Complex Langevin:
Mathematical results and problems

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Overview

1. Introduction
2. General discussion
3. Quadratic actions
4. Mathematical and Practical Problems
5. Extension to manifolds?
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1. Introduction

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)
Resurrection

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

Continuation: Berges et al 2007, Berges & Sexty 2007

Finite density: Aarts & Stamatescu 2008

– Numerically impressive results
– approach appears again promising
– but problems lingering.

Guralnik & Pehlevan 2008-2009 Solutions to some?
2. General discussion

‘Flat’ case: defined on $\mathcal{M} = \mathbb{R}^n$, analytically continued to $\mathcal{M}_c \equiv \mathbb{C}^n$.

Complex Langevin:

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

$dw$ increment of Wiener process on $\mathbb{R}^n$ (formally $dw = \eta(t) dt$, $\eta$ white noise).

This is real stochastic process:

$$dx = K_x dt + dw$$

$$dy = K_y \nabla_x S(x + iy) dt,$$  \hspace{1cm} (1)
\[ K_x = -\text{Re}\nabla_x S(x + iy) \]
\[ K_y = -\text{Im}\nabla_x S(x + iy) \]

(2)

⇒ Real Fokker-Planck equation

\[ \frac{\partial}{\partial t} P(x, y; t) = L_{FP} P(x, y; t); \quad P(x, y; 0) = \delta(x-x_0)\delta(y-y_0) , \]

\( P \) probability density in \( \mathbb{R}^{2n} \),
real Fokker-Planck operator:

\[ L_{FP} \equiv \nabla_x [\nabla_x - K_x] - \nabla_y K_y \]
Complex Fokker-Planck Equation: Given $y_0$, define

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

where $\rho_{y_0}(x; t)$ is complex density defined on $\mathbb{R}^n + iy_0$,

$$L_{y_0}^c \equiv \nabla_x [\nabla_x + (\nabla_x S(x + iy_0))].$$

Special case: $S(x)$ real for $x$ real:
Complex FPE $\rightarrow$ standard FPE
Real FPE lives still in $\mathbb{R}^{2n}$, but has stationary solution

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

$L^c_{y_0}$ operator on $\mathcal{H}_2 \equiv L^2(e^{Re S} dx)$.

Unitary map $U : L^2(dx) \to \mathcal{H}_2$:

$$U \psi = \exp(-\frac{1}{2}S)\psi ,$$

$$H_{FP} \equiv -U^{-1}L^c_{y_0} U = - (\nabla - \frac{1}{2}(\nabla S)) (\nabla + \frac{1}{2}(\nabla S)) ;$$

$S$ real: $H_{FP}$ manifestly positive.

**Fact:** spectrum and numerical range of $-H_{FP}$ and $L^c_{y_0}$ agree.
**Goal and Questions**

**Goal:** Produce expectation values of holomorphic observables $O$:

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

independent of $y_0$ by Cauchy’s theorem.

**Hope:** obtainable as long time limit of

$$\langle O \rangle_{P,t} \equiv \frac{\int O(x+iy)P(x,y;t)d^n x d^n y}{\int P(x,y;t)d^n x d^n y} ;$$

and by ergodicity as

$$\lim_{t \to \infty} \frac{1}{t} \int O(z(t)) dt .$$
**Question:** Relation to ‘$\rho$-expectations’

\[
\langle O \rangle_{\rho,t} \equiv \frac{\int O(x+iy_0)\rho(x;t)d^n x}{\int \rho_y(x;t)d^n x}
\]

Transposer operators:

\[(L^c_{y_0})^T \equiv [\nabla_x - (\nabla_x S(x + iy_0))] \nabla_x ,\]

\[L^T_{FP} \equiv \left[\nabla_x - \text{Re}(\nabla_x S(x + iy))\right] \nabla_x - \text{Im}(\nabla_x S(x + iy)) \nabla_y\]

defined such that

\[\partial_t \langle O \rangle_{\rho,t,y} = \langle (L^c_{y_0})^T O \rangle_{\rho,t} \text{ and } \partial_t \langle O \rangle_{P,t} = \langle L^T_{FP} O \rangle_{P,t} .\]
Result

Assume

- for all \( y_0 \) \( L_{y_0}^c \) generates bounded holomorphic semigroup,
- for all \( y_0 \) \( O(x + iy_0) \in L^1(\mathbb{R}^n, d^n x) \cap L^2(\mathbb{R}^n, d^n x) \),
- \( L_{FP} \) generates quasibounded (strongly continuous) semigroup (i.e. \( \| e^{tL_{FP}} \| \leq C_1 e^{C_2 t} \)).

