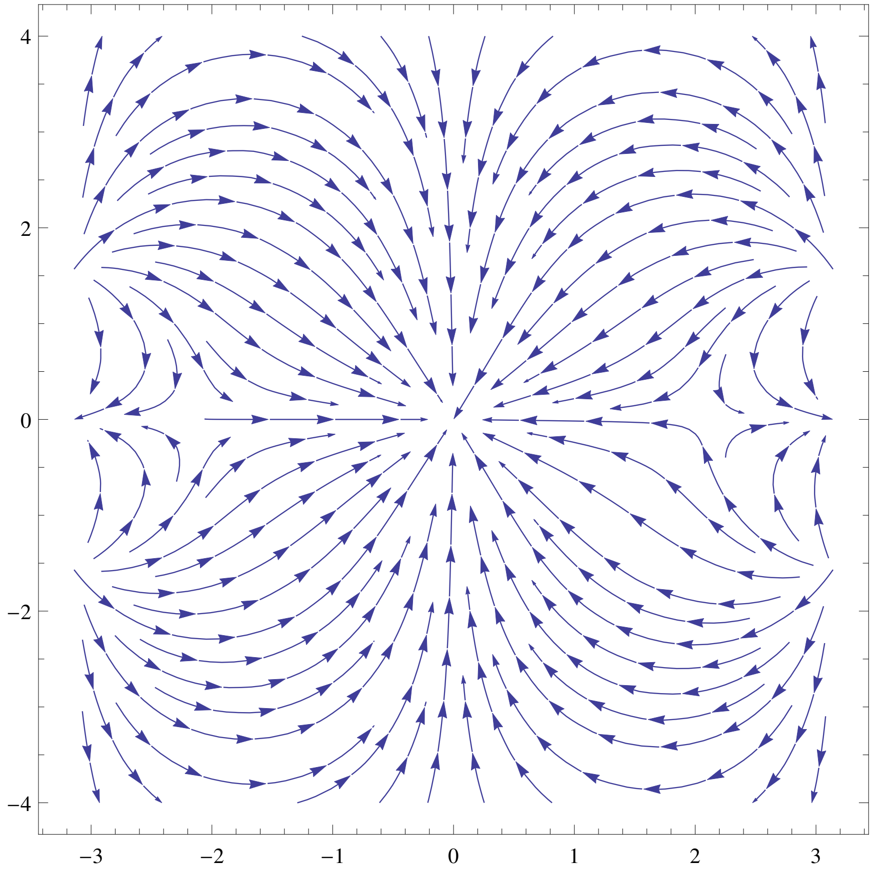
$$\langle \mathcal{O} \rangle_\rho = \frac{\langle \mathcal{O} \rangle_\sigma}{\langle \rho/\sigma \rangle_\sigma}\,,$$

Different kind reweighting: Change drift from $K = \rho'/\rho$ to

$$K_\sigma = \frac{\sigma'}{\sigma} = \frac{\rho'}{\sigma}\,.$$

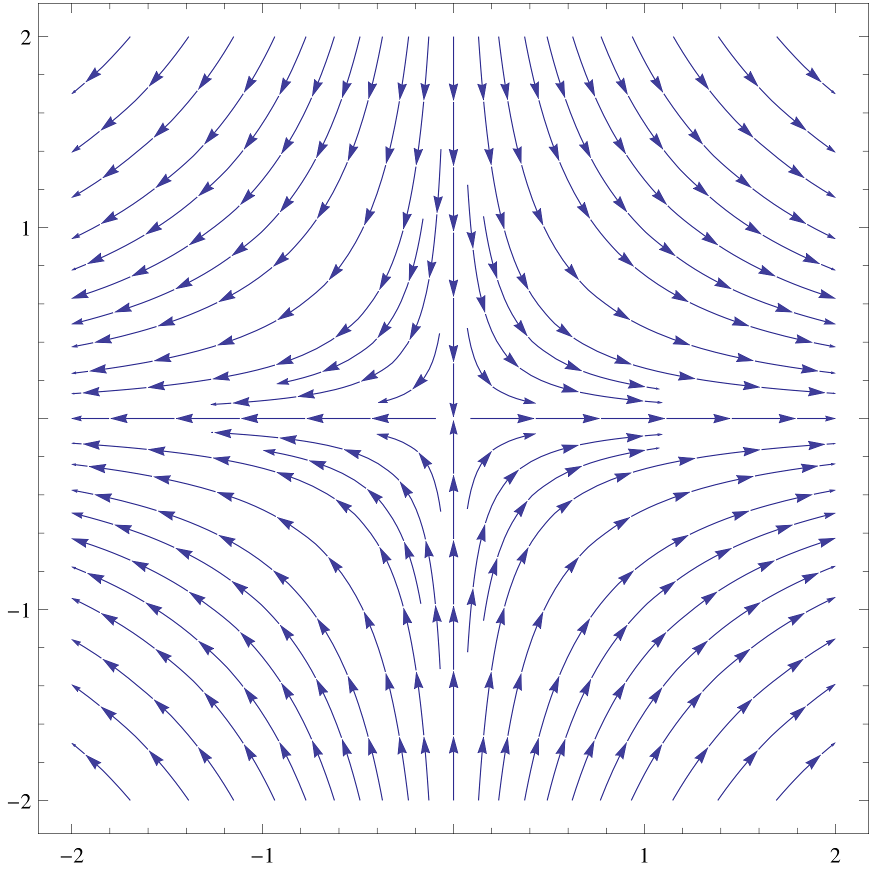
Poles pushed way from real axis!

