Complex Langevin: A universal solution for the sign problem?

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work done in collaboration with

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1.The Sign problem

Via Wick rotation Quantum Field Theory
'reduced to quadratures':

Euclidean functional integral $\longleftrightarrow$ probability measure μ.

$$d\mu(\phi) = \frac{1}{Z}\exp(-S(\phi))$$

provided action S is real.

Numerical simulation

Ergodic stochastic process which has μ as its equilibrium measure.

Example:

$$d\mu(\phi) = \frac{1}{Z}\exp(-S(\phi))$$

(real) Langevin equation

$$d\phi = -\nabla S dt + dw\,.$$

dw increment of Wiener process.

Difficulty

Sometimes

Euclidean functional integral $\longleftrightarrow$ complex measure:

'Sign problem'

Where:

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

Question

Complex measure ρ ‘representable’ by probability measure P?

For holomorphic observables sign problem solved in principle by complex Langevin:

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

First proposed:
G. Parisi 1983, J. Klauder 1983

Successes and Failures

In some simple cases good convergence to the right limit.

Example: $U(1)$ LGT in $2D$ (Ambjørn et al 1986).

Practical Problems:

- Runaways (divergence)
- convergence to wrong limit.

Mathematical questions unresolved:

Quotes: *... conspicuous absence of general spectral theorems*

... (Klauder&Petersen 1984)

... a rather experimental character: for some situations the method works, while it fails for other choices of the action

... (Haymaker&Wosiek 1988)

Revival

Berges&Stamatescu 2005, Berges et al 2007: Simulation of Minkowski space QFT
(Hüffel&Rumpf 1984, Nakamoto&Yamanaka 1986)

Finite density: Aarts&Stamatescu 2008
Complex relativistic Bose gas: Aarts 2009
XY model: Aarts&James 2010
Effective potential: Guralnik&Pehlevan 2008-2009

– Some impressive numerical impressive results
– But problems lingering; sometimes wrong results.

Closer look:

Diseases: etiology, diagnostics, (therapy?) :

Aarts, Seiler, Stamatescu, Phys. Rev. D **81** (2010) 054508 [arXiv:0912.3360 [hep-lat]],

Aarts, Seiler, Stamatescu, Phys. Lett. B **687** (2010) 154 [arXiv:0912.0617 [hep-lat]],

Aarts, Seiler, Stamatescu, James, to appear in Eur. J. Phys., [arXiv:1101.3270 [hep-lat]],

Aarts, Seiler, Stamatescu, James, Sexty, work in progress

2. Formal justification

'Flat' case: defined on $\mathcal{M}_r = \mathbb{R}^n$ or $\mathcal{M}_r = S_1^n$, analytically continued to $\mathcal{M}_c$.

Complex Langevin on $\mathcal{M}_c$

$$dz = -\nabla S dt + dw$$

dw increment of real Wiener process on $\mathcal{M}_r$ (formally $dw = \eta(t)dt$, η white noise).

This means

$$dx = K_x dt + dw,$$
$$dy = K_y dt$$

$$K_x = -\mathrm{Re}\nabla_x S(x+iy)$$
$$K_y = -\mathrm{Im}\nabla_x S(x+iy)$$

Slight generalization:

$$dx = K_x dt + \sqrt{N_R}\, dw_R,$$
$$dy = K_y dt + \sqrt{N_I}\, dw_I,$$

$dw_R,\ dw_I$ independent Wiener processes,
$N_I \geq 0$ and $N_R = N_I + 1$.

Real stochastic process

By Ito calculus ($\langle dw^2 \rangle \propto dt$)

$$\frac{d}{dt} \langle f(x(t), y(t)) \rangle = \langle L f(x(t), y(t)) \rangle \,,$$

Langevin operator

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

$\Longrightarrow$ Dual Fokker-Planck equation

$$\frac{\partial}{\partial t} P(x,y;t) = L^T P(x,y;t) \,; \quad P(x,y;0) = \delta(x - x_0) \delta(y - y_0) \,,$$

P probability density in $\mathcal{M}_c$, Real Fokker-Planck operator:

$$L^T \equiv \nabla_x[N_R\nabla_x - K_x] + \nabla_y[N_I\nabla_y - K_y]$$

Complex Fokker-Planck Equation:

$\rho_{y_0}(x;t)$ complex density on e.g. $\mathbb{R}^n + iy_0$;

$$\frac{\partial}{\partial t}\rho_{y_0}(x;t) = L^T_{y_0}\rho_{y_0}(x;t)\,,$$

$$L^T_{y_0} \equiv \nabla_x\left[\nabla_x + (\nabla_x S(x+iy_0))\right]\,.$$

Special case

If $S(x)$ real for x real, $N_I = 0$:

Complex FPE $\Longrightarrow$ standard real FPE;

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

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

Zoo of operators:

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

$$L_{y_0} = [\nabla_x - (\nabla_x S(x+iy_0))]\nabla_x$$
$$L_{y_0}^T = \nabla_x[\nabla_x + (\nabla_x S(x+iy_0))]$$

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

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

On holomorphic observables $L\mathcal{O} = \tilde{L}\mathcal{O}$ where

$$\tilde{L} = [\nabla_z - (\nabla_z S)]\nabla_z = [\nabla_z + (K_x + iK_y)]\nabla_z$$

Goal

Produce expectation values of holomorphic observables:

$$\langle \mathcal{O} \rangle \equiv \frac{\int \mathcal{O}(x+iy_0)e^{-S(x+iy_0)}dx}{\int e^{-S(x+iy)}dx} \,;$$

(independent of y_0 by Cauchy's theorem).

Hope: obtainable as long time limit of

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

and by ergodicity as

$$\lim_{t\to\infty} \frac{1}{T} \int_0^T \mathcal{O}(z(t))dt \,.$$

Relation of 'P-expectations' to 'ρ-expectations'?

$$\langle\mathcal{O}\rangle_{\rho,t} \equiv \frac{\int \mathcal{O}(x+iy_0)\rho(x;t)dx}{\int \rho_{y_0}(x;t)dx}\,.$$

Two time evolutions:

$$\partial_t \langle\mathcal{O}\rangle_{\rho,t} = \int dx \mathcal{O}(x+iy_0)\, L_{y_0}^T \rho(x;t)$$

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

Consistent?

