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?
6. Outlook

1. Introduction

Complex Langevin first (?) proposed:

Parisi, Phys. Lett. **131 B** (1983) 393; Klauder, Acta Phys. Austriaca Suppl. **XXXV** (1983) 251.

Many studies in 1980's and 1990's, e.g.

Hüffel&Rumpf 1984, Klauder&Petersen 1984, J. Ambjørn and S.-K. Yang 1985, Ambjørn, Flensburg&Peterson 1986, Nakazata&Yamanaka 1986, Gausterer&Klauder 1986, Söderberg 1988, Haymaker&Wosiek 1987, Söderberg 1988, Okamoto, Okano, Schülke and Tanaka 1989, Haymaker&Peng 1989, Gausterer 1993, L. L. Salcedo 1993, 1997, S. Lee 1994, Gausterer&Thaler 1998.

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
(precursor: 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 $dw = \eta(t)dt$, η white noise).

This is real stochastic process:

$$\begin{aligned} dx &= K_x dt + dw \\ dy &= K_y \nabla_x S(x+iy) dt \, , \end{aligned} \qquad (1)$$

$$\begin{aligned} K_x &= -\mathrm{Re}\nabla_x S(x+iy) \\ K_y &= -\mathrm{Im}\nabla_x S(x+iy) \end{aligned} \qquad (2)$$

$\Longrightarrow$ 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

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

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

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

Special case: $S(x)$ real for x real:
Complex FPE $\to$ 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 $U : L^2(dx) \to \mathcal{H}_2$:

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

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

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 'ρ-expectations'

$$\langle O \rangle_{\rho,t} \equiv \frac{\int O(x+iy_0)\rho(x;t)d^n x}{\int \rho_{y_0}(x;t)d^n x} \ ?$$

Transpose operators:

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

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

defined such that

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

Result

Assume

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

$$\Longrightarrow \langle O \rangle_{\rho,t} = \langle O \rangle_{P,t}$$

for all $t \geq 0$ and all y_0.

Proof

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

$$\partial_t O(x+iy_0;t) = (L^c_{y_0})^T O(x+iy_0;t)\,.$$

By Cauchy-Riemann eqations

$$(L^c_{y_0})^T O(x+iy_0) = L^T_{FP} O(x+iy)\Big|_{y_0}\,,$$

and hence

$$\exp(tL^T_{y_0}) O(x+iy_0) = \exp(t(L^c_{FP})^T) O(x+iy)\Big|_{y_0}\,.$$

Integration by parts completes the proof.

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- Need: spectrum of $L^c_{y_0}$ in left half plane.
- $\mathrm{spec}(L^c_{y_0}) \subset \mathrm{spec}(L_{FP})$. Pseudospectrum?

3. Quadratic Actions

Almost trivial, but instructive. Complete analysis possible. (cf. Ambjørn&Yang 1985, Haymaker&Peng 1989)

Setting:

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

$A = A_r + iA_i$ 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: $A = O^T DO$ with $D = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. Generic!

Fact: $\mathrm{Re}\,\lambda_1, \ldots \lambda_n < 0$ because A strictly dissipative.
Converse not true:

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

has eigenvalues $\lambda_{1,2} = -1 \pm \sqrt{8i}$, 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

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

where $\alpha = a_r/a_i$.

Time-dependent solution

(Haymaker&Peng 1989):

$$X = \begin{pmatrix} x \\ y \end{pmatrix}, X_0 = \begin{pmatrix} x_0 \\ y_0 \end{pmatrix}, Z(t) = X - e^{-a_r t} \begin{pmatrix} \cos a_i t & \sin a_i t \\ -\sin a_i t & \cos a_i t \end{pmatrix} X_0$$

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

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:

$$H_{FP} = -\partial_x^2 - \tfrac{1}{2}a + \tfrac{1}{4}a^2(x + iy_0)^2\,,$$

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

$$H_{h.o.} = -\tfrac{1}{2}\tfrac{d^2}{dx^2} + \tfrac{1}{2}\omega^2 x^2 - \tfrac{\omega}{2}$$

Mehler formula

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

with

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

Using unitary map U:

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

Reintroduce y_0:

$$\exp(tL_{y_0}^c)(x, x_0) = \exp(tL_0^c)(x + iy_0, x_0 + iy_0)\,.$$

Higher dimensions

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

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

$$\tfrac{1}{2}(L_{FP} + L_{FP}^\dagger) = \Delta_x + 2\,\mathrm{tr}\,A \,,$$

so L_{FP} is again not dissipative.