Flow pattern for $\alpha = 0$, ($h = 0, \kappa = 2, \mu = 0, \beta = 0.5$):



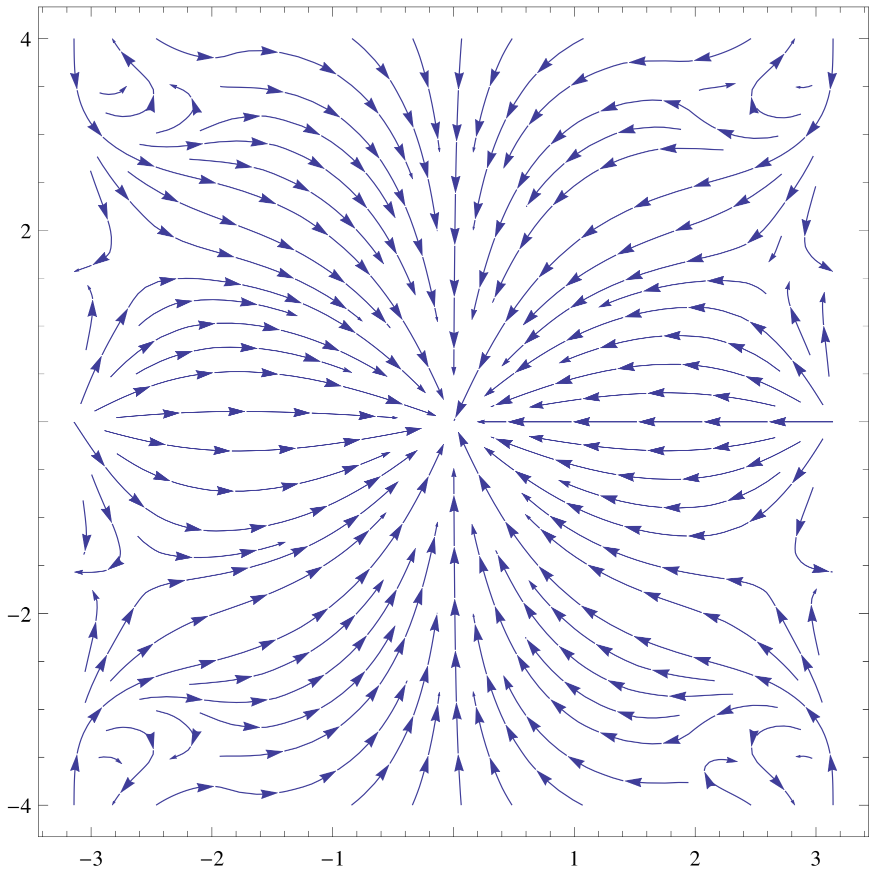
Poles at $x = \pm 2.0944, y = 0$

Flow near pole



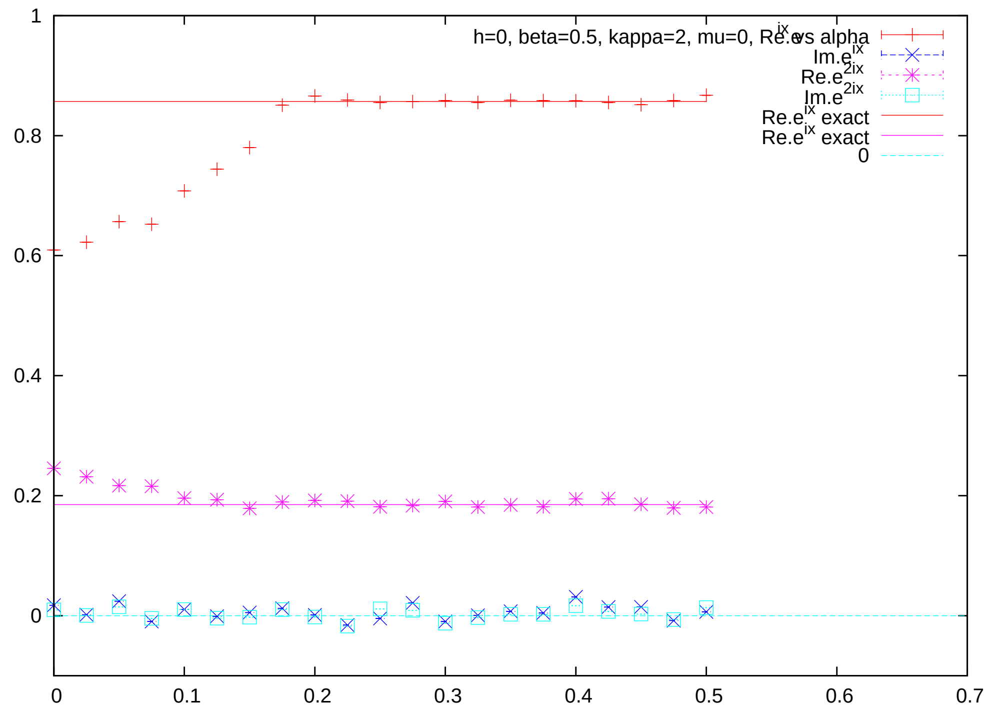
Pattern characteristic for any pole.