Result (semi-rigorous)

Assume

- $P(x, y; 0) = \delta(y)\rho(x; 0) \qquad (\rho(x; 0) \geq 0)$
- $L_0,\ L_0^T$ generate exponentially bounded holomorphic semigroup (i.e. $\|e^{tL_0}\| \leq C_1 e^{C_2 t}$)
- L, L^T generate exponentially bounded (strongly continuous) semigroup on $L^2(\mathcal{M}_c)$
- $\mathcal{O}(x) \in L^2(\mathcal{M}_r)$.

Then

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

"Proof"

1. Initial conditions agree.

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

$$\partial_t \mathcal{O}(x+iy;t) = L_0 \mathcal{O}(x+iy;t) = \tilde{L}\mathcal{O}(x+iy;t) \quad (t \geq 0)\,;$$

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 $\Rightarrow$ crucial identity:

$$\boxed{\frac{\partial}{\partial\tau}F(t,\tau) = 0} \quad \text{(CI)}$$

Justified? Boundary terms?

Historical remark

Early attempt at formal justification Nakazato 1986:

Requires $P(x, y; t)$ to continue to entire function in x.

Not known.

Known: $P(x, y; t)$ not analytic in y in example.

Extension to manifolds

Gausterer&Thaler 1998, Aarts&Stamatescu 2008:
Compact connected Lie groups.

Examples:
$U(1)$ complexified to $U(1) \times \mathbb{R}$
$SU(N)$ complexified to $SL(N, \mathbb{C})$

More generally:
– $\mathcal{M}_r$ Riemannian manifold $\Rightarrow \exists$ Wiener process $\Rightarrow$
noise in real directions well defined
– Real manifold $\mathcal{M}_r$ has to have complexification $\mathcal{M}_c$.

Formal arguments carry over; problems remain.

3. Consistency condition

Recall (CI)

$$0 = \frac{\partial}{\partial\tau}F(t,\tau) = -\int L^T P(x,y;t-\tau)\mathcal{O}(x+iy;\tau)dx\,dy$$
$$+\int P(x,y;t-\tau)\tilde{L}\mathcal{O}(x+iy;\tau)dx\,dy\,.$$

Take $\tau = 0, t \to \infty$, assume convergence to equilibrium:

$$\exp(tL^T)P(x,y;t) \to P(x,y;\infty); \quad L^T P(x,y;\infty) = 0\,,$$

$$\boxed{\langle\tilde{L}\mathcal{O}\rangle \equiv \int P(x,y;\infty)\tilde{L}\mathcal{O}(x+iy)dx\,dy = 0.} \quad \text{(CC)}$$

(CC) Manifestly weaker than (CI).

But: If

- (CC) holds for sufficiently many observables $\mathcal{O}$,
- a certain bound holds,
- spectral conditions assuring convergence hold

then

$$\langle \mathcal{O} \rangle_{P(\infty)} = \frac{1}{Z} \int_{\mathcal{M}_r} \mathcal{O}(x) \exp[-S(x)] dx \, .$$

i.e. Equilibrium measure correct.

Proof

uses density argument and Riesz-Markov theorem.

Morally (CC) equivalent to Schwinger-Dyson equations (SDE).

4. Summary of Problems

Mathematical and practical difficulties:

- *Existence* of the semigroups $\exp(tL)$ etc.?
  Not known; Operators not dissipative.
  But seems ok in examples.

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Mathematical and practical difficulties:

- ***Existence*** of the semigroups $\exp(tL)$ etc.?
  Not known; Operators not dissipative.
  But seems ok in examples.
- ***Spectrum***: Spectrum of Langevin and FP operators in left half plane?
  In relevant examples: seems to be the case.

  (Note: Convergence of $P(x, y; t)$ not strictly necessary, Need only convergence of $\rho(x; t)$).

- *Runaways:* In typical cases deterministic motion can go to ∞ in finite time.
  Reason: Repulsive fixed points, drift ∇S grows in imaginary directions, drift not a gradient.
  In practice: problem solved by adaptive step size (Aarts, Seiler, Stamatescu 2009).
  With noise: Equilibrium measure seems to exist.

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  With noise: Equilibrium measure seems to exist.
- *Convergence to* wrong limit (Noticed already by Klauder&Petersen 1985, Ambjørn et al 1986, Haymaker&Wosiek 1987).
  Most serious, under investigation, see below.

5. Toy models

Example 1: Quadratic Actions (cf. Ambjørn&Yang 1985, Haymaker&Peng 1989)

Setting:

$$S = \frac{1}{2}(x, Ax), \quad x \in \mathbb{R}^n \, ,$$

$A = A_r + iA_i$ complex symmetric matrix; A_r and A_i real symmetric matrices.

Assume: $A_r = \frac{1}{2}(A + A^\dagger) > 0$.

Only fixed point at $x = 0$, attractive, explicit solution (Gaussian).

No problems.

Example 2 ("one-link U(1)")

(Aarts&Stamatescu 2008, Aarts, S., Stamatescu 2009, 2011)

$$S = -\beta \cos x - \kappa \cos(x - i\mu) = -a \cos(x - ic)$$

$$a = \sqrt{(\beta + \kappa e^{\mu})(\beta + \kappa e^{-\mu})}, \quad c = \frac{1}{2} \ln \frac{\beta + \kappa e^{\mu}}{\beta + \kappa e^{-\mu}}$$

From now: $\kappa = 0 \quad \Rightarrow$ CLE becomes

$$dx = K_x dt + dw, \quad dy = K_y dt$$

where

$$K_x = -\beta \, \sin x \, \cosh y, \quad K_y = -\beta \, \cos x \, \sinh y$$

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Attractive fixed point: $x + iy = 0$