Solution by Mehler kernel

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

$$A = O^T D$$

with $D = diag(\lambda_1, \ldots, \lambda_n)$.
Put $Ox = x'$, $Ox_0 = x'_0$:

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

$$e^{L_{y_0} t}(x, x_0) = \exp(-\frac{S(x+iy_0))}{2} \prod_{i=1}^{n} Q_t^{\lambda_i} \left(\frac{(Ox)_i}{\sqrt{2}}, \frac{(Ox_0)_i}{\sqrt{2}} \right) \exp\left[\frac{S(x_0+iy_0)}{2} \right]$$

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- Relaxation to equilibrium if $\mathrm{Re}\,\lambda_i > 0$, $i = 1, \ldots, n$.
- 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.
  Hope: with new scalar product L_{FP} dissipative.

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

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

(integration on curve with dz real multiple of S').

Example (Aarts& Stamatescu 2008)

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

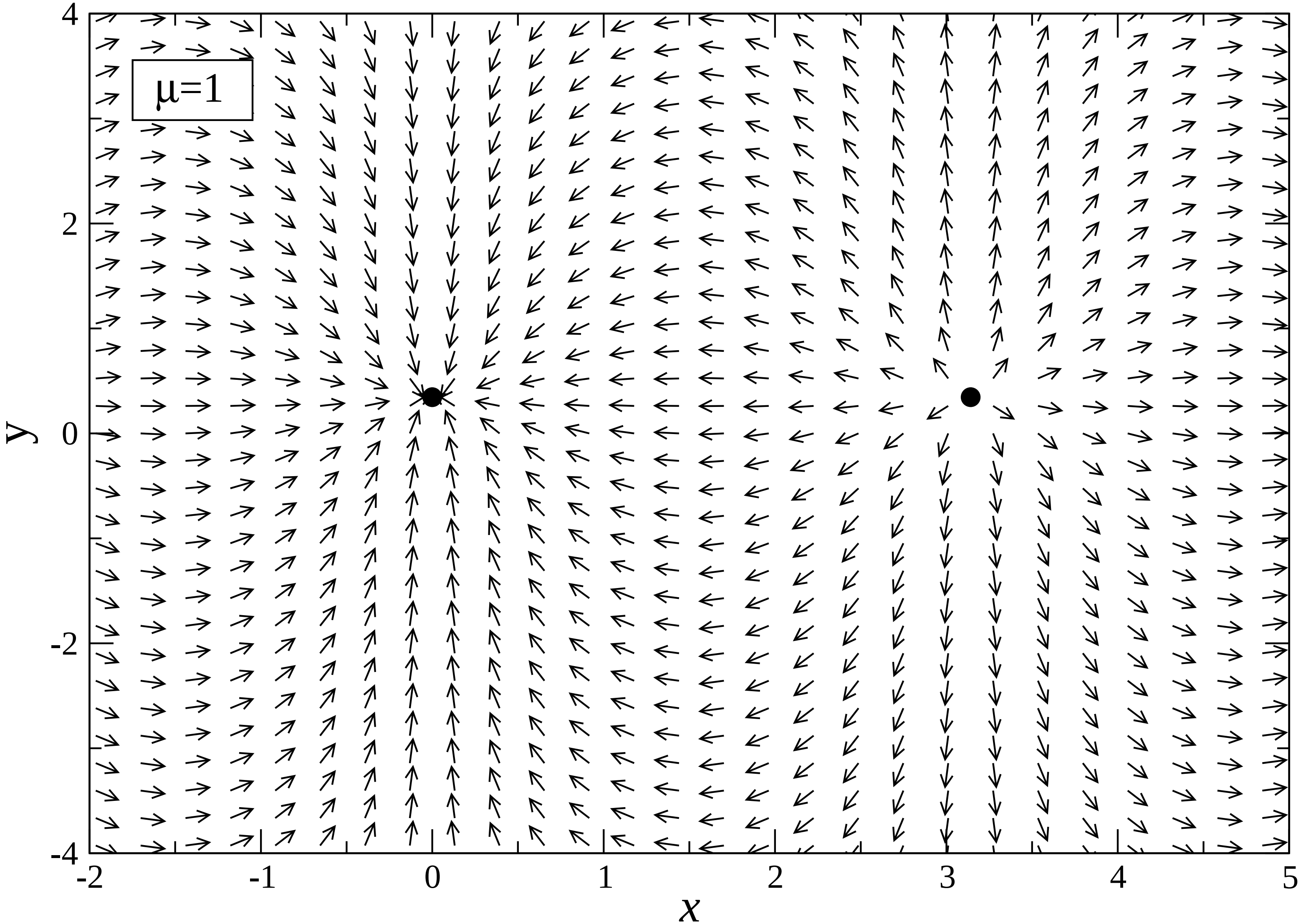
Complex Langevin equation

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

with

$$\begin{aligned} K_x &= -\sin x \left[\beta \cosh y + \kappa \cosh(y - \mu)\right] \\ K_y &= -\cos x \left[\beta \sinh y + \kappa \sinh(y - \mu)\right] \end{aligned} \tag{1}$$

From (Aarts& Stamatescu 2008): Drift pattern



Real FP operator:

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

Complex FP operator:

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

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_*);
$\Rightarrow$ all points attracted to (x, y_*).

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 $(\phi_n)_{n=1}^{\infty}$:

$\exists$ bounded operator S with S^{-1} bounded such that

