Stochastic Quantization - beyond Euclidean Action

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Stochastic processes in Quantum Field Theory

Procedure: Realize a sampling of field configurations by defining a supplementary (noisy) dynamics in a 5-th "time".

Basic example: Parisi Wu stochastic quantization in Euclidean QFT

- proofs of equivalence with path integral formulation, proofs of convergence, etc
  rely on the definition of a probability distribution over the space of field configurations via an associated Fokker-Planck equation
- can define a "perturbation theory" without gauge fixing
- for numerical studies: comparable to MC

  (see also Damgaard and Hueffel; Namiki, ...)

Essential feature: uses a drift force to define the process (the *5-th time dynamics*)

$\longrightarrow$ **versatility**

- can be directly related to expectation values
- can be directly defined from the set up of the problem without needing an action or a probability interpretation for the path integral

This may be of interest in cases where other approaches (e.g., MC) do not work.

In the following: point of view of numerical simulations.

Usual realizations: Langevin Equation and Random Walk.

Here in discretized form, Ito calculus, ϑ: 5-th "time", $\delta\vartheta$: "time" step; for each d.o.f. $\varphi(x)$ (random variable), $K[\varphi]$: drift force,

Langevin equation:

$$\delta\varphi(x;\vartheta) \equiv \varphi(x;\vartheta+\delta\vartheta)-\varphi(x;\vartheta) = K[\varphi(x;\vartheta)]\,\delta\vartheta + \eta(x;\vartheta)$$
$$\langle\eta(x;\vartheta)\rangle = 0, \quad \langle\eta(x;\vartheta)\eta(x';\vartheta')\rangle = 2\,\delta\vartheta\,\delta_{x,x'}\,\delta_{\vartheta,\vartheta'}$$

Random Walk:

$$\delta\varphi(x;\vartheta) = \pm\omega, \quad \text{with pbb}: \ \tfrac{1}{2}(1 \pm \tfrac{1}{2}\omega\,K[\varphi(x;\vartheta)])\,, \ \omega = \sqrt{\delta\vartheta}$$

NB: since η, $\omega \propto \sqrt{\delta\vartheta}$ we need also second derivatives:

$$\delta f[\varphi(\vartheta] = \partial_\varphi f[\varphi(\vartheta)]\,\delta\varphi(x;\vartheta) + \tfrac{1}{2}\partial^2_\varphi f[\varphi(\vartheta)]\,[\delta\varphi(x;\vartheta)]^2$$

Relation to path integral and MC

If the drift is the gradient of a real action, bounded from below **then** there is a probability density $\rho(\varphi, \vartheta)$ satisfying an associated Fokker-Planck Equation in the limit $\delta\vartheta \longrightarrow 0$:

$$\partial_\vartheta \rho(\varphi, \vartheta) = \partial_\varphi \left(\partial_\varphi - K\right) \rho(\varphi, \vartheta), \quad K = -\partial_\varphi S$$

and we have:

$$\rho(\varphi, \vartheta) = c_0 \mathrm{e}^{-S(x)} + \sum_{E_n > 0} c_n \phi_n \mathrm{e}^{-E_n t} \rightarrow \rho_{as}(x) = c_0 \mathrm{e}^{-S(x)}, \ (\vartheta \rightarrow \infty)$$

with E_n the *eigenvalues* of the Fokker–Planck Hamiltonian:

$$H_{FP} = -\partial_x^2 + \frac{1}{4}(\partial_x S)^2 - \frac{1}{2}(\partial_x^2 S)$$

For general drift the FPE still makes sense, but it may not lead to asymptotic distributions (e.g., for GT without gauge fixing there are no as. distributions for the A_μ – only for gauge inv. observables).

- expectation values $\langle f(\varphi)\rangle$ can be calculated as averages over the noise, equivalently as ϑ averages:

$$\overline{f(\varphi)} = \frac{1}{\Theta}\int_0^{\Theta} d\vartheta\, f(\varphi(\vartheta)) = \langle f(\varphi)\rangle + \mathcal{O}(1/\sqrt{\Theta})\,,$$

- the convergence is controlled by the properties of the FP Hamiltonian,

- in practice $\delta\vartheta \neq 0$: $\rho_{as}(\varphi)$ has $\mathcal{O}(\delta\vartheta)$ corrections (controllable).

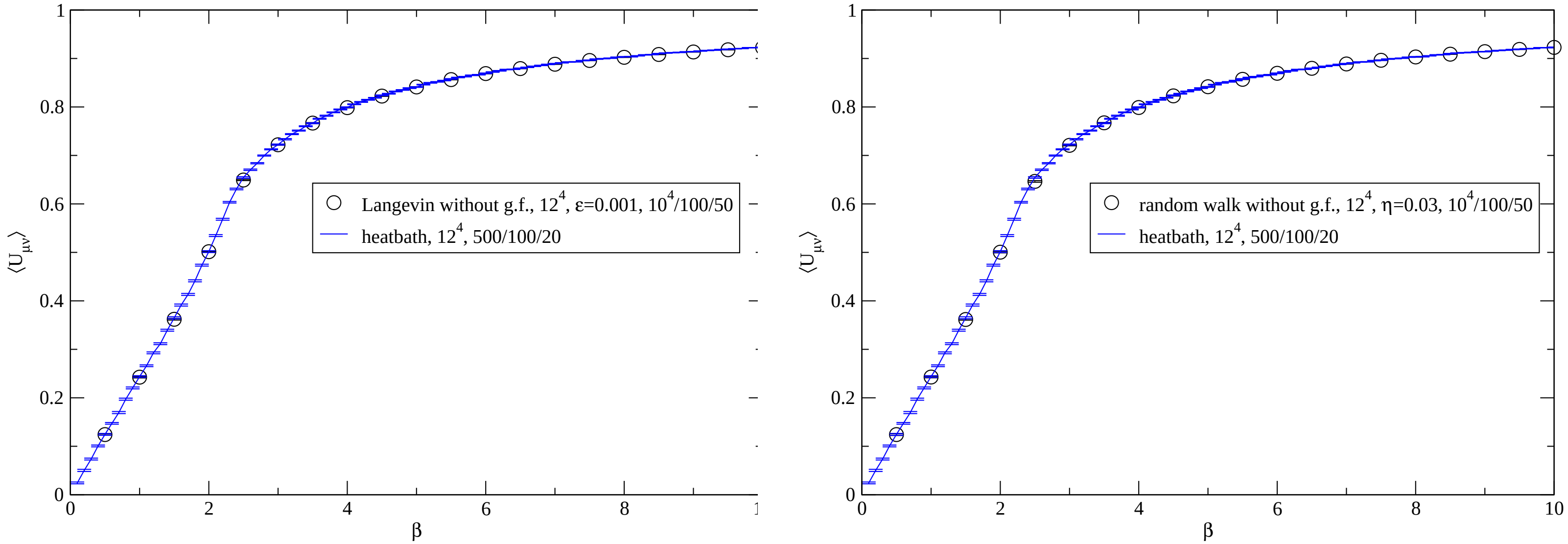


Figure 1: Plaquette averages by LE and RW compared with MC

Beyond Euclidean action

Developments based on the versatility of the method:

- redefining the drift force,
- changing the action,
- redefining the noise (e.g., nonlinear processes: "active brownian motion"),
- ...

Very much used in modeling (statistical physics, complex systems, etc.)
In QM and QFT: open systems, continuous localization, special simulation problems. In the following: two examples.