Flow pattern for $\alpha = 0.4$, ($h = 0, \kappa = 2, \mu = 0, \beta = 0.5$):



Poles at $x = \pm 2.68297, y = \pm 1.60041$

Numerical example:



$h = 0, \kappa = 2, \mu = 0, \beta = 0.5$;

data points: CLE with cure #2 vs $\alpha = ce^{-\beta}/\kappa$,

solid lines: exact results.

More in I.-O. Stamatescu's talk.

Upshot

Real models can be cured.

Ambjørn-Flensburg-Peterson ‘quantum mechanical desasters’ averted.

6. Complex case

Cure #1 generalized to complex situations:
Reweight

$$\mathcal{O}(z) \mapsto \mathcal{O}(z)\,\mathrm{sgn}\,c(z)$$

with (for instance)

$$c(z) = \mathrm{sgn}\,\mathrm{Re}\,\det(x + iy; \kappa, \mu)$$

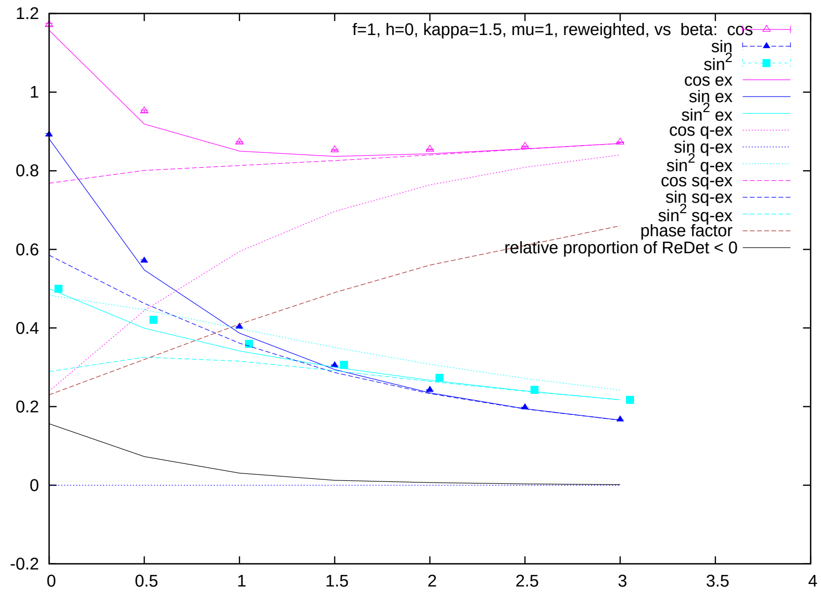
and compute by CLE

$$\langle \mathcal{O} \rangle_{corr} \equiv \frac{\langle \mathcal{O}\, c \rangle}{\langle c \rangle}\,.$$

$\approx$ works in toy models. Overlap problem for lattices.

Numerical example #1

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



Data points: CLE with sign reweighting,

solid lines: unquenched exact results,

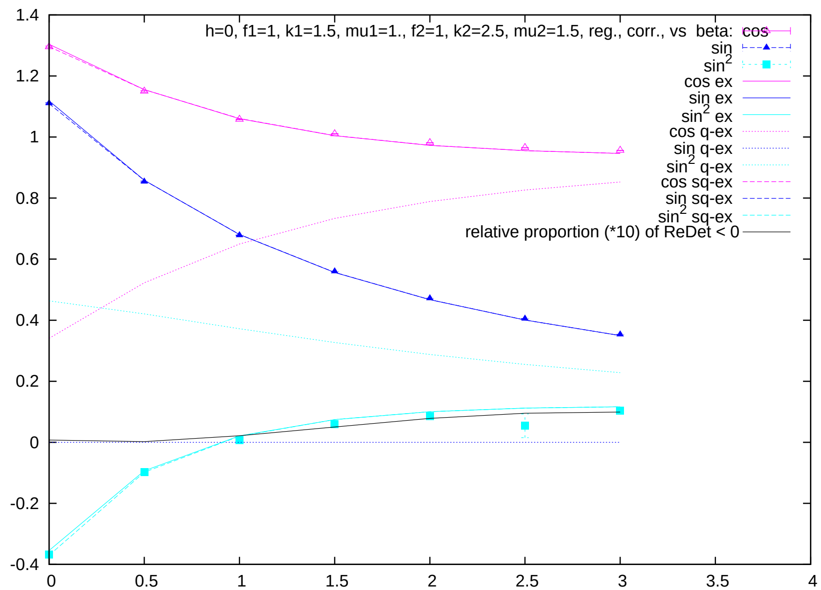
dotted lines: quenched results,

dashed lines: quenched results on the line $y = \mu$)

Numerical example #2

Model with 2 poles:

$$\rho(x) = (1 + \kappa_1 \cos(x - i\,\mu_1))^{f_1} (1 + \kappa_2 \cos(x - i\,\mu_2))^{f_2} e^{\beta \cos(x)}$$



Data points: CLE with correction,
solid lines: unquenched exact results, dotted lines: quenched results.