$$S\phi_n = e_n \quad n = 1, \ldots \infty\,,$$

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

Pseudospectrum:
$\mathrm{spec}_\epsilon(A) \equiv \{z \in \mathbb{C} |\ \|(A-z)^{-1}\| > \epsilon^{-1}\}$

Signifies instability:

$$\mathrm{spec}_\epsilon(A) = \bigcup_B \{\mathrm{spec}(A+B), \|B\| < \epsilon\}$$

Tiny perturbation can eliminate “pseudo”

- Convergence to wrong limit
  Noticed by Klauder&Petersen 1985

  – Ambjørn et al 1986:

  "Quantum mechanical desasters of the first degree":

  $$S = -\beta \cos\theta - i\theta$$

  works for large β, fails for small β.

  "Non-abelian desasters of the third degree":

  $$S = -\beta \mathrm{tr}\, U - \log \mathrm{tr}\, U, \quad U \in SU(2), SU(3)\,,$$

  works for large β, fails for small β.

– Haymaker&Wosiek 1987:

$$S = -\beta cos\theta - \log\cos\theta$$

Simulates restricted range $[-\pi/2, \pi/2]$.
Reason: zero of $\cos\theta$.

– Gausterer 1993: criterion for correctness.
(1) 1D, S poynomial, $e^{-S} \in \mathcal{S}$
(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 $\in \mathcal{S}(\mathbb{R})$.
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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- More general procedures to represent complex measures by positive ones (Salcedo 1997-2007, Bender et al 1998-2008, Weingarten 2002, Bernard& Savage 2001)

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- Practical usefulness has to be checked
- Validation necessary: check with analytic or otherwise known result.
- More general procedures to represent complex measures by positive ones (Salcedo 1997-2007, Bender et al 1998-2008, Weingarten 2002, Bernard& Savage 2001)
- Hope for the best, be prepared for the worst