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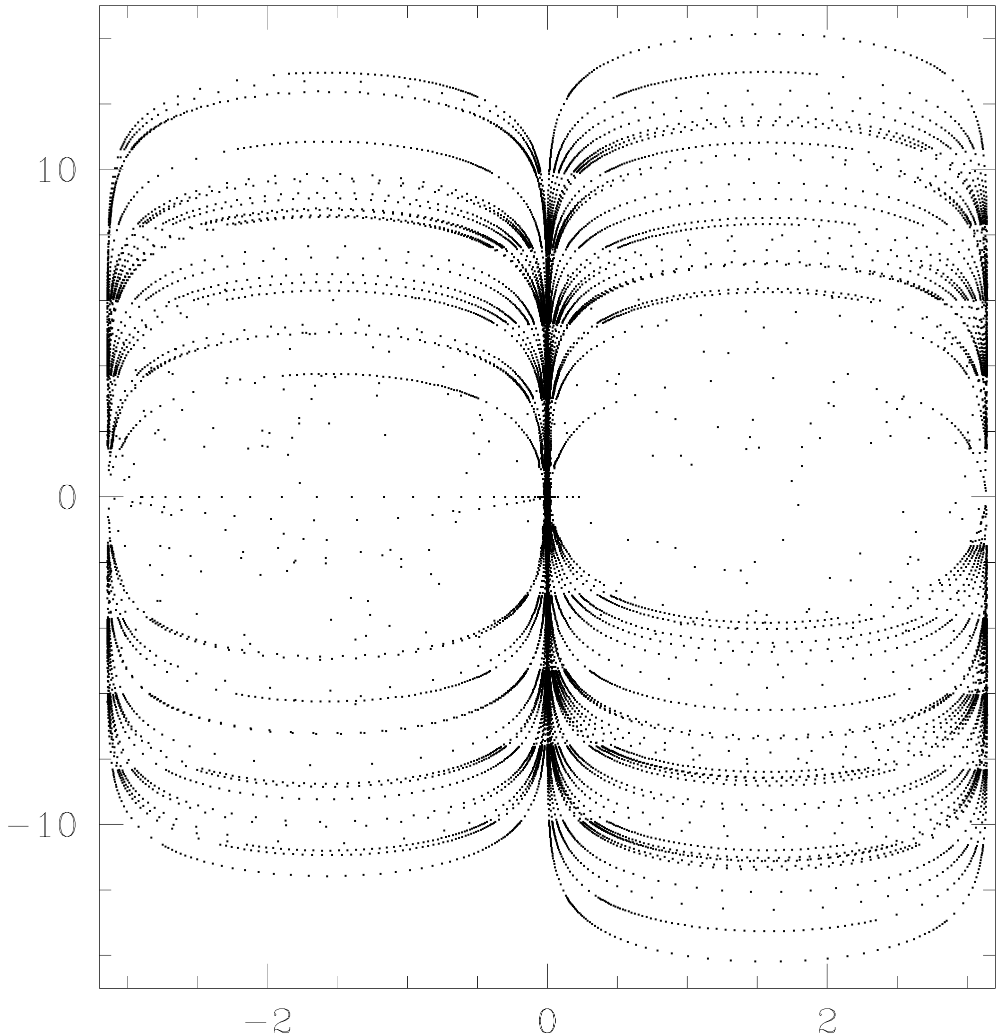
With noise: for $|y|$ large noise irrelevant.
Expect:

- large excursions,
- slow decay of equilibrium measure

Simulation



$\beta = 100.$

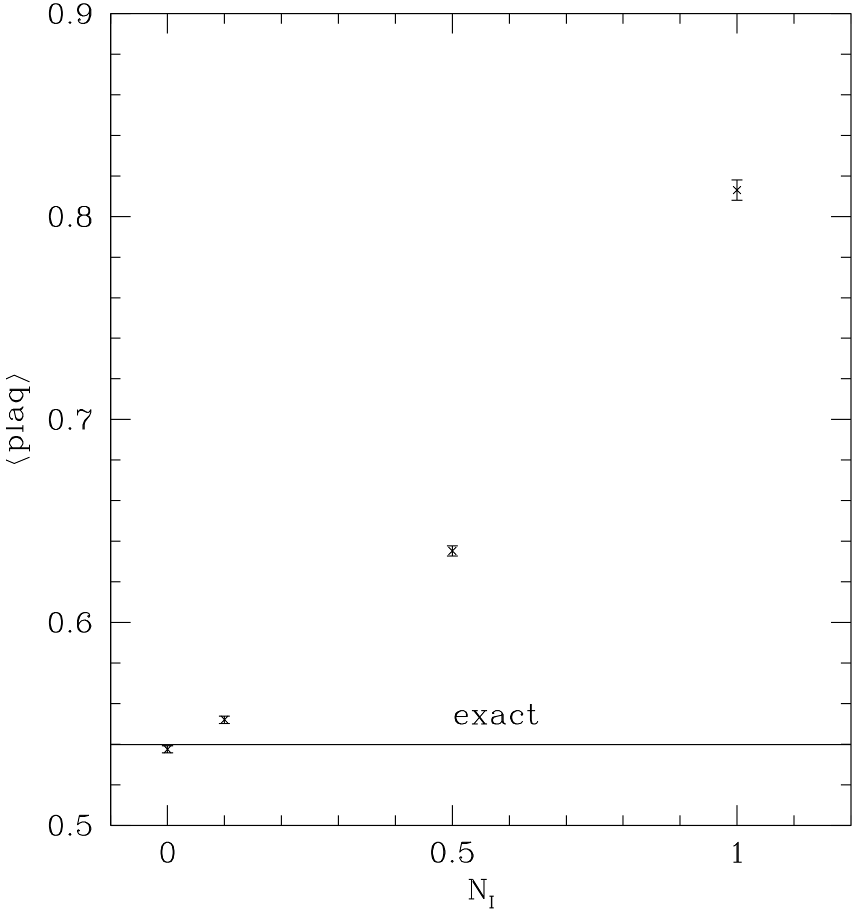
$\kappa = 0.0$

$N_I = 1.0$

$\approx$ classical trajectories

Problem

Convergence to wrong limit for $N_I > 0$.