Cure #2:

Consider $\mathcal{O}$ with

$$\int \mathcal{O} = 0 \,.$$

Define as before

$$\sigma \equiv \rho + c \,,$$

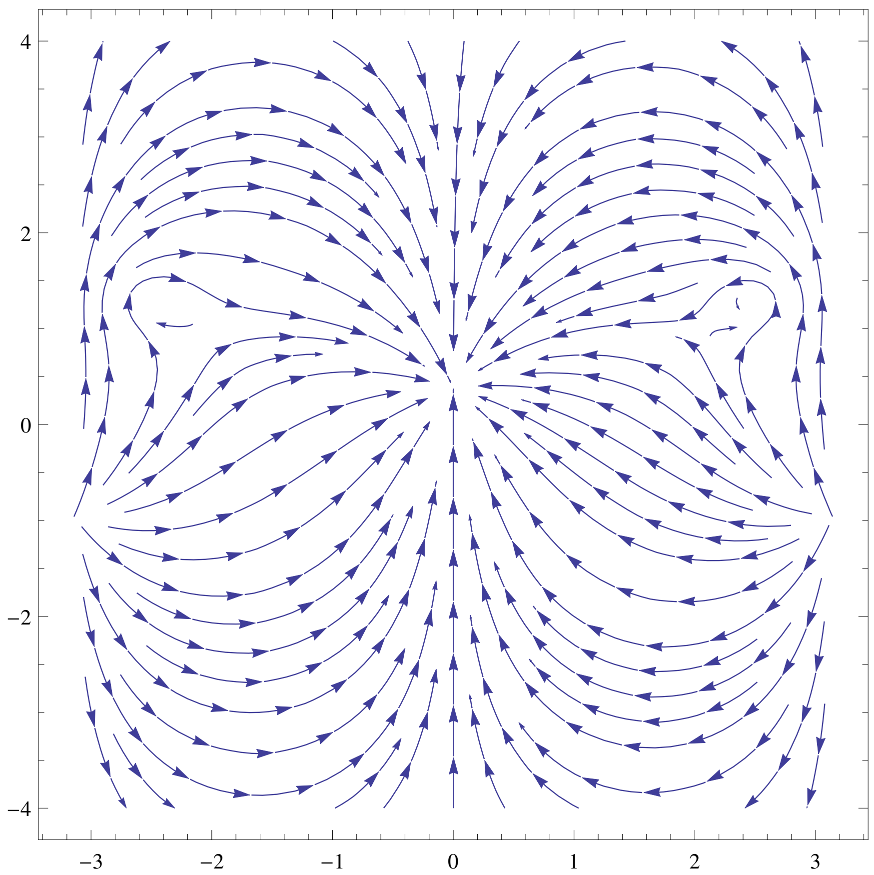
$$\langle \mathcal{O} \rangle_\rho = \frac{\langle \mathcal{O} \rangle_\sigma}{\langle \rho/\sigma \rangle_\sigma} \,.$$

Fixed points not moved; poles shifted.

Mollgaard&Splittorff 2013 (random matrix model):

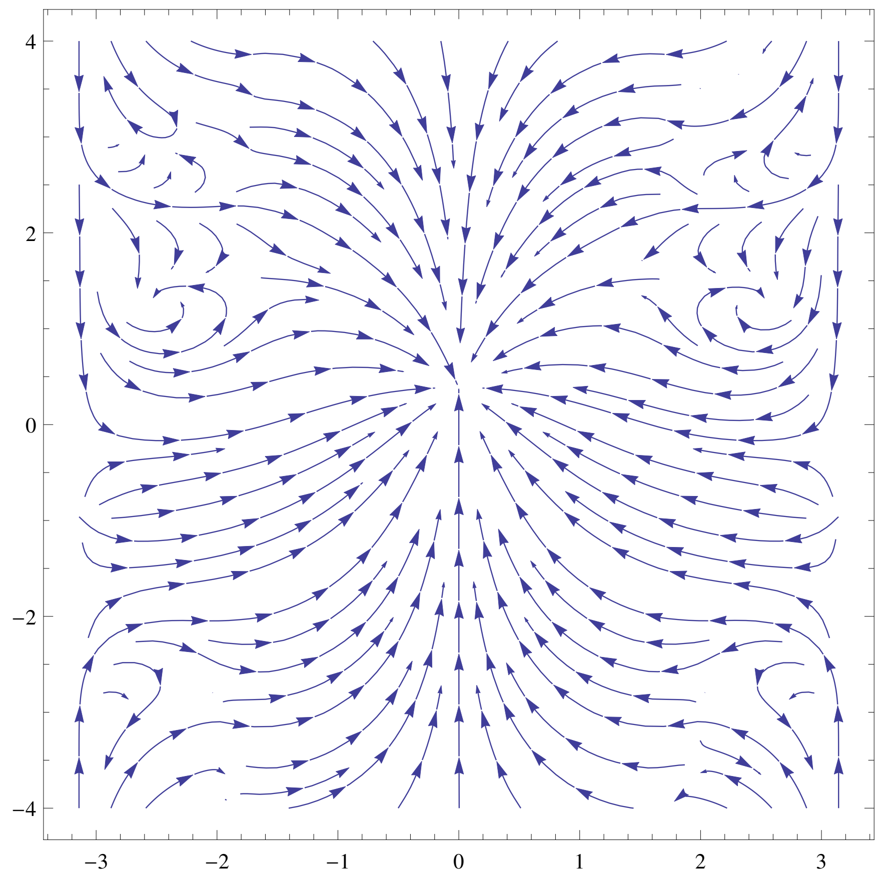
If paths ‘do not wind around’ poles CLE ok.