\[ \Rightarrow \langle O \rangle_{\rho,t} = \langle O \rangle_{P,t} \]

for all \( t \geq 0 \) and all \( y_0 \).
Proof

1. Initial conditions agree (Cauchy)
2. By assumption, \( \exp \left[ t\left( L_{y_0}^c \right)^T \right] O(x + iy_0; t) \) is in \( L^2 \) and unique solution of DE

\[
\partial_t O(x + iy_0; t) = \left( L_{y_0}^c \right)^T O(x + iy_0; t).
\]

By Cauchy-Riemann equations

\[
\left( L_{y_0}^c \right)^T O(x + iy_0) = L_{FP}^T O(x + iy)\big|_{y_0},
\]

and hence

\[
\exp(t L_{y_0}^T) O(x + iy_0) = \exp(t \left( L_{FP}^c \right)^T) O(x + iy)\big|_{y_0}.
\]

Integration by parts completes the proof.
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- Convergence of \( P(x, y; t) \) not necessary. Need only convergence of \( \rho(x; t) \).
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• Need: spectrum of $L_{y0}^c$ in left half plane.

• $\text{spec}(L_{y0}^c) \subset \text{spec}(L_{FP})$. Pseudospectrum?
3. Quadratic Actions

Almost trivial, but instructive. Complete analysis possible.

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.

Assumptions:

- **A strictly dissipative:** \( A_r = \frac{1}{2} (A + A^\dagger) < 0 \).
- **A diagonalizable by a complex orthogonal matrix \( O \):**
  \[ A = O^T D O \] with \( D = \text{diag}(\lambda_1, \ldots, \lambda_n) \). Generic!
**Fact:** \( \text{Re } \lambda_1, \ldots \lambda_n < 0 \) because \( A \) strictly dissipative.
Converse not true:

\[
A = -\begin{pmatrix} 1 & 2 + 2i \\ 2 + 2i & 1 \end{pmatrix}
\]

has eigenvalues \( \lambda_{1,2} = -1 \pm \sqrt{8}i \), but

\[
\frac{1}{2}(A + A^\dagger) = -\frac{1}{2} \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix}
\]

not negative definite (eigenvalues \(-1, 3\)).
**1D example**

\[ S = \frac{1}{2} ax^2, \quad a = a_r + ia_i, \quad a_r > 0 \]

\[ L_{FP} = \partial_x^2 + a_r (\partial_x x + \partial_y y) + a_i (-\partial_x y + \partial_y x). \]

\( L_{FP} \) not dissipative:

\[ \frac{1}{2} (L_{FP} + L_{FP}^\dagger) = \partial_x^2 + 2a_r. \]

But stationary solution:

\[ P(x, y; \infty) = c \exp \left[ -a_r x^2 - \frac{2a_r^2}{a_i} xy - \frac{a_r}{a_i^2} (2a_r^2 + a_i^2) y^2 \right]. \]

Integrable for \( a_r > 0 \).
Remark: Level lines of $P(x, y; \infty)$ are tilted ellipses:

$$P(x, y; \infty) = c \exp[-Q(x, y)]$$

with

$$Q(x, y) = \frac{a_r}{2} \left[ x + y(\alpha + \sqrt{1 + \alpha^2}) \right]^2 +$$

$$\frac{a_r}{2} \frac{1+\alpha^2-\sqrt{1+\alpha^2}}{1+\alpha^2+\sqrt{1+\alpha^2}} \left[ x(\alpha + \sqrt{1 + \alpha^2}) - y \right]^2.$$  \hspace{1cm} (2)

where $\alpha = a_r/a_i$. 
Time-dependent solution

(Haymaker & Peng 1989):

\[ X = \begin{pmatrix} x \\ y \end{pmatrix}, \quad X_0 = \begin{pmatrix} x_0 \\ y_0 \end{pmatrix}, \quad Z(t) = X - e^{-at} \begin{pmatrix} \cos at & \sin at \\ -\sin at & \cos at \end{pmatrix} X_0; \]

\[ P(x, y; t) = \exp \left[ -\frac{1}{2} Z(t)^T \Sigma^{-1}(t) Z(t) \right] \]

with \( \Sigma(t) = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{pmatrix} \)
\[ \sigma_{11} = \frac{1}{a_r} + \frac{a_r}{2(a_r^2 + a_i^2)} + e^{-2a_r t}\left[\frac{-a_r \cos(2a_i t) + a_i \sin(2a_i t)}{2(a_r^2 + a_i^2)} - \frac{1}{2a_r}\right] \]