$\beta = 1.0$

$\kappa = 0.25$

$\mu = 0.5$

Example 3 ("GP": Guralnik&Pehlevan 2009)

$$S = -i\beta(z + \frac{1}{3}z^3)$$

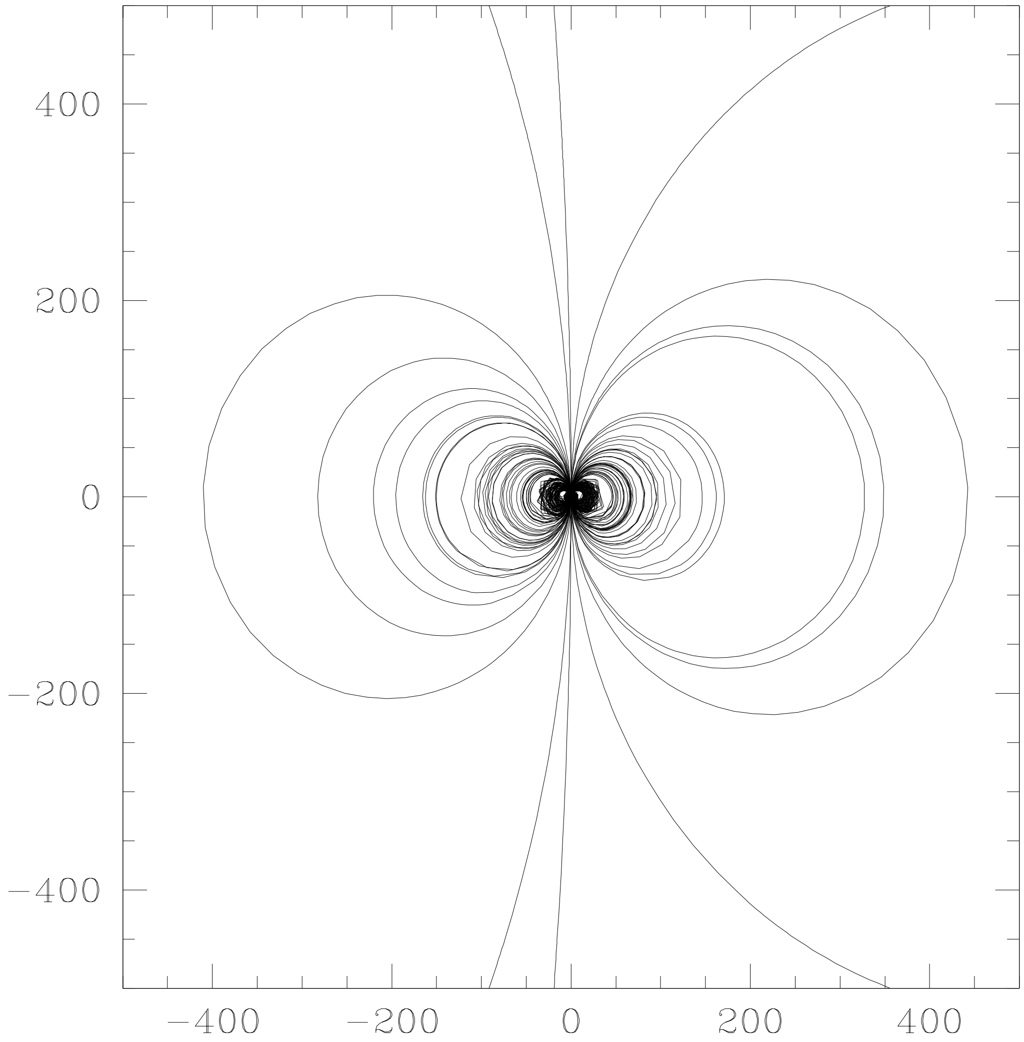
Attractive fixed point: $z = i$
Repulsive fixed point: $z = -i$, drift grows as $|z| \to \infty$

Classical orbits: Circles $z(t) = \frac{z_o + i \tanh t}{1 - i z_o \tanh t}$ $^{*)}$
$z_0 = -iy \, , y > 1$: escape to ∞ in finite time.

Expect trouble: large excursions, slow decay of equilibrium measure

$^{*)}$ Möbius transf. $\tanh t \equiv w \mapsto z(t) \; ; z(0) = z_o \, , z(\infty) = i$

Simulation



$N_I = 1.0, \beta = 1.0$

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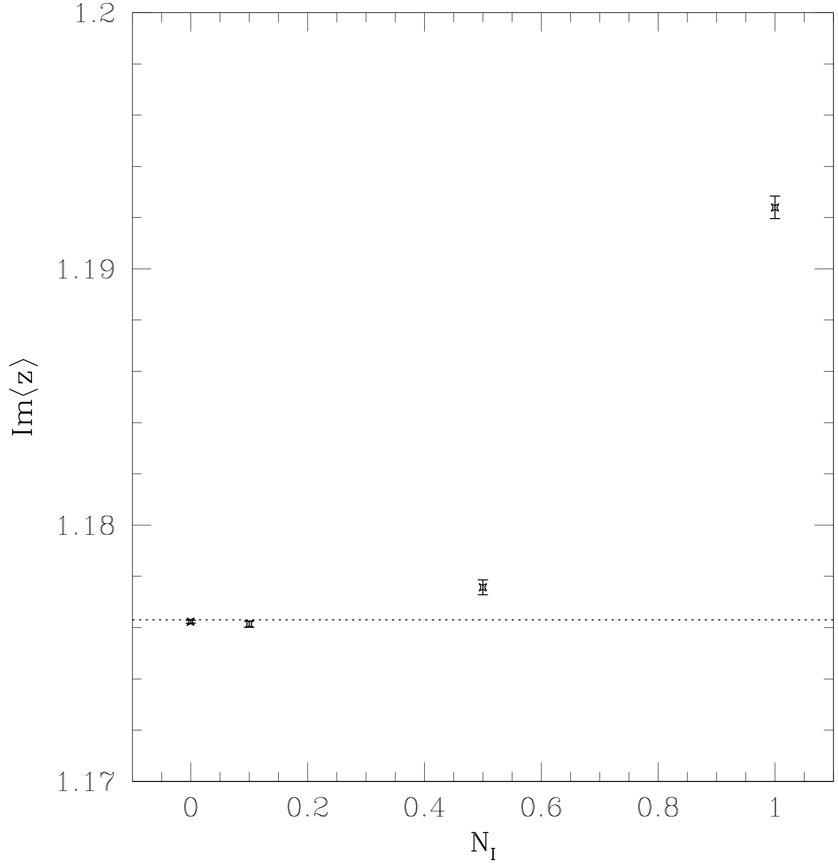