Flow without shift



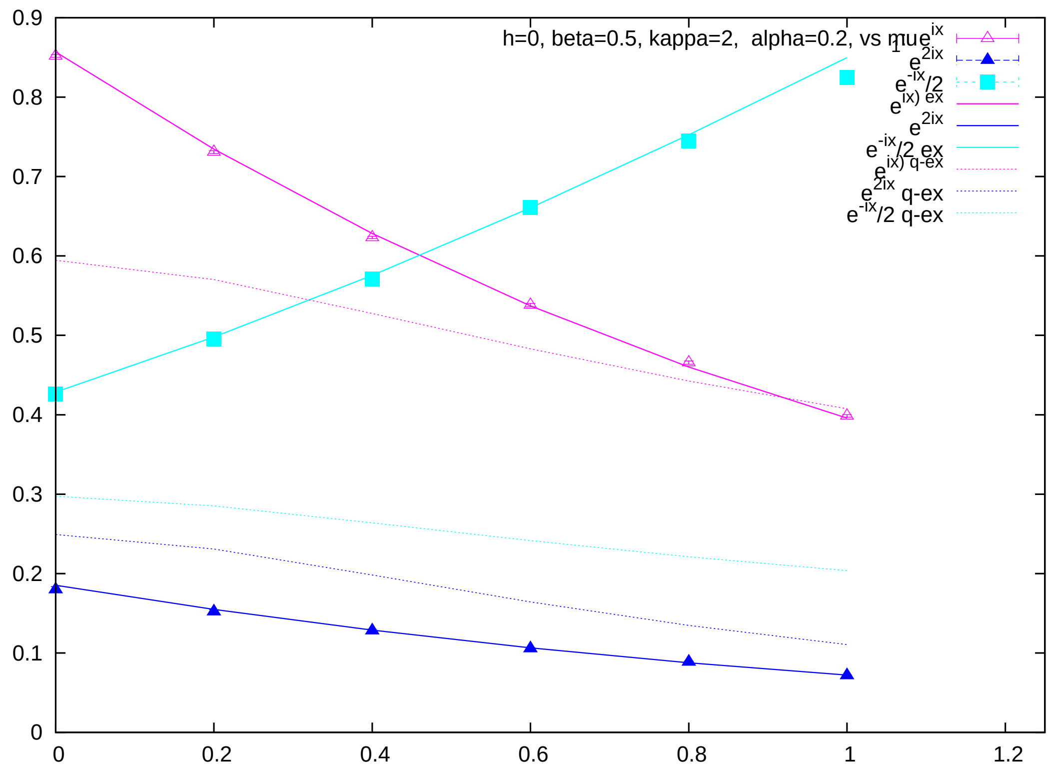
Poles at $x = \pm 2.094395, y = 1$

Flow with shift $c = 1$



Poles at $z = \pm 1.684981 + 1.52266i$ and $x = \pm\pi - 0.261275i$

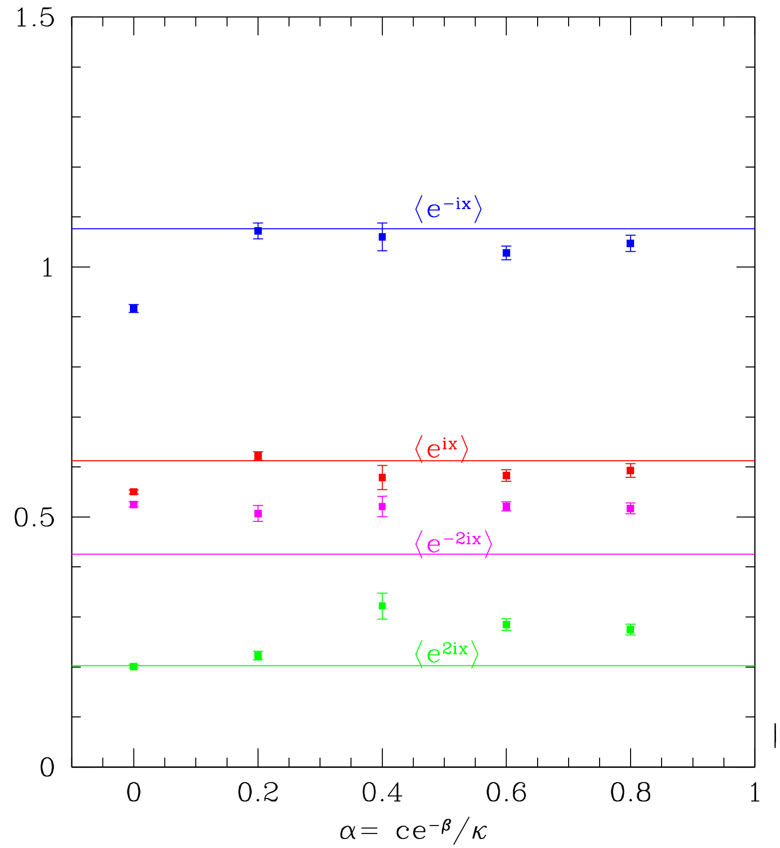
$h = 0,\ \beta = 0.5,\ \kappa = 2.0,\ \mu = 0 \text{ to } 1$