\[ \sigma_{12} = -\frac{a_r}{2(a_i^2 + a_i^2)} + e^{-2a_r t}\left[\frac{a_r \sin(2a_i t) + a_i \cos(2a_i t)}{2(a_r^2 + a_i^2)}\right] \]

\[ \sigma_{22} = \frac{1}{a_r} - \frac{a_r}{2(a_r^2 + a_i^2)} + e^{-2a_r t}\left[\frac{a_r \cos(2a_i t) - a_i \sin(2a_i t)}{2(a_r^2 + a_i^2)} - \frac{1}{2a_r}\right] \]
Complex FP equation

\[ L^c_{y_0} = \partial_x^2 + a \partial_x (x + iy_0); \]

not dissipative if \( a_i \neq 0 \).

FP Hamiltonian:

\[ H_{FP} = -\partial_x^2 - \frac{1}{2} a + \frac{1}{4} a^2 (x + iy_0)^2, \]

For \( y_0 = 0 \) and rescaled \( x \mapsto x\sqrt{2} \): standard harmonic oscillator

\[ H_{h.o.} = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} \omega^2 x^2 - \frac{\omega}{2} \]
**Mehler formula**

\[ \exp(-tH_{h.o.}(x, x_0)) \equiv Q_t(x, x_0), \]

with

\[ Q_{\omega t}^\omega (x, x_0) = \sqrt{\frac{\omega}{\pi(1-e^{-2\omega t})}} \exp \left[ -\frac{\omega(x^2+x_0^2)}{2 \tanh(\omega t)} - \frac{\omega xx_0}{\sinh(\omega t)} \right]. \]

Using unitary map \( U \):

\[ \exp(tL_0^c)(x, x_0) = e^{-ax^2/4} Q_t^\omega \left( \frac{x}{\sqrt{2}}, \frac{x_0}{\sqrt{2}} \right) e^{ax_0^2/4}. \]

Reintroduce \( y_0 \):

\[ \exp(tL_{y_0}^c)(x, x_0) = \exp(tL_0^c)(x + iy_0, x_0 + iy_0). \]
Higher dimensions

\[ L_{FP} = \Delta_x + \nabla_x \cdot A_r x + \nabla_y \cdot A_r y - \nabla_x \cdot A_i y + \nabla_y \cdot A_i x , \]

\[ L_{FP}^\dagger = \Delta_x - (A_r x) \cdot \nabla_x - (A_r y) \cdot \nabla_y + \nabla_x \cdot A_i y - \nabla_y \cdot A_i x . \]

\[ \frac{1}{2} (L_{FP} + L_{FP}^\dagger) = \Delta_x + 2 \text{tr} A , \]

so \( L_{FP} \) is again not dissipative.
Solution by Mehler kernel

First $A_i = 0$: exists $O$ (orthogonal)

$$A = O^T D$$

with $D = \text{diag}(\lambda_1, \ldots, \lambda_n)$.

Put $Ox = x'$, $Ox_0 = x'_0$:

$$\exp(-tH_{FP})(x, x_0) = \prod_{i=1}^{n} Q^\lambda_i \left( \frac{(Ox)_i}{\sqrt{2}}, \frac{(Ox_0)_i}{\sqrt{2}} \right).$$

$$e^{L_{y_0} t}(x, x_0) = \exp\left(-\frac{S(x+iy_0)}{2}\right) \prod_{i=1}^{n} Q^\lambda_i \left( \frac{(Ox)_i}{\sqrt{2}}, \frac{(Ox_0)_i}{\sqrt{2}} \right) \exp\left[\frac{S(x_0+iy_0)}{2}\right].$$
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• Relaxation to equilibrium if $\Re \lambda_i > 0$, $i = 1, \ldots, n$.

• Moral reason: all classical trajectories attracted to origin.
4. Problems

Mathematical and practical difficulties:

- **Existence** of the semigroup generated by $L_{FP}$. Not known: $L_{FP}$ never manifestly dissipative.
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- **Runaways:** In typical cases deterministic motion can go to $\infty$ in finite time. Reason: Drift $\nabla S$ grows in some directions. 1D:

  $$\dot{z} = -S' \implies t - t_0 = -\int \frac{dz}{S'}$$

  (integration on curve with $dz$ real multiple of $S'$).
**Example** (Aarts& Stamatescu 2008)

\[ S = -\beta \cos x - \kappa \cos(x - i\mu) \]