$\beta = 1.$

6. Etiology I: finite times

Revisiting ‘crucial identity’ (CI):

Recall

$$F(t,\tau) \equiv \int P(x,y;t-\tau)\mathcal{O}(x+iy;\tau)dxdy$$

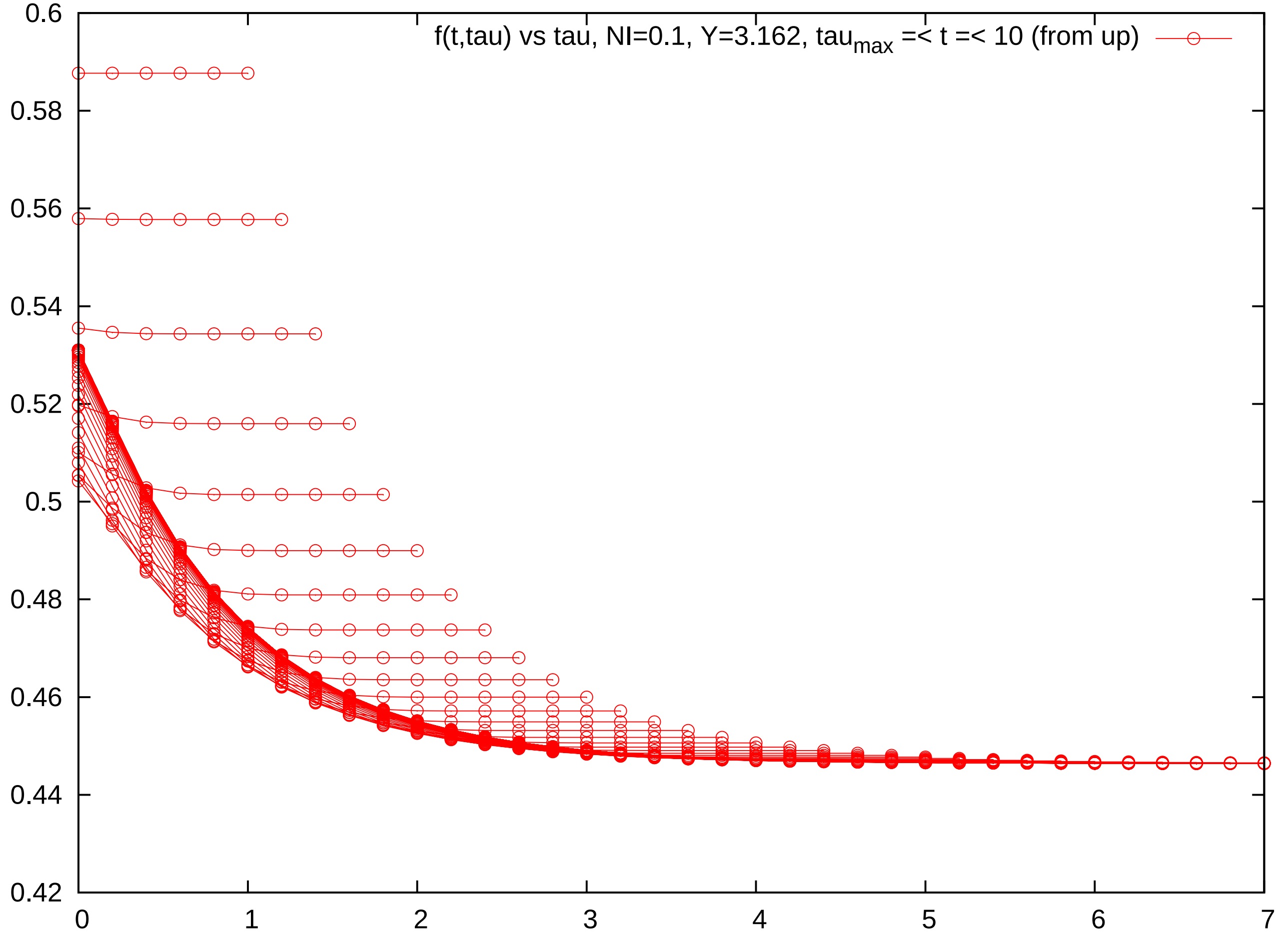
(CI)

$$\frac{\partial}{\partial\tau}F(t,\tau) = 0$$

But is this true?

Fails in U(1) toy model for $N_I > 0$:

Numerical test for U(1) via FPE



$F(t, \tau)$ vs. τ

Explanation

Langevin evolution of observables:

$$\tilde{L} = \frac{d^2}{dz^2} - a\sin(z - ic)\frac{d}{dz}\,.$$

But $\exp(t\tilde{L})\mathcal{O}$ grows super-exponentially:

$$\sup_x |\mathcal{O}(x + iy; t)| = |\mathcal{O}(\pi - iy)| \gtrsim \exp\left[\text{const}\exp(y/c)\right]\,.$$

for $t > 0$.

$P(x, y; t)$ (presumably) decays only like Gaussian $\Rightarrow$ formal argument fails, $F(t, \tau)$ not well defined.

Formal argument collapses.