1. There is no S (non-conservative drift)

Simulation of non-compact Y-M theory with stochastic gauge fixing [E.Seiler, I.O.S., D.Zwanziger, . . . , Hüffel, . . . , Nakamura , . . . , J.Pawlowski, D.Spielmann, I.O.S.]

There are a number of problems which require gauge fixing:

- putting into evidence dynamically relevant degrees of freedom (monopoles, etc),

- testing confinement scenarios (Kugo-Ojima, Gribov, Zwanziger, ..)

- ...

Gauge fixing on the lattice is difficult when implemented as minimization of a gauge functional (metastabilities, Gribov copies)

$\longrightarrow$ try to ensure that the simulation fixes the gauge properly and the fields are confined to the first Gribov zone.

One adds a gauge fixing force tangent to orbits:

$$
\begin{aligned}
K^a_\mu[A^c_\nu] &= K^a_{YM,\mu}[A^c_\nu] + K^a_{g.f.,\mu}[A^c_\nu] \\
K^a_{g.f.,\mu}(A) &= \alpha\, D^{ab}_\mu(A)\,(\partial.A)^b = -\frac{\delta S_{GF}}{\delta A^a_\mu} + g\, f^{abc}\, A^b_\mu\,(\partial.A)^c
\end{aligned}
$$

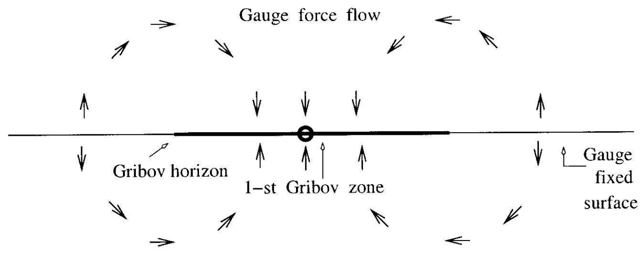
$K_{g.f.}$ is not conservative since it contains a curl: no action, therefore no MC possible.

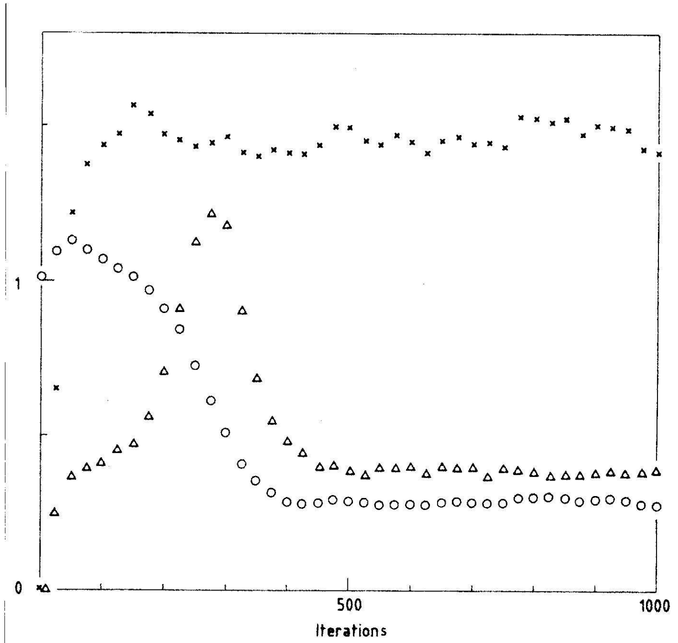
LE simulation is possible. It can be shown that it leads to a stable distribution.

Can be implemented for the compact, non abelian theory on the lattice, for various gauge fixing conditions.

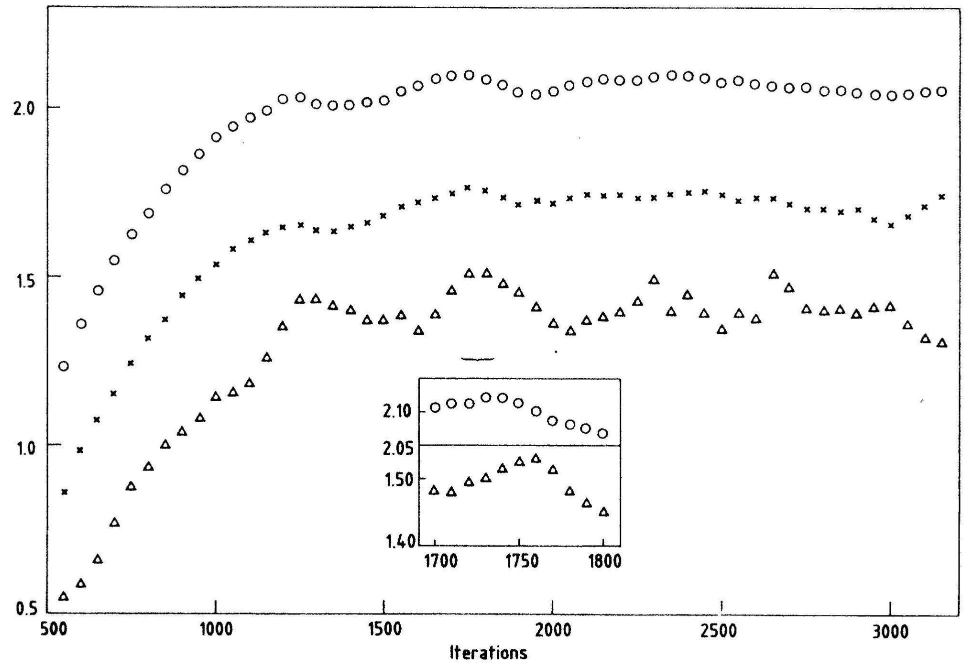
Provable properties of the gauge fixing force:

- it is tangent to the gauge orbits, therefore it does not modify the dynamics of the theory,
- it vanishes on the *gauge fixing surface*,
- it is strictly restoring near the surface *inside the first Gribov zone*,
- it has destabilizing modes near the surface *outside* the first Gribov zone,
- it is directed toward the origin ($A^c_\mu = 0$) everywhere far from the gauge fixing surface (large A^c_μ).





3. Action, $A_\mu^2(\times\frac{1}{5})$ and $(D_\mu A_\mu)^2(\times\frac{1}{2})$. Averages over 25 sweeps: $\beta = 0.25$, $\alpha = 1$ and $\eta = \frac{1}{8}$ on 4^4 lattice started outside the Gribov horizon. Same symbols as before.



1. Action $(\times\frac{1}{100})$: crosses, $A_\mu^2(\times\frac{1}{10})$: circles and $(D_\mu A_\mu)^2(\times\frac{1}{10})$: triangles. Each point represents an average over the 50 sweeps (respectivel the box) between it and the preceding point. Here $\beta = 0.0001$, $\alpha = 1$ and the step size $\eta = \frac{1}{8}$ on a 6^4 lattice. All the averages are given per lir

Figure 2: Stochastic gauge fixing (Random Walk simulation).

2. Complex action

- accounting for complex terms in the action (non-zero density),
- reformulation of the stochastic quantization for the Minkowski path integral: Langevin equation with complex driving force
- in both cases: (more or less formal) proofs of convergence and equivalence to the path integral formulation under certain conditions [Hüffel and Rumpf, Okamoto, etc]
- interesting if Euclidean formulation is not possible or ambiguous:

  Non-equilibrium dynamics in real time

Some recent applications

Lattice calculations [J. Berges, S. Borsanyi, D. Sexty and I.O.S.; J. Berges and D. Sexty]

Here only a short "warm up" and an illustration of the relation between LE and FPE.