Data points: CLE with shift by $c = \alpha\kappa \exp(\beta) \approx 0.66$,
solid lines: exact results.

Looks good

$h = 0, \ \beta = 1.0, \ \kappa = 2.0, \ \mu = 0.5$



Data points: CLE with shift by $c = \alpha\kappa\exp(\beta)$,
solid lines: exact results.
Cure #2 $\approx$ doesn't work very well in complex models.

7. Outlook

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Backup slides

Problems:

Extensively studied: Slow decay of P in imaginary direction (always noncompact). Partial help:

- *no diffusion in imaginary direction*
- *Gauge cooling*

Under study: Poles in the drift.

Cause: zeroes of ρ on $\mathcal{M}_c$.

Special case

If $S(x)$ real for x real:

Complex FPE $\Longrightarrow$ standard real FPE;

real FPE still lives in $\mathcal{M}_c$, but stationary solution

$$P(x,y) \propto \exp[-S(x)]\delta(y)\,.$$

Four operators:

'Complex' operators on functions on $\mathcal{M}_r$:

$$L_c = [\nabla_x - (\nabla_x S(x))]\nabla_x$$

$$L_c^T = \nabla_x[\nabla_x + (\nabla_x S(x))]$$

'Real' operators on functions on $\mathcal{M}_c$:

$$L = [\nabla_x + K_x]\nabla_x + K_y\nabla_y$$

$$L^T = \nabla_x[\nabla_x - K_x] - \nabla_y K_y$$

On holomorphic observables $L\mathcal{O} = L_c\mathcal{O}$

Side remark

Independent rescaling of times $\Longrightarrow$

$$
\begin{aligned}
dx =& \tilde{K}_x dt + \sqrt{N_R} dw_x , \\
dy =& \tilde{K}_y dt + \sqrt{N_I} dw_y
\end{aligned}
$$

with $\tilde{K}_x = N_R K_x$, $\tilde{K}_y = N_I K_y$

Choose $N_R - N_I = 1$

get standard CLE form.

But: $\tilde{K}_x + i\tilde{K}_y$ still not holomorphic.

General U(1) toy models

$$\rho(x) = \sum a_n \mathrm{e}^{inx}, \quad a_n = A_n + iB_n$$

with technical condition on growth of a_n's for $n \to \infty$.
Then $\exists$ solution of the form

$$P(y) = \sum_{n=-\infty}^{\infty} \frac{\lambda_n \mathrm{e}^{inx}}{2\sqrt{2\pi\sigma}} \exp\left(-\frac{(y-1)^2}{2\sigma}\right) + \sum_{n=-\infty}^{\infty} \frac{\mu_n \mathrm{e}^{inx}}{2\sqrt{2\pi\sigma}} \exp\left(-\frac{(y+1)^2}{2\sigma}\right)$$

with $\lambda_0 = \mu_0 = 1/2$ and for $n \neq 0$

$$\lambda_n = \exp\left(-\frac{n^2\sigma}{2}\right)\left\{A_n \frac{\cosh(ny_0)}{\cosh(2ny_0)} - iB_n \sinh(ny_0)\right\},$$

$$\mu_n = \exp\left(-\frac{n^2\sigma}{2}\right)\left\{-A_n \frac{\sinh(ny_0)}{\cosh(2ny_0)} + iB_n \cosh(ny_0)\right\}.$$

Side remark: rescaling

Define

$$\xi = \sqrt{N_R} x, \quad \eta = \sqrt{N_I} y \,.$$

The $Q(\xi,\eta) \equiv P(\xi/\sqrt{N_R}, \eta/\sqrt{N_I})$ is a solution to the FPE

$$\left(N_R \partial_\xi^2 + N_I \partial_\eta^2 + \partial_\xi \tilde{K}_\xi + \partial_\eta \tilde{K}_\eta\right) Q(\xi,\eta) = 0 \,,$$