7. Etiology II: equilibrium

Slow decay for $N_I > 0$

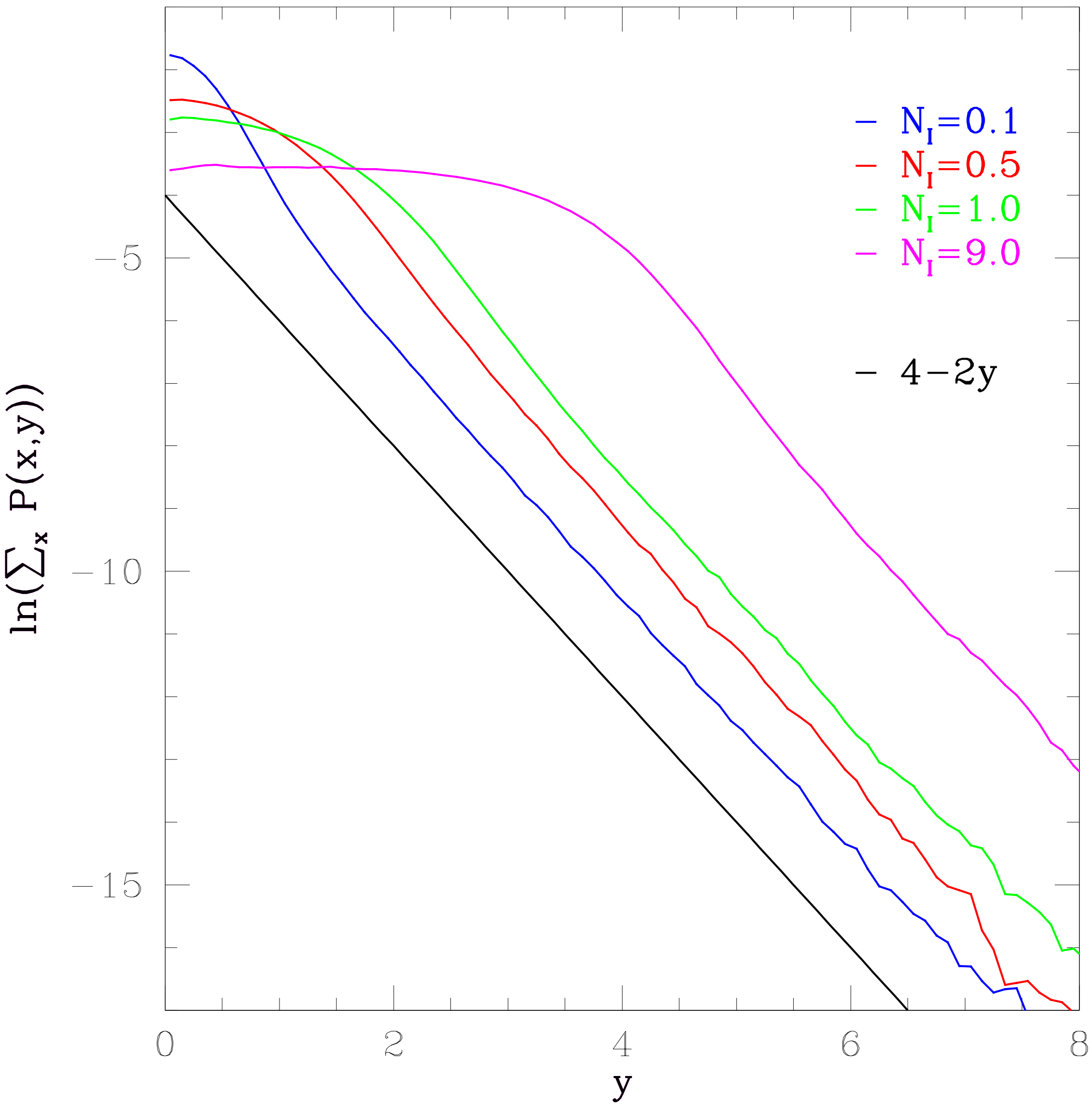
U(1) one-link model:
Analytic and numerical studies reveal (for $N_I > 0$)

$$\int dx P(x, y; \infty) \sim e^{-2|y|}$$

no super-exponential decay!
$\Rightarrow \exp(ikz)\, P(x, y; \infty)$ not absolutely integrable for $k \geq 2$.

$\Rightarrow \langle \exp(ikz) \rangle$ ambiguous.
Numerically: Large excursions $\Rightarrow$ Huge fluctuations.

Numerics: U(1) model



$\beta = 1.$

$\kappa = 0.0$

Falloff of modes:

$$P_k(y;t) \equiv \int \frac{dx}{2\pi}\, e^{ikx} P(x,y;t)$$

Analytic and numerical studies indicate for $N_I > 0$

$$P_k(y) \sim c_k e^{(-|k|+2)|y|}\ .$$

Hence $\int P_k(y) e^{-ky} dy$ exists

But $\int \exp(ikz)\, P(x,y;\infty) dx dy$ ambiguous ($k \geq 2$).

GP model:

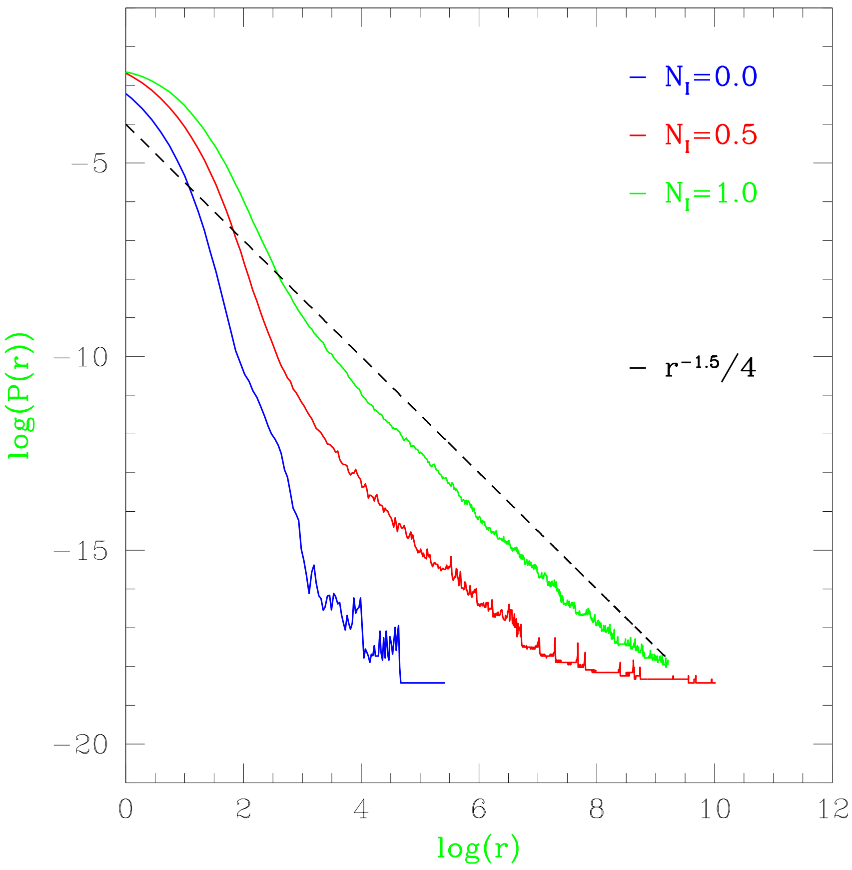
$$r \equiv \sqrt{x^2 + (y-1)^2}$$

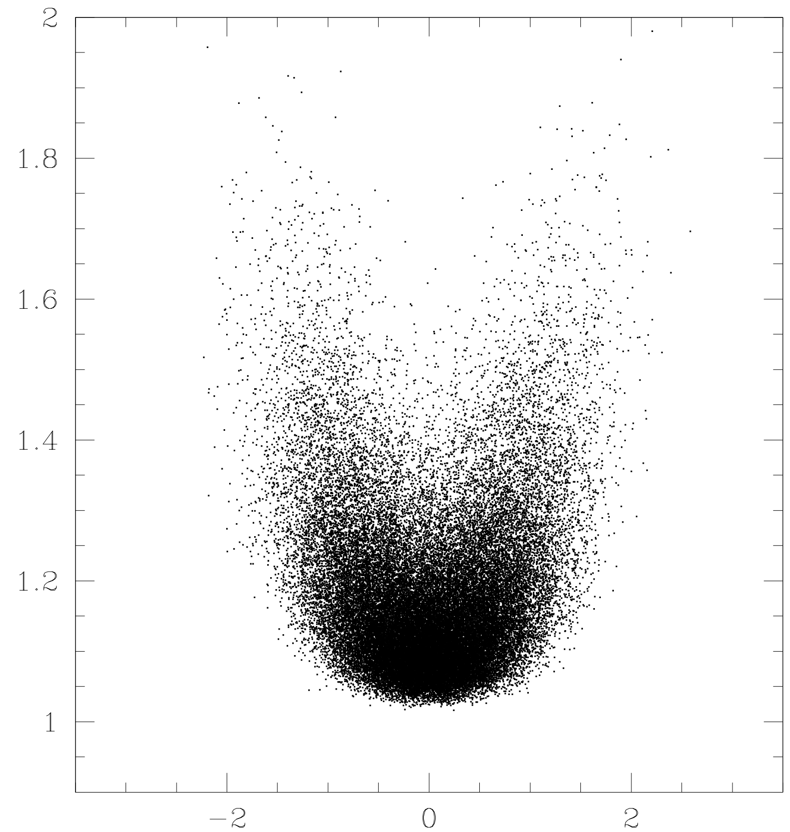
$P(r;\infty)$ density with respect to dr:
Numerical study indicates for $N_I > 0$

$$P(r;\infty)\,dr \sim r^{-1.5}\,dr$$

$\Rightarrow$ z not absolutely integrable. $\langle z \rangle$ Ambiguous.

Numerics: GP model





$N_I = 0$

8. CC as diagnostic tool

Recall:

$$\lim_{t\to\infty} \frac{d}{d\tau} F(t,\tau)\bigg|_{\tau=0} = 0\,.$$

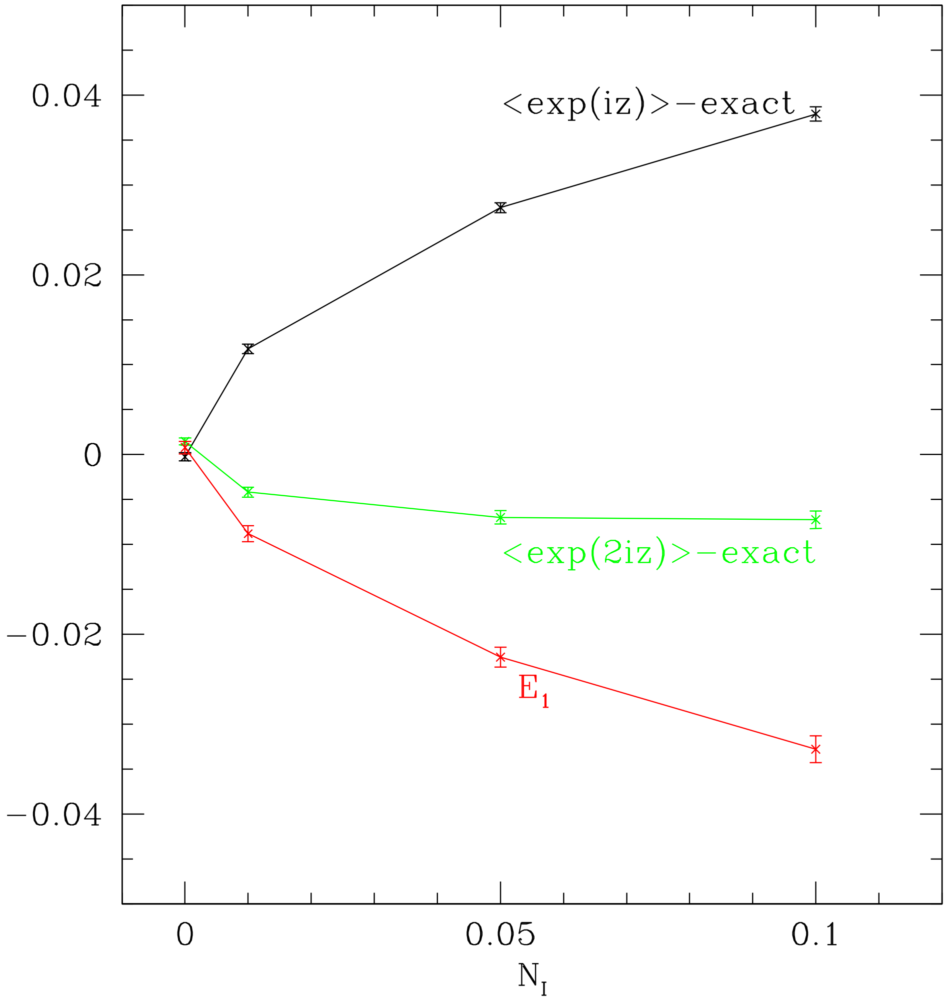
reduces to (CC):