The real extent of both the capabilities of the method and the problems it raises – see talk by Denes Sexty.

Scalar field simulations on the lattice

$\hat\varphi = a\varphi$, $\hat m = am$, $\hat{\mathbf{x}} = \mathbf{x}/a$, $\hat t = t/a_t$, $\gamma = a/a_t$

$\hat\vartheta = \vartheta/a^2$, $\epsilon = \delta\vartheta/a^2$,

$\hat\eta = \sqrt{a^3 a_t \delta\vartheta}\,\eta = \sqrt{\epsilon/\gamma}\,a^3\eta$, $\quad \langle \hat\eta(\hat x,\hat\vartheta)\,\hat\eta(\hat x',\hat\vartheta')\rangle_\eta = 2\,\delta_{\hat x,\hat x'}\delta_{\hat\vartheta,\hat\vartheta'}$

$$
\begin{aligned}
\hat\varphi(\hat x;\hat\vartheta+\epsilon) &= \hat\varphi(\hat x;\hat\vartheta) + \sqrt{\epsilon\gamma}\,\hat\eta(\hat x;\hat\vartheta) \\
&\quad - i\,\epsilon\left(\Box_\gamma\hat\varphi(\hat x;\hat\vartheta) + \hat m^2\hat\varphi(\hat x;\hat\vartheta) + \lambda\hat\varphi(\hat x;\hat\vartheta)^3\right). \\
\Box_\gamma\hat\varphi(\hat x;\hat\vartheta) &= \gamma^2\left(\hat\varphi(\hat x+\hat e_0;\hat\vartheta) + \hat\varphi(\hat x-\hat e_0;\hat\vartheta) - c_t\hat\varphi(\hat x;\hat\vartheta)\right) \\
&\quad - \sum_i\left(\hat\varphi(\hat x+\hat e_i;\hat\vartheta) + \hat\varphi(\hat x-\hat e_i;\hat\vartheta) - 2\hat\varphi(\hat x;\hat\vartheta)\right)
\end{aligned}
$$

Notice that the fields are the complex extensions of the original, real ones and all observables have to be understood as analytic extensions of the original observables.

The problem is set by giving the initial conditions in *physical time* t, here for simplicity [J.Berges and I.O.S.]:

$\varphi(x, 0; \vartheta) = \varphi_0(x)$, $\varphi(x, 1; \vartheta) = \varphi(x, 0; \vartheta)$ with some chosen "initial configuration" $\varphi_0(x)$

These values are not updated in the LE. Since the drift force contains time "derivatives" (finite differences), the initial conditions shapes the drift at small t and therefore also the asymptotic the solution $\varphi(x, t)$. (More complicated initial conditions can be introduced.)

The simulation is started by providing a "starting configuration" $\varphi(x, t; \vartheta = 0)$ (which of course must comply with the "initial conditions"). It turns out in the simulations that the large ϑ behaviour does not depend on the starting configuration (as it should).

The figures show the correlations $\langle \sum_x \varphi(x, t)\varphi(x, 0)\rangle$ and other quantities for the quantum ("$n = 1$") or classical ("$n = 0$") problem.

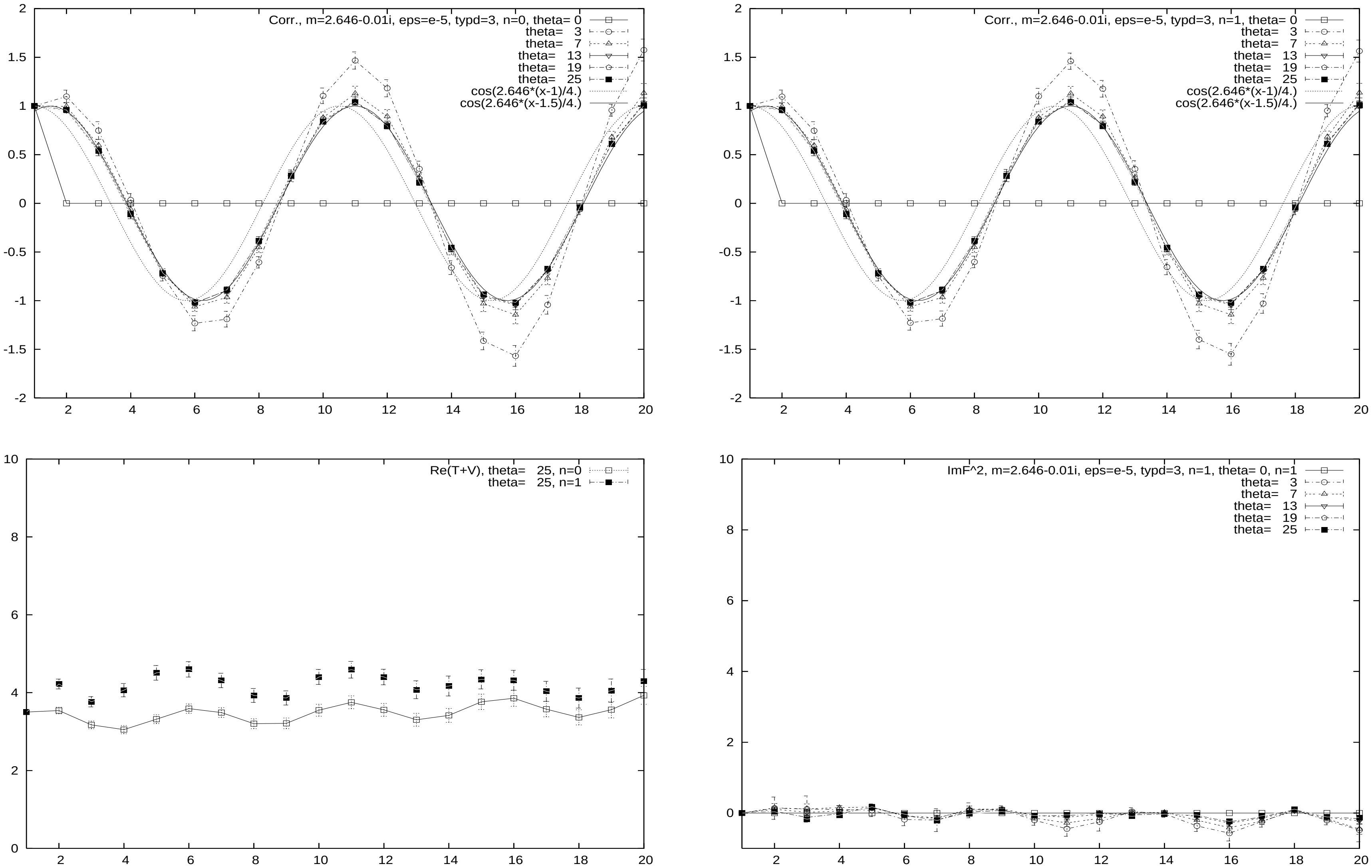


Figure 3: 3+1 dim free field, $12^3.20, \gamma = 4, M = 2.63 - i0.01, \lambda = 0$. Correlations (classical, quantum), energy and $Im < \varphi^2 >$.