where

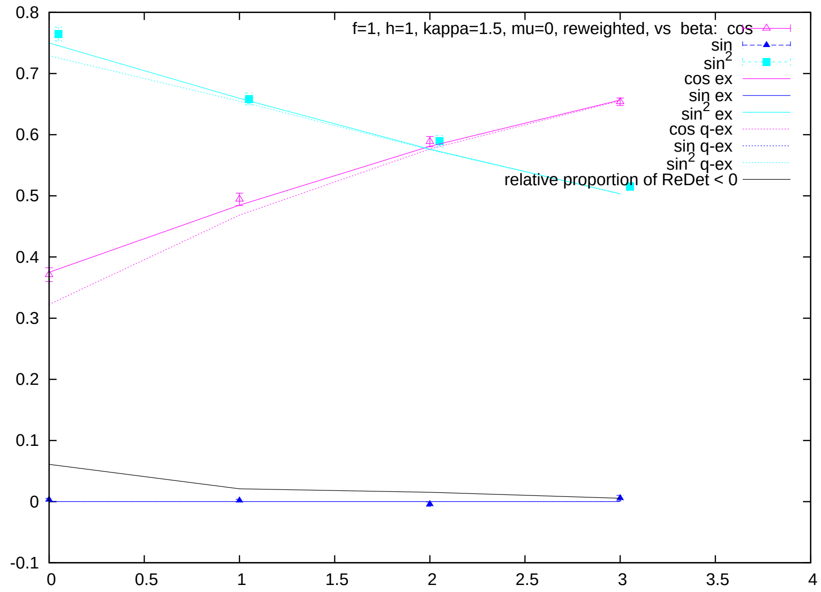
$$\tilde{K}_x(\xi,\eta) \equiv N_R K_x(\xi/\sqrt{N_R}, \eta/\sqrt{N_I})$$
$$\tilde{K}_y(\xi,\eta) \equiv N_R K_x(\xi/\sqrt{N_R}, \eta/\sqrt{N_I}) \,.$$

Again for $N_R - N_I = 1$ standard CLE form, but $\tilde{K}_\xi + i\tilde{K}_\eta$ not holomorphic.

Toy model

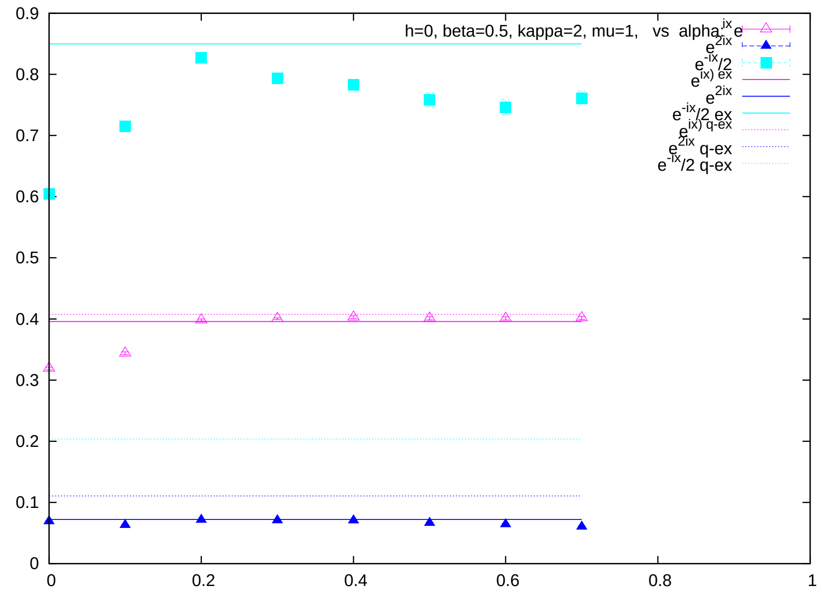
$$\rho(x) \equiv \exp(-S) = (\sin^2(x))^h\,(1+\kappa\cos(x-i\mu))^{N_f}\,\exp[\beta\cos(x)]\,.$$

$$h = 1, \kappa = 1.5, \mu = 0$$



data points: CLE with sign reweighting,
solid lines: exact results,
dotted lines: sign quenched results.

cure #2



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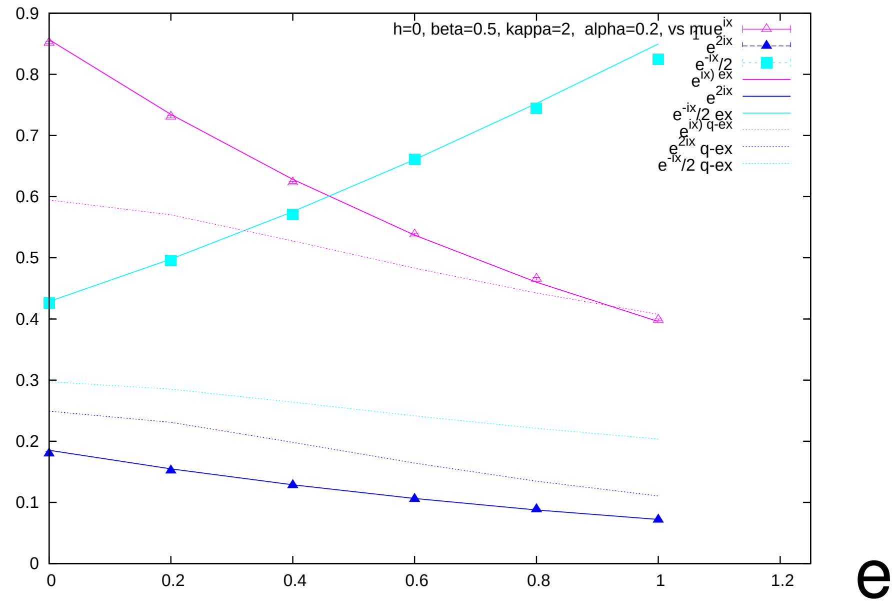