Complex Langevin equation

\[ dx = K_x dt + dw, \quad dy = K_y dt \]

with

\[ K_x = -\sin x [\beta \cosh y + \kappa \cosh(y - \mu)] \]
\[ K_y = -\cos x [\beta \sinh y + \kappa \sinh(y - \mu)] \]

(1)
From (Aarts & Stamatescu 2008): Drift pattern
Real FP operator:

\[ L_{FP} = \partial_x [\partial_x - K_x] - \partial_y K_y \]

Complex FP operator:

\[ L_{y_0}^c = \partial_x [\partial_x + \beta \sin(x + iy_0) + \kappa \sin(x + iy_0 - i\mu)] \]

Drift \( K_x, K_y \) parallel to gradient of

\[ G(x, y) = \exp \left[ - \frac{\cos x}{\beta \cosh y + \kappa \cosh(y - \mu)} \right]. \]
$G$ is Lyapunov function:

$$\frac{d}{dt} G(x(t), y(t)) = (K_x \partial_x + K_y \partial_y) G(x, y) =$$

$$- \left[ \sin^2 x + \cos^2 x \left( \frac{\beta \sinh y + \kappa \sinh(y-\mu)}{\beta \cosh y + \kappa \cosh(y-\mu)} \right)^2 \right] G \leq 0,$$

Vanishes only on stable fixed point $(x, y_*)$;
⇒ all points attracted to $(x, y_*)$.  

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$G$ also candidate stochastic Lyapunov function:

$$L_{FP}^T G < 0$$

for $|y|$ large enough.

Need (Khasminskii 1980):

$$L_{FP}^T G \to -\infty \quad \text{for } |y| \to \infty .$$

Open problem.

*Practically* large excursions cause problems even if stationary $P(x, y)$ exists.
• *Spectral* projections of complex FP operator: Example Davies&Kuilaars, 2004: Spectral projections $P_n$ of complex harmonic oscillator grow:

$$\|P_n\| \geq a C^{2n+1}, \quad C > 1;$$

poor convergence of eigenfunction expansions:

$$e^{-Ht}\psi = \sum_n e^{-\omega(n+1/2)t} P_n\psi$$

– Eigenfunctions do not form Riesz basis
– $e^{-Ht}$ not bounded semigroup
– $\exists$ pseudospectrum far from spectrum!

(Davies 1999)
**Riesz basis** \( (\phi_n)_{n=1}^{\infty} \):

\[ \exists \text{ bounded operator } S \text{ with } S^{-1} \text{ bounded such that} \]

\[ S\phi_n = e_n \quad n = 1, \ldots \infty, \]

where \( (e_n)_{n=1}^{\infty} \) orthonormal basis.

**Pseudospectrum:**

\[ \text{spec}_\epsilon(A) \equiv \{ z \in \mathbb{C} \mid \|(A - z)^{-1}\| > \epsilon^{-1} \} \]

Signifies instability:

\[ \text{spec}_\epsilon(A) = \bigcup_B \{ \text{spec}(A + B), \|B\| < \epsilon \} \]

Tiny perturbation can eliminate “pseudo”
• Convergence to wrong limit
  Noticed by Klauder&Petersen 1985
  – Ambjørn et al 1986:
  “Quantum mechanical disasters of the first degree”:

  \[ S = -\beta \cos \theta - i\theta \]

  works for large \( \beta \), fails for small \( \beta \).

  “Non-abelian disasters of the third degree”:

  \[ S = -\beta \text{tr}\ U - \log \text{tr}\ U, \quad U \in SU(2), SU(3) \]

  works for large \( \beta \), fails for small \( \beta \).
– Haymaker&Wosiek 1987:

\[ S = -\beta \cos \theta - \log \cos \theta \]

Simulates restricted range \([-\pi/2, \pi/2]\).

**Reason:** zero of \(\cos \theta\).


1. 1D, \(S\) polynomial, \(e^{-S} \in S\)
2. \(\int_{\mathbb{R}} e^{-S(x)} \, dx \neq 0\)
3. \(\forall k \in \mathbb{R} \quad \lim_{t \to \infty} \langle e^{ikz} \rangle_{P,t} \) exists and is \(\in S(\mathbb{R})\).

Not really practical.
5. 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:
– $\mathcal{M}$ Riemannian manifold $\Rightarrow \exists$ Wiener process $\Rightarrow$
  noise in real directions well defined
– Real manifold $\mathcal{M}$ has to have complexification $\mathcal{M}_C$.

Formal arguments carry over; problems remain.
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- Hope for the best, be prepared for the worst