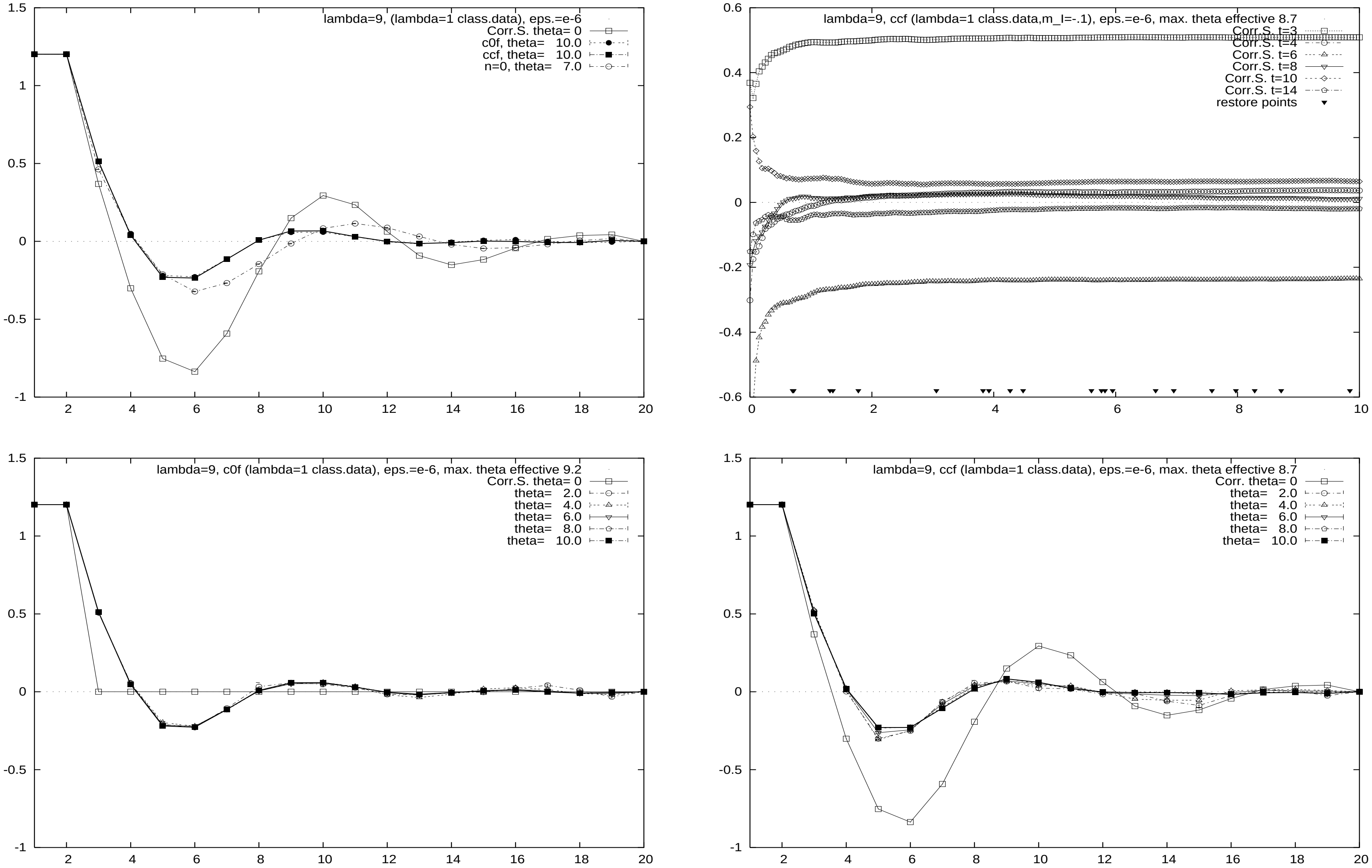


Figure 4: 3+1 dim , φ^4 theory, $8^3.20, M = 0, \lambda = 9, \gamma = 4$. Large ϑ correlations from different starting configurations, ϑ dependence, correlations from different start configuration at various ϑ.

Gauge Theory in real time

The process is defined in the group algebra, the links are recalculated and used to derive the drift:

$$U'_{x,\mu} = \exp\left\{i\lambda_a\left(\epsilon\, K_{x\mu a}[U] + \sqrt{\epsilon}\,\eta_{x\mu a}\right)\right\} U_{x,\mu}\,,$$
$$K_{x\mu a} = -\frac{1}{2N}\sum_{\nu\neq\mu}\beta \mathrm{Tr}\left(\lambda_a U_{x,\mu} R_{x,\mu\nu} - \bar{R}_{x,\mu\nu} U^{-1}_{x,\mu}\lambda_a\right)\,.$$

with λ_a the $SU(N)$ generators and $R_{x,\mu\nu}, \bar{R}_{x,\mu\nu}$ the "rest-Plaquette" staples. The process runs in $SL(N,C)$. One can use various procedure to ensure this: reduced Haar measure, projection onto SL, etc. For $SU(2)$ we can use $U = a_0 + i\,\vec{\sigma}\,\vec{a}$, with a_ν complex, $a_0^2 + \vec{a}^2 = 1$ and we also have $U^{-1} = a_0 - i\,\vec{\sigma}\,\vec{a}$.

Questions

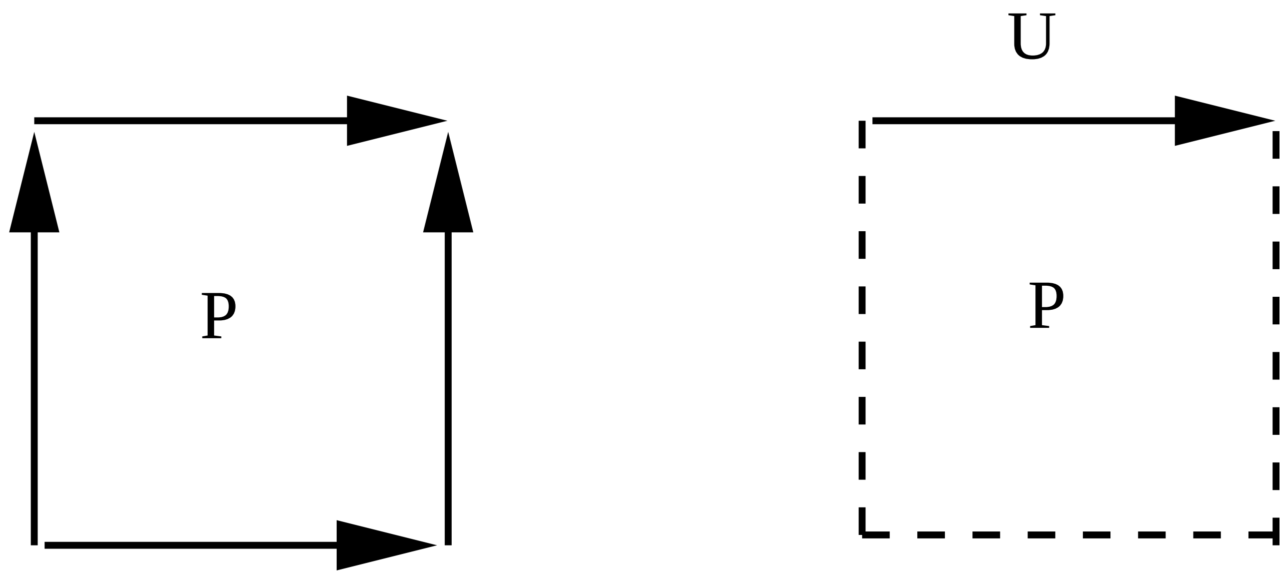
- systematic discretization errors
- run-away trajectories
- convergence

One can try to better control the method by redesigning the process. For instance:

- Kernel controlled LE (to generate positive real parts in the spectrum of the FP Hamiltonian) without changing the EV,

- reweighting (changing the drift to ensure convergence and recalculating the EV).