$$\langle \tilde{L}\mathcal{O}(x+iy;0)\rangle \equiv \int P(x,y;\infty)\tilde{L}\mathcal{O}(x+iy;0)dx\,dy = 0$$

for ‘all’ observables $\mathcal{O}$.

In practice: test a few observables.

For $N_I > 0$ results incorrect, (CC) violated:



Test results for toy models

- Simple test successful to select correct simulations.

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- $N_I = 0$ preferable, but no guarantee for correctness.

9. Lattice models – examples

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- Four-fermion models (J. Pawlowski, I. O. Stamatescu, C. Zielinski, in preparation): Consistency Criterion tricky.

10. Generalizations as therapy?

Equilibrium measure $P(x, y)dxdy)$ not fixed by

$$\int_{\mathbb{C}^n} dx\, dy\, P(x, y)\mathcal{O}(x + iy) = \int_n dx \rho(x)\mathcal{O}(x)$$

for holomorphic $\mathcal{O}$.

Freedom: $P \to P + Q$ with

$$\int_{\mathbb{C}^n} dx\, dy\, Q(x, y)\mathcal{O}(x + iy) = 0\,.$$

Ignoring boundary terms

$$Q(x,y) = (\partial_{x_j} + i\partial_{y_j})H_j(x,y) \quad (j = 1,\ldots,n)\,.$$

More detailed characterization of Q possible, but useful?

Problem: How to modify process?

Modifying the CL process

Try:

$$L \to L + L_m$$

s.t.

$$L_m \mathcal{O} = 0$$

for holomorphic $\mathcal{O}$.

Ansatz:

$$L_m \equiv \sum_j F_j^2 \partial_{x_j}^2 + \sum_j G_j^2 \partial_{y_j}^2 + R_x \cdot \nabla_x + R_y \cdot \nabla_y \quad \Rightarrow$$

(1) $G_j^2 = F_j^2, \quad j = 1, \ldots n$,
(2) $R_x = R_y = 0$.

Stochastic process:

$$dx = K_x dt + (1+F) dw_x ,$$
$$dy = K_y dt + F dw_y \, .$$

Need

$$F \to 0 \quad \text{for} \quad |y_j| \to \infty \, .$$

because of problem with $N_I > 0$.

Useful?

Holomorphic kernel

cf. Okamoto et al 1989 $H(z)$ holomorphic on $\mathcal{M}_c$.

Generalized CLE:

$$
\begin{aligned}
dx =& \hat{K}_x\, dt + \mathrm{Re}\, H dw, \\
dy =& \hat{K}_y\, dt + \mathrm{Im}\, H dw
\end{aligned}
$$

where

$$
\begin{aligned}
&\hat{K} \equiv -H^2 \nabla_z S + \nabla_z H^2\,, \\
&\hat{K}_x \equiv \mathrm{Re}\, \hat{K}\,, \\
&\hat{K}_y \equiv \mathrm{Im}\, \hat{K}
\end{aligned}
$$

$$L_H = \left((\mathrm{Re}\, H)^2\nabla_x + \hat{K}_x\right)\nabla_x + \left((\mathrm{Im}\, H)^2\nabla_y + \hat{K}_y\right)\nabla_y$$
$$+ 2(\mathrm{Re}\, H)(\mathrm{Im}\, H)\nabla_x\nabla_y\,,$$

$$L_H^T = \nabla_x\left(\nabla_x(\mathrm{Re}\, H)^2 - \hat{K}_x\right) + \nabla_y\left(\nabla_y(\mathrm{Im}\, H^2 - \hat{K}_y\right)$$
$$+ 2\nabla_x\nabla_y(\mathrm{Re}\, H)(\mathrm{Im}\, H)\,.$$

$$L_{H,0}^T = \nabla_x H^2\left(\nabla_x + (\nabla_x S)\right)$$

$$L_{H,0}^T = \nabla_x H^2\left(\nabla_x + (\nabla_x S)\right)$$

$$\tilde{L}_H = H^2\Delta_z + \hat{K}\nabla_z\,.$$

Formal argument unchanged, but many problems for nonconstant kernel.

Reweighting

Idea:

Shift weight between ‘bare’ measure and Boltzmann factor $\exp(-S)$

$$e^{-S(\phi)} d\nu(\phi) = e^{-S_r(\phi)} d\nu_1(\phi)\,.$$

Some success in toy models

Berges and Sexty 2007, Sexty 2008, 2009, Stamatescu 2007

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  perfect specificity (no false positives),
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- Test for lattice models: checked for Karsch-Wyld
  $SU(3)$ spin model (Aarts & James 2011)

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  perfect specificity (no false positives),
  good sensitivity (‘not really’ false negatives found)
- Test for lattice models: checked for Karsch-Wyld $SU(3)$ spin model (Aarts & James 2011)
- Therapy for wrong limits: use nonuniqueness of correct P? Kernel? Other?

11. Conclusions and outlook

- Method shows some promise
- Main problem: insufficient falloff of probability
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  perfect specificity (no false positives),
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