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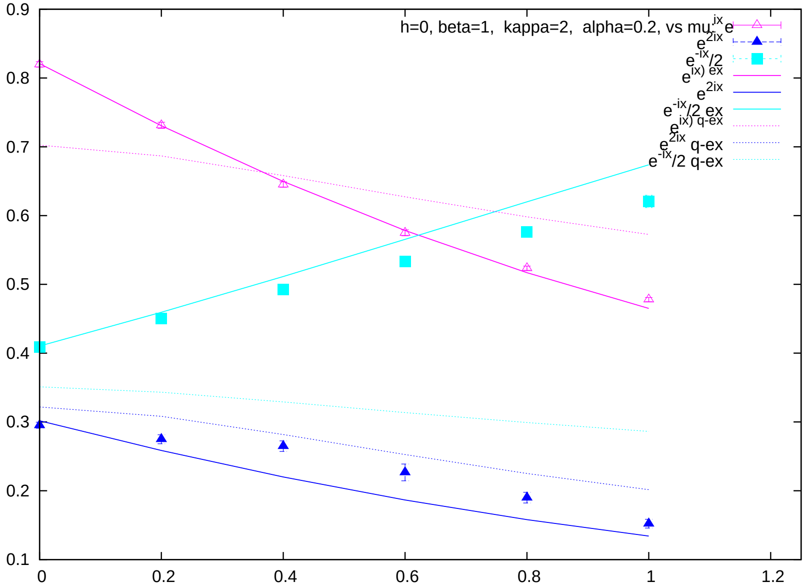

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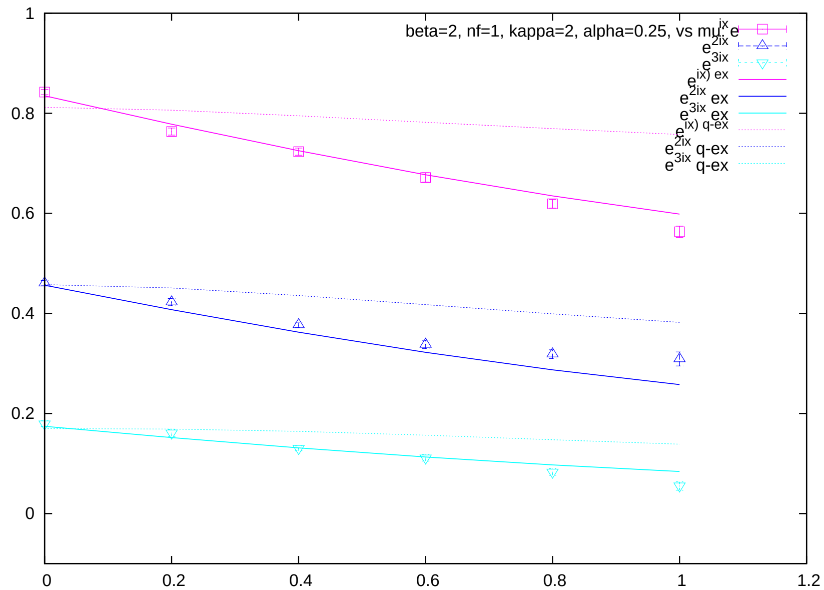

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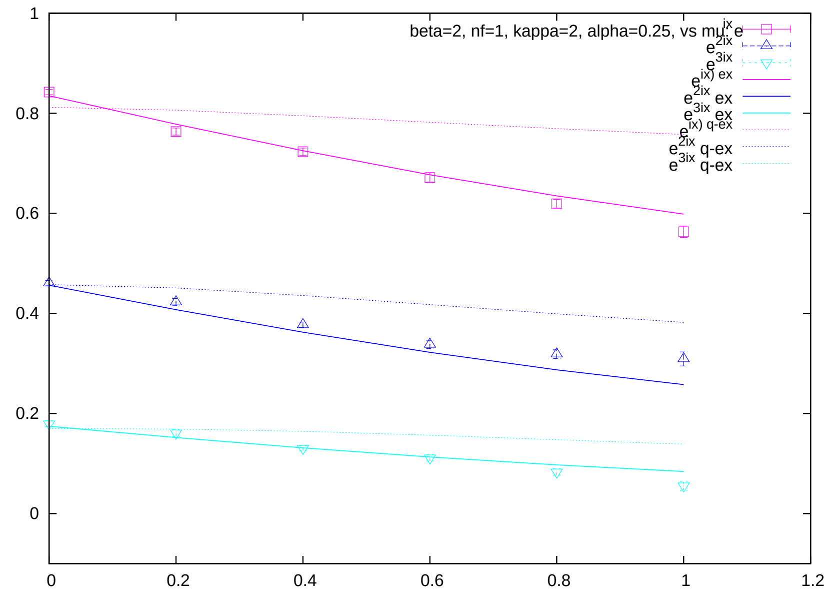

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