Illustration - the One Plaquette U(1) model



Can be used to study the features of the process

Notations

$< O >$: exact EV (from integration)

$\overline{O}$: average over the LE process (noise, time, ensemble)

$\mathcal{E}\left\{O\right\}$: EV with real distribution $P(x, y, t)$

$\langle O \rangle$: EV with complex distribution $\rho(x)$

Integral

$$Z_p(\beta) = \int_{-\pi}^{\pi} dx \, \mathrm{e}^{i\,p\,x - i\,\beta\,\cos x} \tag{1}$$

We consider the analytic functions

$$f(z) = \mathrm{e}^{i\,q\,z}\,, \quad z = x + i\,y\,, \quad f(x) \equiv f(z)|_{y=0} \tag{2}$$

Exact expectation values, direct and using p as reweighting

$$< \mathrm{e}^{i\,q\,x} >_p \;=\; \frac{\int_{-\pi}^{\pi} dx \, \mathrm{e}^{i\,q\,x}\,\mathrm{e}^{i\,p\,x - i\,\beta\,\cos x}}{\int_{-\pi}^{\pi} dx \, \mathrm{e}^{i\,p\,x - i\,\beta\,\cos x}} \tag{3}$$

$$< \mathrm{e}^{i\,q\,x} >_0 \;=\; \frac{\int_{-\pi}^{\pi} dx \, \mathrm{e}^{i\,q\,x}\,\mathrm{e}^{-i\,\beta\,\cos x}}{\int_{-\pi}^{\pi} dx \, \mathrm{e}^{-i\,\beta\,\cos x}} = \frac{< \mathrm{e}^{i\,(q-p)\,x} >_p}{< \mathrm{e}^{i\,(-p)\,x} >_p} \tag{4}$$

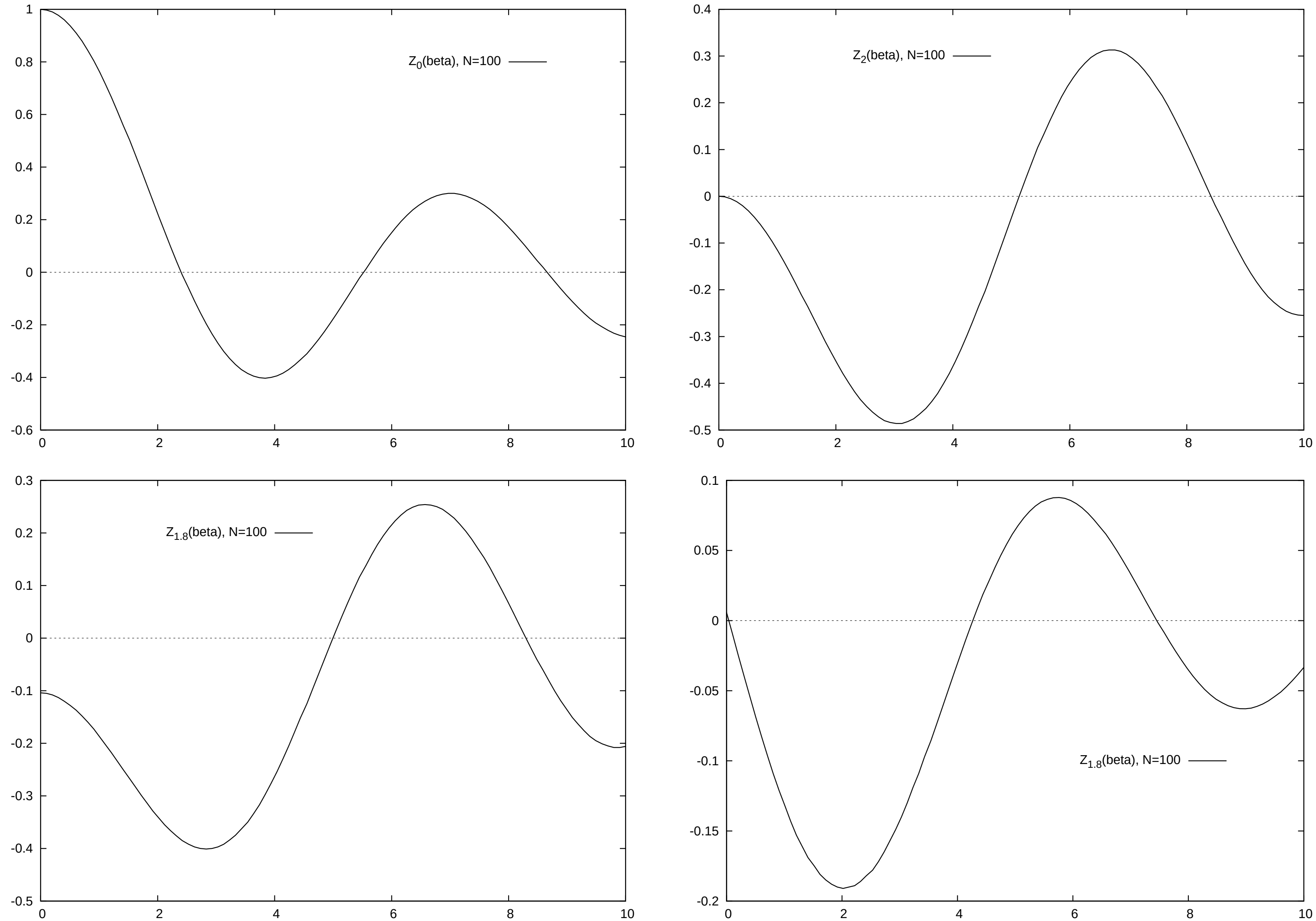


Figure 5: $Z_p(\beta)$ for $p = 0$ and $p = 2$ and for $p = 1.8$, with $N = 100$ x-discretization. Notice that the imaginary part vanishes for even p.

Complex Langevin eq. for complex measure

[J.Berges, D.Sexty; E.Seiler, I.O.S.]

$$e^{i\,p\,z - i\,\beta\,\cos z}\,dz \tag{5}$$

$$S = -i\,p\,z + i\,\beta\,\cos z\,, \qquad K = -\partial_z S = i\,p + i\,\beta\,\sin z \tag{6}$$

We have

$$z = x + i\,y \tag{7}$$

$$K = i\,(p + \beta\,\sin x\,\cosh y) - \beta\,\sinh y\,\cos x \tag{8}$$

Lang. eq. (in the following t denotes the Langevin time instead of ϑ):

$$\dot{z} = i\,p + i\,\beta\,\sin z + \eta \tag{9}$$

$$\dot{x} = -\beta\,\cos x\,\sinh y + \eta \tag{10}$$

$$\dot{y} = p + \beta\,\sin x\,\cosh y \tag{11}$$

$$Im\,\eta = 0\,, \quad \overline{\eta(t)\,\eta(t')} = 2\,\lambda\,\delta(t - t') \tag{12}$$

One builds averages of $f(z)$ over the LE process

$$\overline{f(z)} = \frac{1}{T}\sum_{t=1}^{T} f(x_t + i\, y_t) \tag{13}$$

$\overline{f(z)}_p$ should reproduce the ensemble averages over the distribution realized by the LE process, and thus the exact EW (3,4). Using reweighting (for $p = 0$) it holds, numerically:

$$< \mathrm{e}^{i\,q\,x} >_p \;=\; \overline{\{e^{i\,q\,z}\}_p}\,, \quad p \neq 0 \tag{14}$$

$$< \mathrm{e}^{i\,q\,x} >_0 \;=\; \frac{\overline{\left\{e^{i\,(q-p)\,z}\right\}_p}}{\overline{\left\{e^{-i\,p\,z}\right\}_p}} \tag{15}$$

In the tables $t = 1000$, $\delta t = 10^{-5}$. Agreement/disagreement can be systematically studied and general criteria established *[Berges and Sexty]*.

One can define a FPE for a complex "distribution" $\rho(z)$, z : complex ($\lambda = 1$ is the quantum problem, $\lambda = 0$ the clasical limit):

$$\dot{\rho}_p(z,t) = \big(\lambda\,\partial_z^2 - i\,\partial_z\,(p + \beta\,\sin z)\big)\;\rho_p(z,t). \tag{16}$$

Formally this has as asymptotic solution e^{-S}.

Alternatively one can define a true probability distribution $P(x,y,t)$ for the real variables x, y:

$$\dot{P}_p(x,y,t) = \tag{17}$$
$$\big(\lambda\,\partial_x^2 + \beta\,\partial_x\,\cos\,x\,\sinh\,y - \partial_y(p + \beta\,\sin\,x\,\cosh\,y)\big)\;P_p(x,y,t)$$

P is realized in the Langevin process, ρ indicates the relation to the measure.

For analytic $f(z)$ we have (Parisi, etc)

$$\int dx\, dy\, P_p(x,y,t)\, f(x+iy) = \int dx\, \rho_p(x,t)\, f(x) \tag{18}$$

hence, in particular

$$\int dx\, dy\, P_p(x,y,t)\, \mathrm{e}^{i\,k\,x - k\,y} \;=\; \int dy\, \mathrm{e}^{-k\,y}\, \tilde{P}_p(k,y,t) \tag{19}$$

$$= \int dx\, \rho_p(x,t)\, \mathrm{e}^{i\,k\,x} \;=\; \widetilde{\rho}_p(k,t) \tag{20}$$

where $\widetilde{\rho}_p(k,t)$ are the Fourier modes of $\rho_p(x,t)$. We thus have:

$$\mathcal{E}\left\{e^{i\,q\,x - q\,y}\right\}_p = \overline{\left\{e^{i\,q\,z}\right\}_p} = \langle \mathrm{e}^{i\,q\,x} \rangle_p \tag{21}$$

Complex FP Equation

$$\dot{\rho}_p(x,t) \;=\; \left(\partial_x^2 - i\,\partial_x\,(p+\beta\,\sin x)\right)\,\rho_p(x,t) \tag{22}$$

FT:

$$\widetilde{\rho}_p(k,t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} dx \mathrm{e}^{i\,k\,x}\rho_p(x,t)\,, \quad \rho_p(x,t) = \sum_k \mathrm{e}^{-i\,k\,x}\widetilde{\rho}_p(k,t) \tag{23}$$

For calculation x is discretized in N points: $x = \frac{2\pi}{N}\,l$ and the FPE in momentum space reads:

$$\begin{aligned} \dot{\widetilde{\rho}}_p \quad & (k,t) = \\ - \quad & (\lambda k^2 + k\,p)\,\widetilde{\rho}_p(k,t) + \frac{i}{2}\,\beta\,k\,\widetilde{\rho}_p(k+1,t) - \frac{i}{2}\,\beta\,k\,\widetilde{\rho}_p(k-1,t) \end{aligned} \tag{24}$$

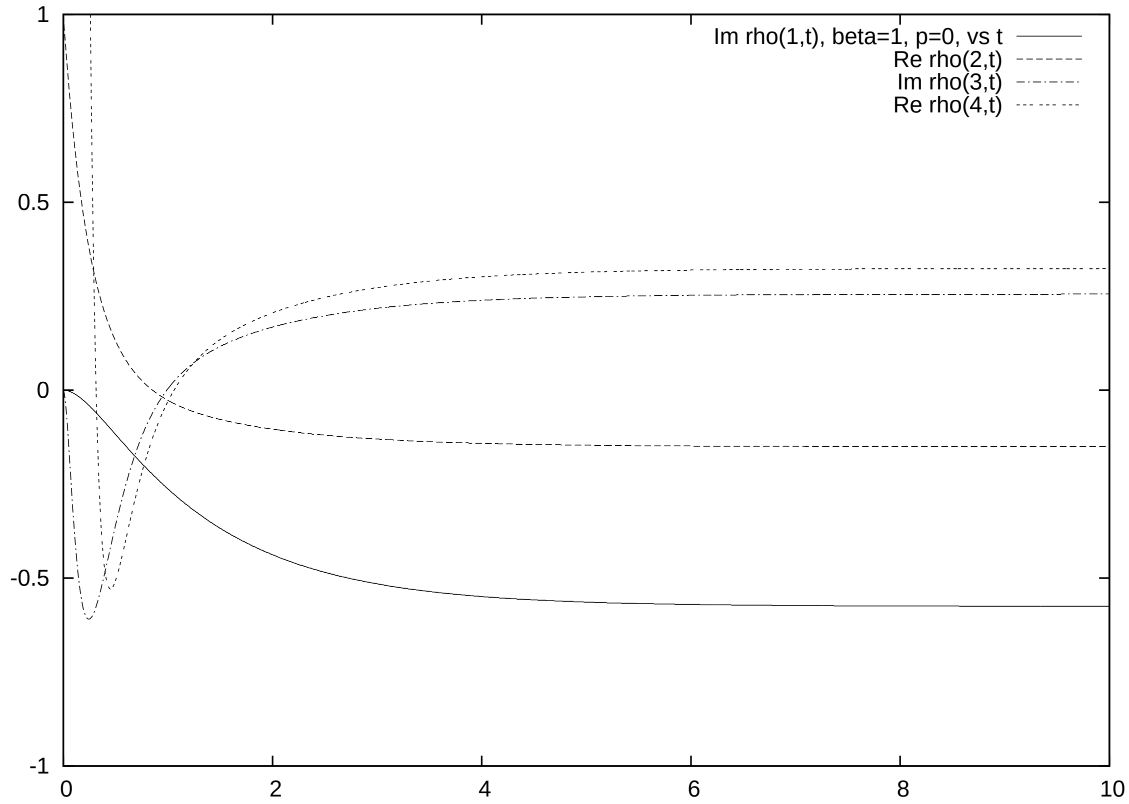


Figure 6: $\widetilde{\rho}_p(k,t)$ (Re, Im) for $p = 0$ and $\beta = 1$, $k = 1, 2, 3, 4$ from FPE (24) vs t.

EV from ρ *averages*:

$$\langle e^{i\,q\,x}\rangle_p = \frac{\int_{-\pi}^{\pi} dx\, \mathrm{e}^{i\,q\,x} \rho_p(x,t)}{\int_{-\pi}^{\pi} dx\, \rho_p(x,t)} = \frac{\widetilde{\rho}_p(q,t)}{\widetilde{\rho}_p(0,t)} \tag{25}$$

$$\langle e^{i\,q\,x}\rangle_0 = \frac{\int_{-\pi}^{\pi} dx\, \mathrm{e}^{i\,q\,x} \rho_0(x,t)}{int^{\pi}_{-\pi} dx\, \rho_0(x,t)} = \frac{\widetilde{\rho}_0(q,t)}{\widetilde{\rho}_0(0,t)} \tag{26}$$

$$= \frac{\int_{-\pi}^{\pi} dx\, \mathrm{e}^{i\,(q-p)\,x} \rho_p(x,t)}{\int_{-\pi}^{\pi} dx\, \mathrm{e}^{i\,(-p)\,x} \rho_p(x,t)} = \frac{\widetilde{\rho}_p(q-p,t)}{\widetilde{\rho}_p(-p,t)} \tag{27}$$

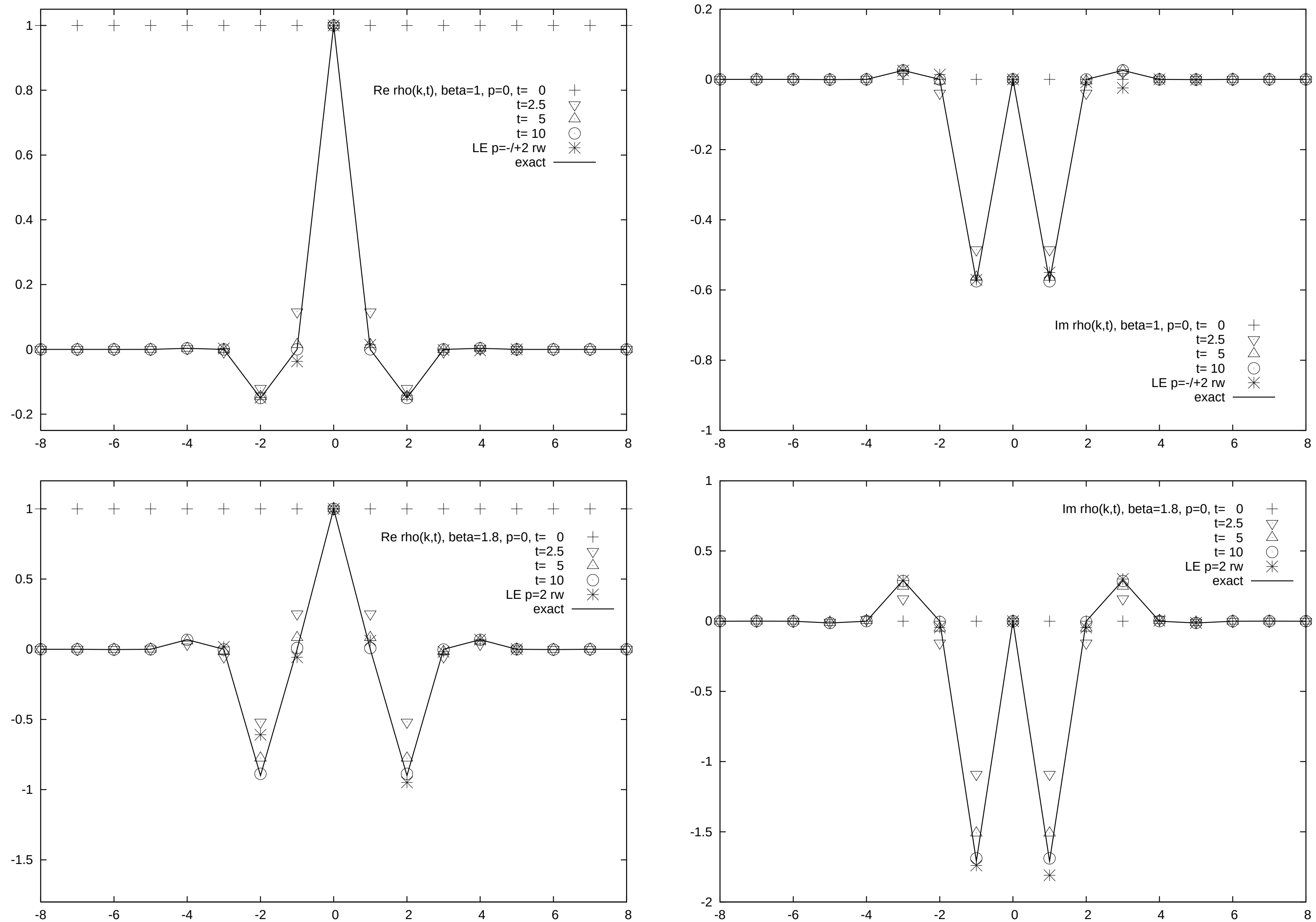


Figure 7: $\widetilde{\rho}_0(k,t)$ (Re, Im) for $p = 0$ and $\beta = 1$ and 1.8 from FPE (24) with $N = 100$ x-discretization, $\delta\, t = 10^{-6}$, for $t = 0, 2.5, 5, 10$. Solid line: from exact measure (5). Stars: from stochastic simulation.

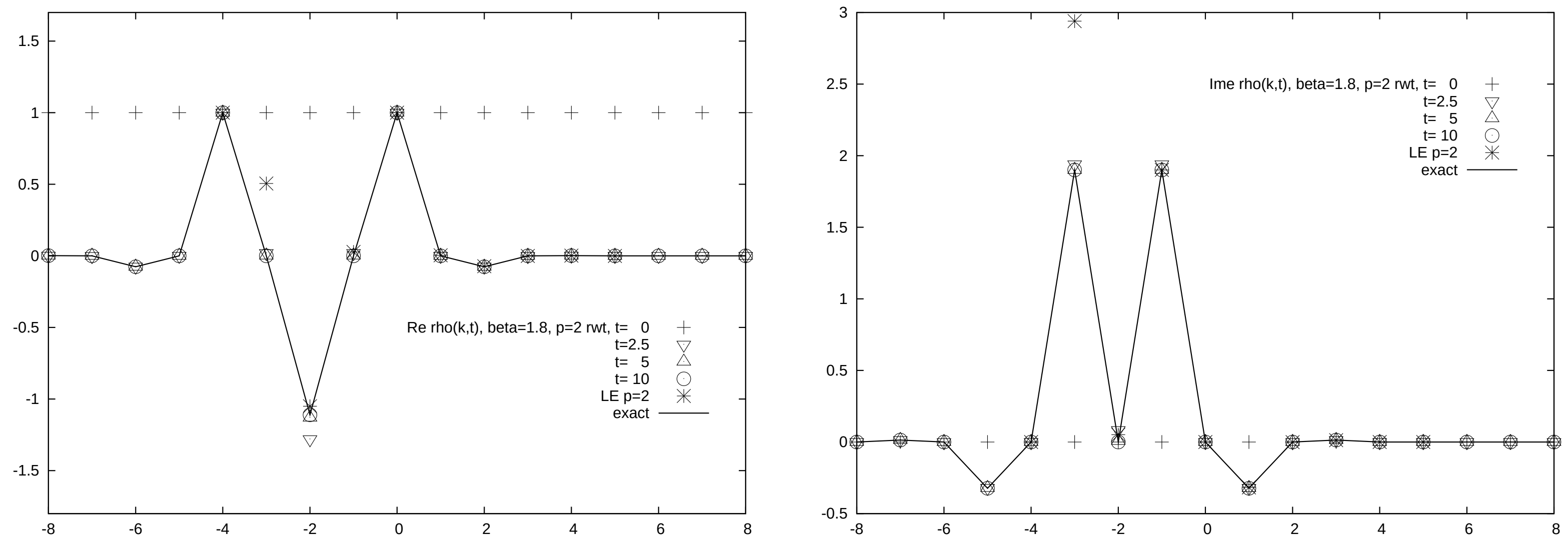


Figure 8: $\widetilde{\rho}_p(k,t)$ (Re, Im) for $p=2$ and $\beta=1.8$ from FPE (24) at $p=0$ and 'reweighting' compared with the exact results from (5) (solid line) and the stochastic data from the LE simulation (stars); $N=100$ x-discretization, $\delta\, t = 10^{-6}$, $t=0, 2.5, 5, 10$.

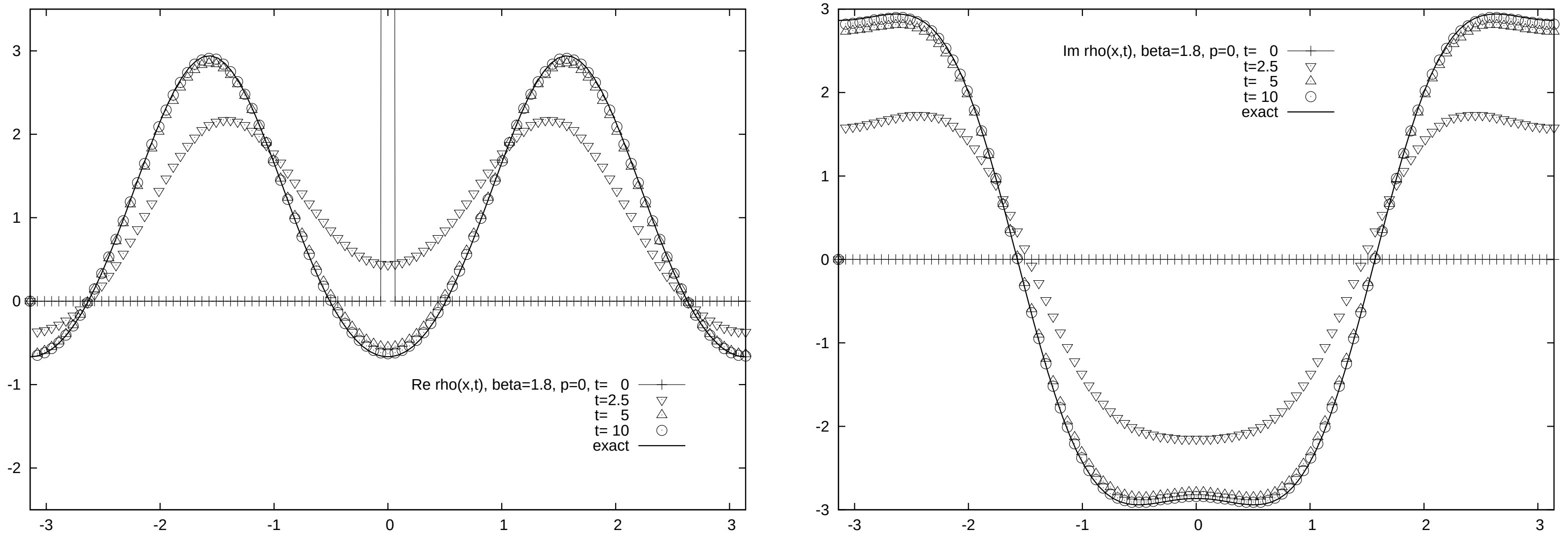


Figure 9: $\rho_0(x,t)$ (Re, Im), $p = 0$, $\beta = 1.8$ with $N = 100$ x-discretization, $\delta t = 10^{-6}$, for $t = 0, 2.5, 5, 10$ compared with exact measure e^{-S} (discretized).

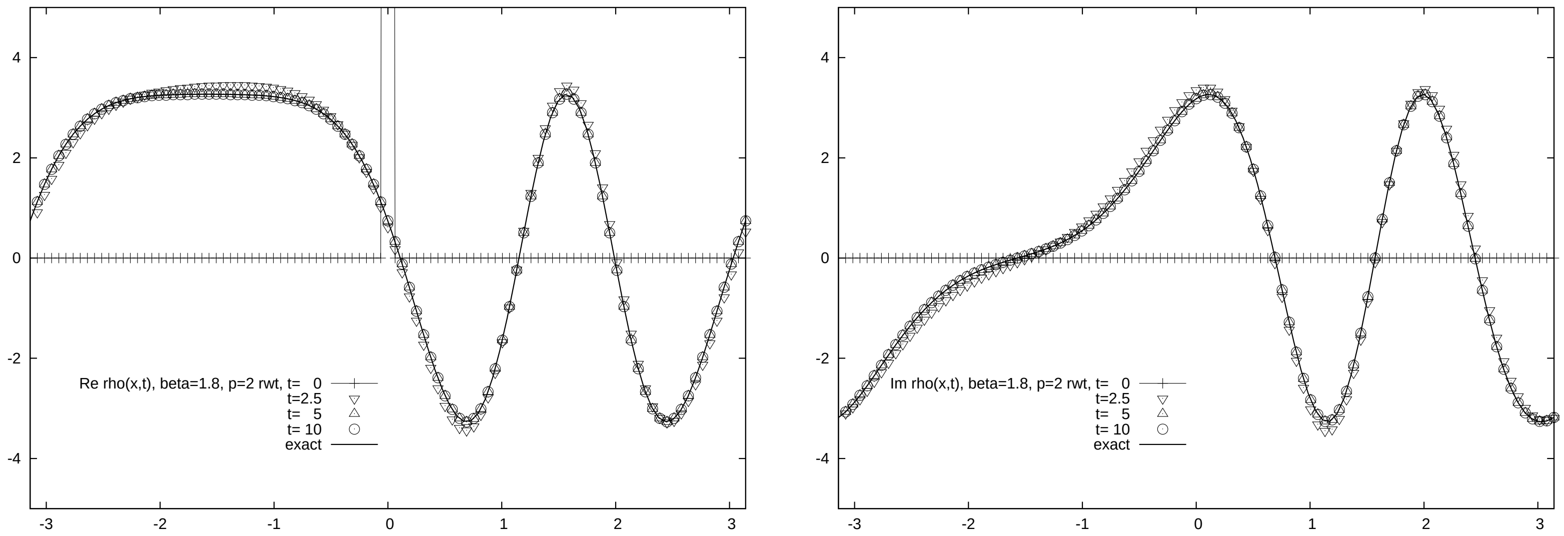


Figure 10: $\rho_p(x,t)$ (Re, Im), $p = 2$, $\beta = 1.8$ obtained from the FPE at $p = 0$ followed by'reweighting' according to (27), compared with exact measure e^{-S} (discretized); $N = 100$ x-discretization, $\delta t = 10^{-6}$, $t = 0, 2.5, 5, 10$.

Discussion

- There is high motivation to try to define numerical simulations for real time problems, where mainly approximate methods have been used so far:
  - High energy physics and QCD Plasma
  - Cosmology
  - Ultra-Cold quantum gases ...
- In these studies we encountered a number of problems,
  - some of them easily manageable (run away's, $\delta\vartheta$ dependence),
  - some demanding more work and understanding (fixed point structure)

See Sexty's talk!